# WORLDWIDE wwPDB PROTEIN DATA BANK

# wwPDB NMR Structure Validation Summary Report ⓘ

Feb 25, 2020 – 04:42 PM CST

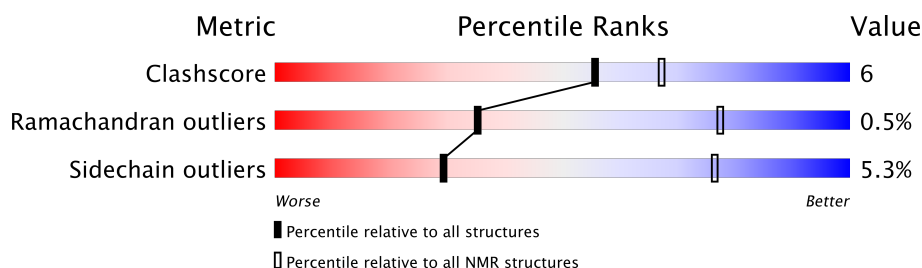|  |  |  |
|---|---|---|
| PDB ID | : | 2KO1 |
| Title | : | Solution NMR structure of the ACT domain from GTP pyrophosphokinase of Chlorobium tepidum. Northeast Structural Genomics Consortium Target CtR148A |
| Authors | : | Eletsky, A.; Garcia, E.; Wang, H.; Ciccosanti, C.; Jiang, M.; Nair, R.; Rost, B.; Acton, T.B.; Xiao, R.; Everett, J.K.; Lee, H.; Prestegard, J.H.; Montelione, G.T.; Szyperski, T.; Northeast Structural Genomics Consortium (NESG) |
| Deposited on | : | 2009-09-08 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 64%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

| Metric | Percentile Ranks | Value |
|---|---|---|
| Clashscore | | 6 |
| Ramachandran outliers | | 0.5% |
| Sidechain outliers | | 5.3% |

*Worse*      *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all NMR structures

| Metric | Whole archive (#Entries) | NMR archive (#Entries) |
|---|---|---|
| Clashscore | 136327 | 12091 |
| Ramachandran outliers | 132723 | 10835 |
| Sidechain outliers | 132532 | 10811 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 88 | 76%   13%   11% |
| 1 | B | 88 | 76%   14%   10% |

# 2   Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues | | | |
|---|---|---|---|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:4-A:81, B:3-B:81 (157) | 0.32 | 1 |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 3 single-model clusters were found.

| Cluster number | Models |
|---|---|
| 1 | 1, 5, 6, 8, 9, 10, 18 |
| 2 | 2, 13, 16, 17 |
| 3 | 7, 12, 15 |
| 4 | 3, 19, 20 |
| Single-model clusters | 4; 11; 14 |

# 3  Entry composition  ⓘ

There is only 1 type of molecule in this entry. The entry contains 2858 atoms, of which 1452 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called GTP pyrophosphokinase.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 88 | Total | C | H | N | O | S | 0 |
| | | | 1429 | 442 | 726 | 128 | 128 | 5 | |
| 1 | B | 88 | Total | C | H | N | O | S | 0 |
| | | | 1429 | 442 | 726 | 128 | 128 | 5 | |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1 | MET | - | INITIATING METHIONINE | UNP Q8KC80 |
| A | 16 | ASN | ILE | ENGINEERED | UNP Q8KC80 |
| A | 81 | LEU | - | EXPRESSION TAG | UNP Q8KC80 |
| A | 82 | GLU | - | EXPRESSION TAG | UNP Q8KC80 |
| A | 83 | HIS | - | EXPRESSION TAG | UNP Q8KC80 |
| A | 84 | HIS | - | EXPRESSION TAG | UNP Q8KC80 |
| A | 85 | HIS | - | EXPRESSION TAG | UNP Q8KC80 |
| A | 86 | HIS | - | EXPRESSION TAG | UNP Q8KC80 |
| A | 87 | HIS | - | EXPRESSION TAG | UNP Q8KC80 |
| A | 88 | HIS | - | EXPRESSION TAG | UNP Q8KC80 |
| B | 1 | MET | - | INITIATING METHIONINE | UNP Q8KC80 |
| B | 16 | ASN | ILE | ENGINEERED | UNP Q8KC80 |
| B | 81 | LEU | - | EXPRESSION TAG | UNP Q8KC80 |
| B | 82 | GLU | - | EXPRESSION TAG | UNP Q8KC80 |
| B | 83 | HIS | - | EXPRESSION TAG | UNP Q8KC80 |
| B | 84 | HIS | - | EXPRESSION TAG | UNP Q8KC80 |
| B | 85 | HIS | - | EXPRESSION TAG | UNP Q8KC80 |
| B | 86 | HIS | - | EXPRESSION TAG | UNP Q8KC80 |
| B | 87 | HIS | - | EXPRESSION TAG | UNP Q8KC80 |
| B | 88 | HIS | - | EXPRESSION TAG | UNP Q8KC80 |

# 4 Residue-property plots ⓘ

## 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: GTP pyrophosphokinase

Chain A:



• Molecule 1: GTP pyrophosphokinase

Chain B:
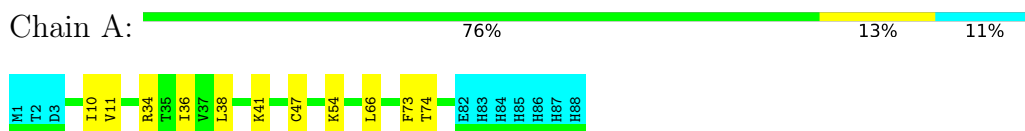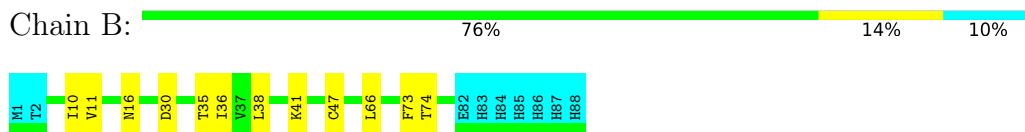


## 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

• Molecule 1: GTP pyrophosphokinase

Chain A:



• Molecule 1: GTP pyrophosphokinase

Chain B:
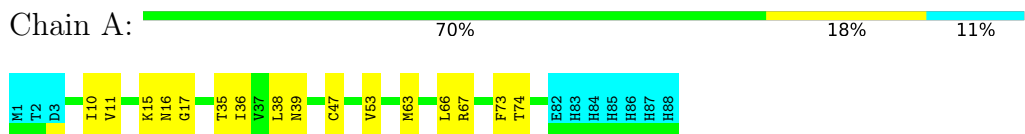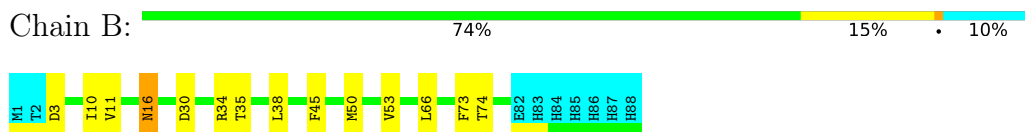
# 5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function.*

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification | Version |
|---|---|---|
| CYANA | structure solution | 3.0 |
| CNS | refinement | 1.2.1 |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| Chemical shift file(s) | 2ko1_nmr.cif |
|---|---|
| Number of chemical shift lists | 1 |
| Total number of shifts | 2170 |
| Number of shifts mapped to atoms | 1348 |
| Number of unparsed shifts | 312 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 510 |
| Assignment completeness (well-defined parts) | 64% |

No validations of the models with respect to experimental NMR restraints is performed at this time.

# 6 Model quality ⓘ

## 6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 610 | 650 | 650 | 8±2 |
| 1 | B | 618 | 654 | 654 | 9±3 |
| All | All | 24560 | 26080 | 26080 | 288 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

5 of 104 unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|--------|--------|----------|-------------|--------|---|
| | | | | Worst | Total |
| 1:B:10:ILE:HD11 | 1:B:66:LEU:HD13 | 0.71 | 1.62 | 3 | 11 |
| 1:B:36:ILE:HD11 | 1:B:47:CYS:SG | 0.66 | 2.29 | 14 | 10 |
| 1:A:10:ILE:HD11 | 1:A:66:LEU:HD13 | 0.66 | 1.65 | 18 | 14 |
| 1:A:36:ILE:HD11 | 1:A:47:CYS:SG | 0.65 | 2.31 | 5 | 9 |
| 1:A:15:LYS:O | 1:A:17:GLY:N | 0.59 | 2.35 | 20 | 3 |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------|----------|---------|----------|:---:|:---:|
| 1 | A | 78/88 (89%) | 75±2 (96±3%) | 3±2 (4±3%) | 0±0 (0±1%) | 40 | 79 |
| 1 | B | 79/88 (90%) | 75±2 (95±2%) | 4±2 (4±2%) | 0±1 (1±1%) | 31 | 76 |
| All | All | 3140/3520 (89%) | 2996 (95%) | 129 (4%) | 15 (0%) | 35 | 77 |

5 of 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | B | 16 | ASN | 5 |
| 1 | A | 16 | ASN | 4 |
| 1 | A | 42 | ASP | 2 |
| 1 | B | 17 | GLY | 2 |
| 1 | B | 43 | GLY | 1 |

### 6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------|-----------|----------|:---:|:---:|
| 1 | A | 70/80 (88%) | 66±2 (95±2%) | 4±2 (5±2%) | 29 | 76 |
| 1 | B | 71/80 (89%) | 67±1 (95±2%) | 4±1 (5±2%) | 30 | 77 |
| All | All | 2820/3200 (88%) | 2670 (95%) | 150 (5%) | 29 | 76 |

5 of 41 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | B | 73 | PHE | 19 |
| 1 | A | 41 | LYS | 17 |
| 1 | B | 41 | LYS | 13 |
| 1 | A | 73 | PHE | 13 |
| 1 | B | 30 | ASP | 11 |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 6.7 Other polymers ⓘ

There are no such molecules in this entry.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

# 7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 64% for the well-defined parts and 59% for the entire structure.

## 7.1 Chemical shift list 1

File name: 2ko1_nmr.cif

Chemical shift list name: *nef_chemical_shift_list_aco.tbl*

### 7.1.1 Bookkeeping ⓘ

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

| | |
|---|---|
| Total number of shifts | 2170 |
| Number of shifts mapped to atoms | 1348 |
| Number of unparsed shifts | 312 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 510 |
| Number of shift outliers (ShiftChecker) | 0 |

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. First 5 (of 312) occurences are reported below.

| Shift ID | Chain | Res | Type | Atom | Shift Data | | |
|---|---|---|---|---|---|---|---|
| | | | | | Value | Uncertainty | Ambiguity |
| 4 | A | 2 | THR | HG2% | 1.335 | 0.020 | 1 |
| 5 | A | 2 | THR | HG2% | 1.335 | 0.020 | 1 |
| 21 | A | 4 | PHE | HB% | 3.080 | 0.020 | 1 |
| 23 | A | 4 | PHE | HD% | 7.184 | 0.020 | 1 |
| 38 | A | 5 | LEU | HD1% | 0.475 | 0.020 | 1 |

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atoms found in structure. First 5 (of 510) occurences are reported below.

| Chain | Res | Type | Atom | Shift Data | | |
|---|---|---|---|---|---|---|
| | | | | Value | Uncertainty | Ambiguity |
| A | 21 | GLN | HBx | 2.243 | 0.02 | 2 |
| B | 44 | ILE | HG1x | 1.482 | 0.02 | 2 |

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| Chain | Res | Type | Atom | Shift Data | | |
|-------|-----|------|------|-------|-------------|-----------|
| | | | | Value | Uncertainty | Ambiguity |
| A | 62 | LEU | HBx | 1.26 | 0.02 | 2 |
| B | 41 | LYS | HB% | 1.815 | 0.02 | 1 |
| A | 33 | ILE | HG1x | 1.751 | 0.02 | 2 |

### 7.1.2   Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction ± precision, *ppm* | Suggested action |
|---------|----------|-------------------------------|------------------|
| $^{13}C_\alpha$ | 164 | -0.11 ± 0.13 | None needed ($< 0.5$ ppm) |
| $^{13}C_\beta$ | 152 | -0.03 ± 0.11 | None needed ($< 0.5$ ppm) |
| $^{13}C'$ | 162 | 0.07 ± 0.13 | None needed ($< 0.5$ ppm) |
| $^{15}N$ | 162 | -0.06 ± 0.17 | None needed ($< 0.5$ ppm) |

### 7.1.3   Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 64%, i.e. 1256 atoms were assigned a chemical shift out of a possible 1959. 30 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^1H$ | $^{13}C$ | $^{15}N$ |
|-----------|----------------|----------------|----------------|------------------|
| Backbone | 771/785 (98%) | 302/314 (96%) | 312/314 (99%) | 157/157 (100%) |
| Sidechain | 445/1084 (41%) | 72/622 (12%) | 347/406 (85%) | 26/56 (46%) |
| Aromatic | 40/90 (44%) | 20/50 (40%) | 20/40 (50%) | 0/0 (—%) |
| Overall | 1256/1959 (64%) | 394/986 (40%) | 679/760 (89%) | 183/213 (86%) |

### 7.1.4   Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

### 7.1.5   Random Coil Index (RCI) plots ⓘ

The images below report *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:
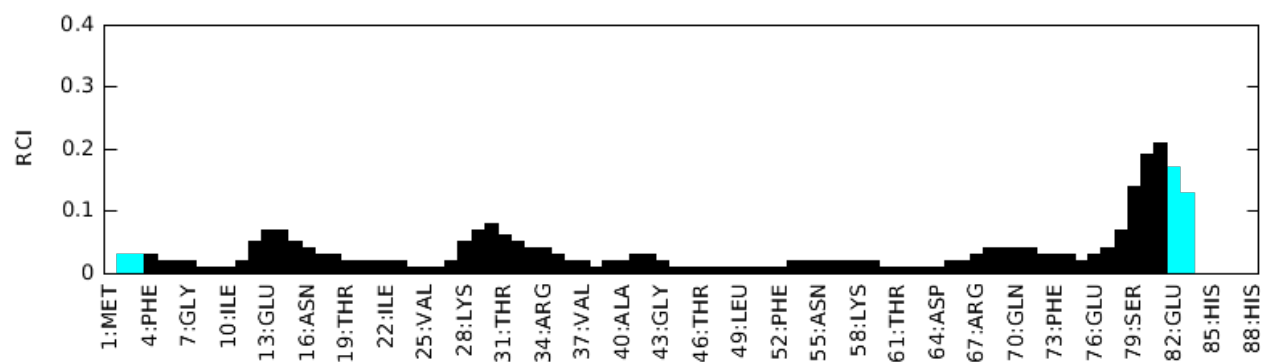


Random coil index (RCI) for chain B:
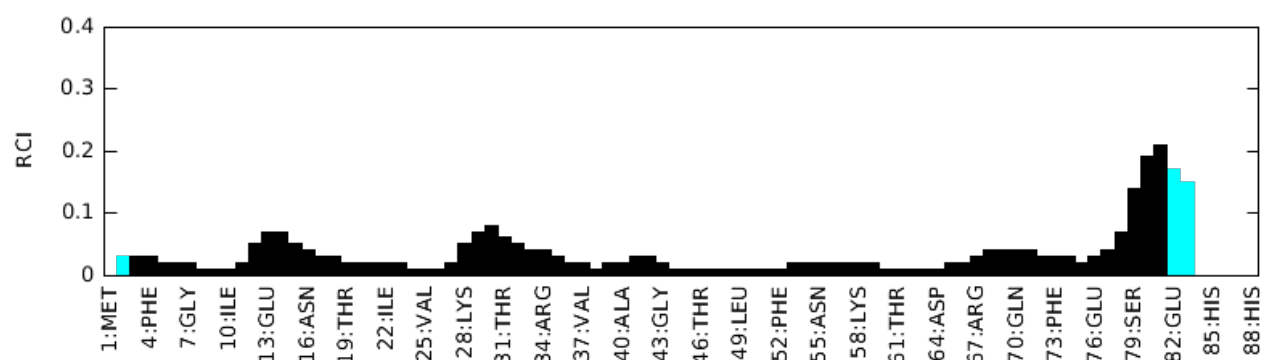
# 8 Distance restraints analysis

## 8.1 Distance restraints summary

Restraints are counted in different categories based on the atoms involved in each restraint.

| Restraints type | B-B$^1$(H$^4$) | B-S$^2$(H$^4$) | S-S$^3$(H$^4$) | Total | | |
|---|---|---|---|---|---|---|
| | | | | Total(H$^4$) | RR$^5$ | %$^6$ |
| Intraresidue (\|i-j\|=0) | 0(0) | 715(0) | 173(0) | 888(0) | 0.6 | 16.9 |
| Sequential (\|i-j\|=1) | 230(0) | 783(0) | 212(0) | 1225(0) | 0.8 | 23.3 |
| Medium range (\|i-j\|>1 and \|i-j\|<5) | 172(0) | 550(0) | 351(0) | 1073(0) | 0.7 | 20.4 |
| Long range (\|i-j\|≥5) | 178(0) | 843(0) | 919(0) | 1940(0) | 1.3 | 36.9 |
| Inter chain | 8(0) | 84(0) | 45(0) | 137(0) | 0.1 | 2.6 |
| Total | 588(0) | 2975(0) | 1700(0) | 5263(0) | 3.6 | 100.0 |

$^1$number of backbone to backbone restraints, $^2$number of backbone to sidechain restraints, $^3$number of sidechain to sidechain restraints, $^4$number of hydrogen bonds in that category, $^5$number of restraints per residue, $^6$percentage of restraints in that category. There are 0 unmapped restraints

### 8.1.1 Pie chart : Distance restraints summary

## 8.2 Distance violations summary

The following table provides the summary of violated restraints. Restraints that are violated at least in one model are counted as violated.

| Restraints type | B-B[1](%[4]) | B-S[2](%[4]) | S-S[3](%[4]) | Total | | |
|---|---|---|---|---|---|---|
| | | | | Total(%[4]) | RR[5] | %[6] |
| Intraresidue (\|i-j\|=0) | 0(0.0) | 114(15.9) | 17(9.8) | 131(14.8) | 0.1 | 10.6 |
| Sequential (\|i-j\|=1) | 15(6.5) | 160(20.4) | 110(51.9) | 285(23.3) | 0.2 | 23.0 |
| Medium range (\|i-j\|>1 and \|i-j\|<5) | 8(4.7) | 141(25.6) | 144(41.0) | 293(27.3) | 0.2 | 23.7 |
| Long range (\|i-j\|≥5) | 12(6.7) | 169(20.0) | 314(34.2) | 495(25.5) | 0.3 | 40.0 |
| Inter chain | 0(0.0) | 16(19.0) | 18(40.0) | 34(24.8) | 0.0 | 2.7 |
| Total | 35(6.0) | 600(20.2) | 603(35.5) | 1238(23.5) | 0.8 | 100.0 |

[1]number of backbone to backbone restraints, [2]number of backbone to sidechain restraints,[3]number of sidechain to sidechain restraints, [4]percentage of violations with respect to total restrains in that category, [5]number of restraints per residue, [6]percentage of violation with respect to total violations.

### 8.2.1 Pie-chart : Distance violations summary

## 8.3 Consistent distance violations summary

The following table provides the summary of consistently violated restraints. Restraints that are violated all models are counted as violated.

| Restraints type | B-B[1]($\%^4$) | B-S[2]($\%^4$) | S-S[3]($\%^4$) | Total Total($\%^4$) | Total RR[5] | Total $\%^6$ |
|---|---|---|---|---|---|---|
| Intraresidue ($\|i\text{-}j\|$=0) | 0(0.0) | 5(0.7) | 0(0.0) | 5(0.6) | 0.0 | 4.9 |
| Sequential ($\|i\text{-}j\|$=1) | 4(1.7) | 17(2.2) | 4(1.9) | 25(2.0) | 0.0 | 24.5 |
| Medium range ($\|i\text{-}j\|$>1 and $\|i\text{-}j\|$<5) | 1(0.6) | 7(1.3) | 16(4.6) | 24(2.2) | 0.0 | 23.5 |
| Long range ($\|i\text{-}j\|$≥5) | 1(0.6) | 15(1.8) | 32(3.5) | 48(2.5) | 0.0 | 47.1 |
| Inter chain | 0(0.0) | 0(0.0) | 0(0.0) | 0(0.0) | 0.0 | 0.0 |
| Total | 6(1.0) | 44(1.5) | 52(3.1) | 102(1.9) | 0.1 | 100.0 |

[1]number of backbone to backbone restraints, [2]number of backbone to sidechain restraints,[3]number of sidechain to sidechain restraints, [4]percentage of violations with respect to total restrains in that category,[5]number of restraints per residue,[6]percentage of violation with respect to total violations

### 8.3.1 Pie-chart : Consistent distance violations
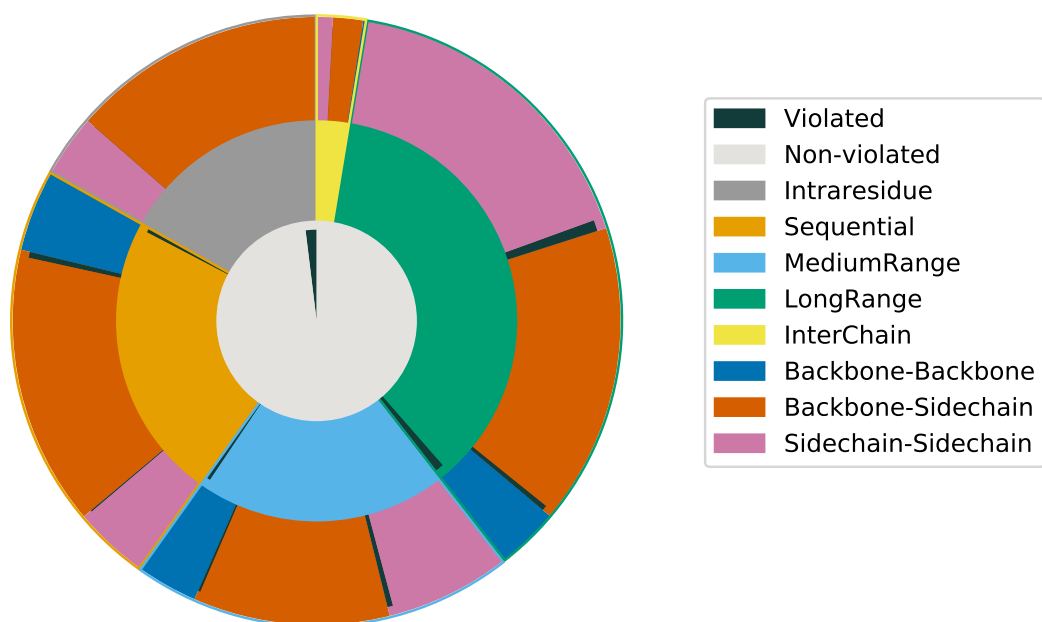
## 8.4 Residual distance violations

Violation are counted in different bin sizes and listed below

| Range (Å) | No. of violated restraints per model | Max violation (Å) |
|:---:|:---:|:---:|
| 0-0.2 | 247.4 | 0.2 |
| 0.2-0.5 | 69.8 | 0.5 |
| 0.5-1.0 | 78.0 | 1.0 |
| 1.0-2.0 | 48.0 | 2.0 |
| 2.0-5.0 | 22.2 | 4.07 |
| 5.0< | None | None |

## 8.5 Distance violations in ensemble

The restraints are grouped based on the number of violated models and listed here.

| No. of violated restraints | | | | | | No. of violated models |
|:---:|:---:|:---:|:---:|:---:|:---:|:---:|
| IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | |
| 34 | 49 | 57 | 98 | 15 | 253 | 1 |
| 20 | 35 | 41 | 52 | 8 | 156 | 2 |
| 17 | 20 | 30 | 39 | 2 | 108 | 3 |
| 9 | 24 | 14 | 20 | 2 | 69 | 4 |
| 6 | 9 | 13 | 29 | 3 | 60 | 5 |
| 8 | 13 | 7 | 22 | 0 | 50 | 6 |
| 7 | 15 | 6 | 26 | 0 | 54 | 7 |
| 3 | 8 | 7 | 16 | 1 | 35 | 8 |
| 1 | 13 | 12 | 22 | 1 | 49 | 9 |
| 2 | 14 | 6 | 9 | 1 | 32 | 10 |
| 2 | 9 | 6 | 14 | 1 | 32 | 11 |
| 1 | 10 | 10 | 8 | 0 | 29 | 12 |
| 2 | 5 | 13 | 20 | 0 | 40 | 13 |
| 0 | 4 | 6 | 6 | 0 | 16 | 14 |
| 3 | 2 | 2 | 13 | 0 | 20 | 15 |
| 3 | 9 | 9 | 13 | 0 | 34 | 16 |
| 4 | 1 | 11 | 9 | 0 | 25 | 17 |
| 4 | 10 | 9 | 12 | 0 | 35 | 18 |
| 0 | 10 | 10 | 19 | 0 | 39 | 19 |
| 5 | 25 | 24 | 48 | 0 | 102 | 20 |

[1]intraresidue restraints, [2]sequential restraints, [3]medium range restraints, [4]long range restraints, [5]inter chain restraints

### 8.5.1   Bar graph : No. of models vs No. of violations
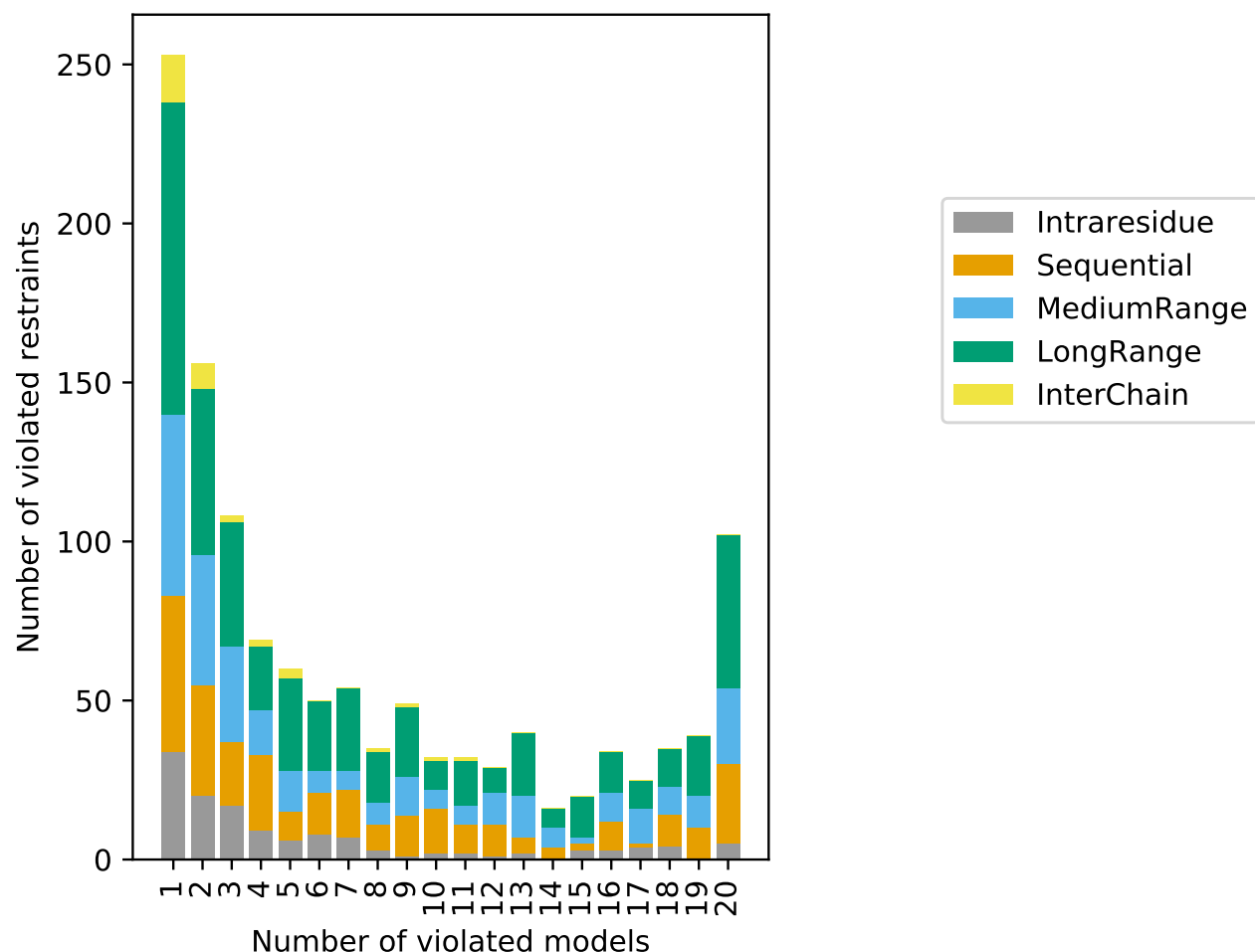


757 intraresidue restraints, 940 sequential restraints, 780 medium range restraints,1445 long range restraints and 103 inter chain restraints are not violated. There are totally 4025 restrains not violated in any of the models

## 8.6   Violations in each model

The following table lists the violation count in each model in the ensemble

| Model ID | No. of violations | | | | | | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|---|---|---|
| | IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | | |
| 1 | 36 | 127 | 114 | 198 | 2 | 477 | 0.47 | 3.88 |
| 2 | 32 | 103 | 111 | 202 | 10 | 458 | 0.5 | 3.98 |
| 3 | 40 | 108 | 124 | 183 | 5 | 460 | 0.5 | 3.85 |
| 4 | 42 | 105 | 119 | 194 | 5 | 465 | 0.43 | 3.27 |
| 5 | 37 | 111 | 116 | 187 | 3 | 454 | 0.48 | 4.05 |

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| Model ID | No. of violations | | | | | | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|---|---|---|
| | IR[1] | SQ[2] | MR[3] | LR[4] | IC[5] | Total | | |
| 6 | 44 | 123 | 117 | 208 | 6 | 498 | 0.46 | 3.78 |
| 7 | 40 | 119 | 117 | 197 | 5 | 478 | 0.5 | 3.97 |
| 8 | 32 | 110 | 118 | 202 | 3 | 465 | 0.49 | 4.07 |
| 9 | 29 | 109 | 125 | 196 | 1 | 460 | 0.5 | 3.89 |
| 10 | 39 | 125 | 110 | 193 | 3 | 470 | 0.47 | 3.9 |
| 11 | 32 | 114 | 112 | 191 | 4 | 453 | 0.49 | 3.78 |
| 12 | 44 | 110 | 115 | 197 | 5 | 471 | 0.53 | 3.87 |
| 13 | 32 | 118 | 98 | 204 | 10 | 462 | 0.48 | 3.87 |
| 14 | 38 | 110 | 120 | 185 | 3 | 456 | 0.48 | 3.59 |
| 15 | 45 | 97 | 110 | 199 | 7 | 458 | 0.44 | 3.95 |
| 16 | 34 | 112 | 103 | 202 | 6 | 457 | 0.51 | 3.56 |
| 17 | 36 | 103 | 116 | 212 | 5 | 472 | 0.49 | 3.73 |
| 18 | 37 | 103 | 125 | 209 | 6 | 480 | 0.5 | 3.68 |
| 19 | 33 | 112 | 110 | 208 | 5 | 468 | 0.47 | 4.06 |
| 20 | 32 | 106 | 110 | 194 | 4 | 446 | 0.46 | 3.66 |

[1]intraresidue restraints, [2]iequential restraints, [3]iedium range restraints, [4]long range restraints, [5]inter chain restraints

## 8.6.1 Bar graph : Violations in each model
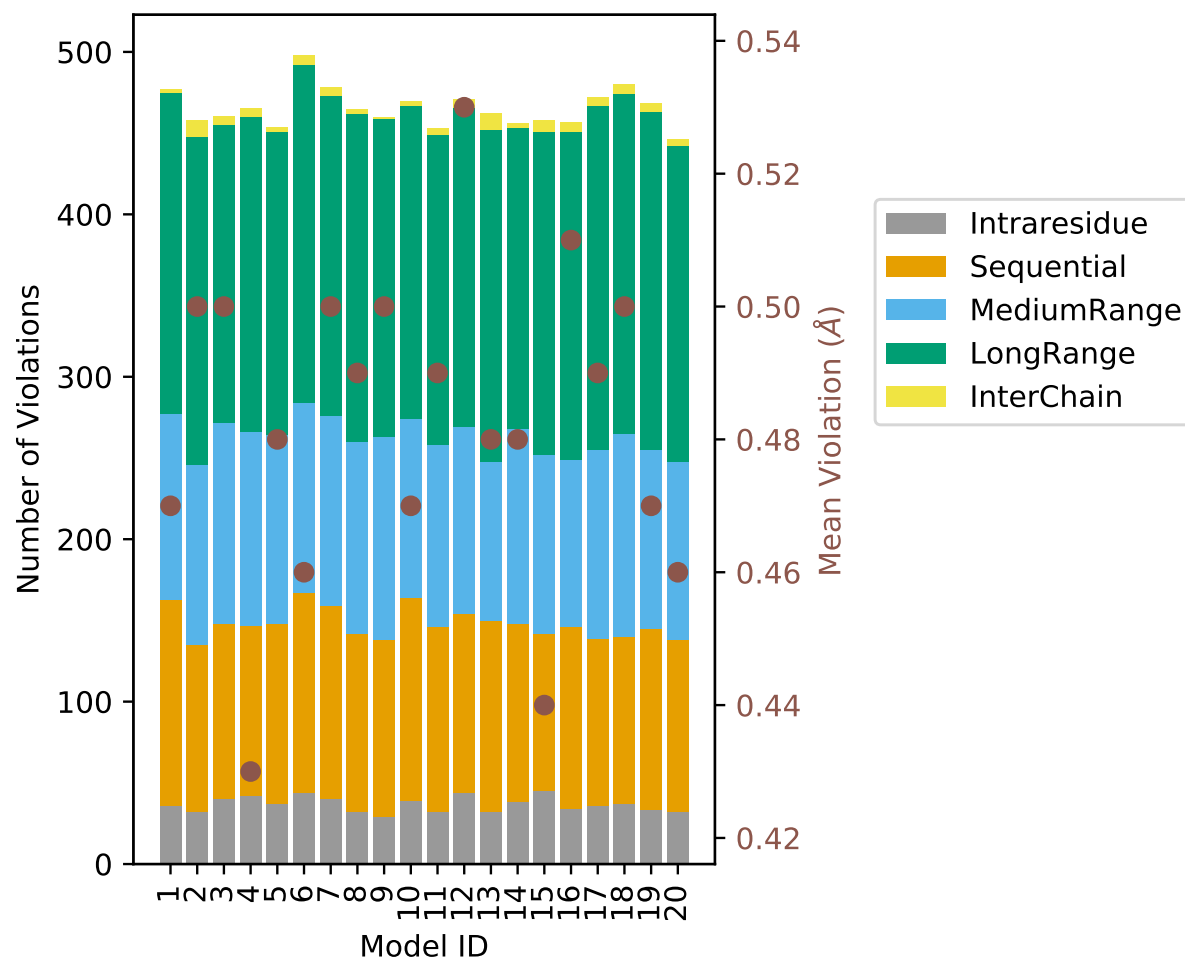
## 8.7 Most violated distance restraints

### 8.7.1 Histogram : Distribution of mean distance violation

The following histogram shows the distribution of average violation of each restraint.
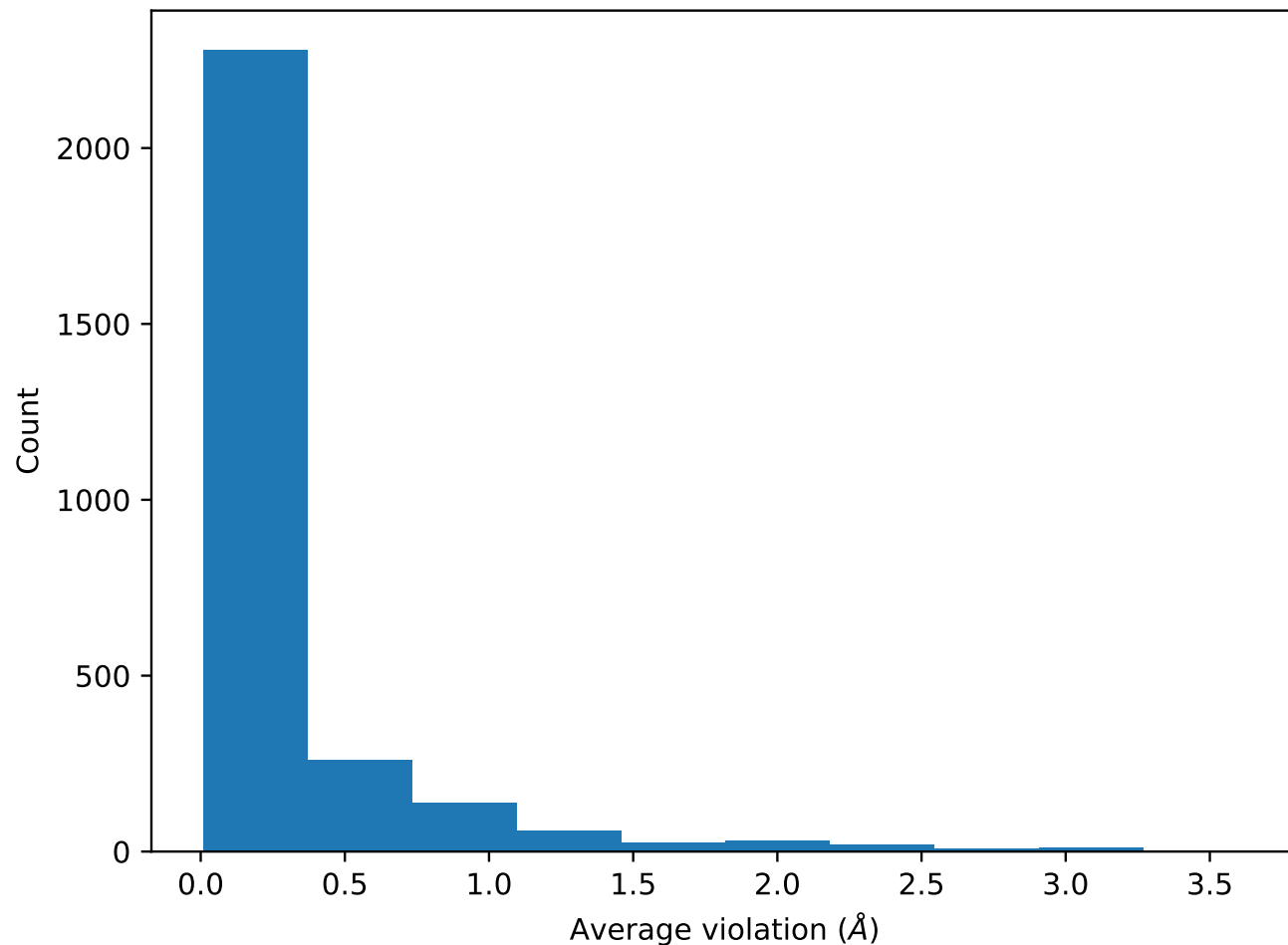


### 8.7.2 Table: Most violated distance restraints

The following tale lists the average violation of each restraint sorted by number of violated models

| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 20 | 0.05 | 0.09 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 20 | 0.06 | 0.1 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 20 | 0.11 | 0.22 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 20 | 0.13 | 0.21 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 20 | 0.29 | 0.68 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 20 | 0.57 | 0.66 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 20 | 1.04 | 1.58 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 20 | 0.9 | 1.23 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 20 | 0.93 | 1.12 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 20 | 0.93 | 1.12 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 20 | 0.93 | 1.12 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 20 | 0.59 | 0.92 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 20 | 0.59 | 0.92 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 20 | 0.59 | 0.92 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 20 | 0.23 | 0.31 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 20 | 0.69 | 1.15 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 20 | 0.23 | 0.31 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 20 | 0.68 | 1.17 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 20 | 0.68 | 1.17 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 20 | 0.68 | 1.17 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 20 | 0.86 | 1.52 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 20 | 1.23 | 2.14 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 20 | 0.6 | 0.82 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 20 | 0.6 | 0.82 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 20 | 0.6 | 0.82 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 20 | 1.15 | 1.51 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 20 | 1.15 | 1.51 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 20 | 1.15 | 1.51 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 20 | 0.14 | 0.19 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 20 | 2.79 | 4.07 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 20 | 0.93 | 1.78 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 20 | 0.93 | 1.78 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 20 | 0.52 | 0.67 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 20 | 0.28 | 0.67 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 20 | 0.37 | 0.48 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 20 | 0.58 | 0.66 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 20 | 0.58 | 0.89 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 20 | 0.58 | 0.89 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 20 | 0.58 | 0.89 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 20 | 0.23 | 0.28 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 20 | 0.21 | 0.37 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 20 | 0.37 | 0.54 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 20 | 0.37 | 0.54 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 20 | 0.37 | 0.54 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 20 | 0.63 | 1.13 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 20 | 0.63 | 1.13 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 20 | 0.63 | 1.13 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 20 | 2.9 | 4.06 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 20 | 0.58 | 0.81 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 20 | 0.58 | 0.81 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 20 | 0.58 | 0.81 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 20 | 0.13 | 0.17 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 20 | 0.97 | 1.27 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 20 | 0.97 | 1.27 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 20 | 0.97 | 1.27 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 20 | 0.95 | 1.22 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 20 | 0.47 | 0.57 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 20 | 0.07 | 0.13 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 20 | 0.07 | 0.13 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 20 | 0.07 | 0.13 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 20 | 2.45 | 2.61 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 20 | 2.45 | 2.61 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 20 | 2.45 | 2.61 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 20 | 2.43 | 2.77 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 20 | 2.43 | 2.77 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 20 | 2.43 | 2.77 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 20 | 1.79 | 2.28 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 20 | 1.79 | 2.28 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 20 | 1.79 | 2.28 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 20 | 1.74 | 2.11 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 20 | 1.74 | 2.11 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 20 | 1.74 | 2.11 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 20 | 0.49 | 1.24 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 20 | 0.49 | 1.24 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 20 | 0.49 | 1.24 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 20 | 0.46 | 1.22 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 20 | 0.46 | 1.22 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 20 | 0.46 | 1.22 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 20 | 0.04 | 0.09 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 20 | 0.05 | 0.08 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 20 | 0.41 | 3.32 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 20 | 0.41 | 3.32 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 20 | 0.09 | 0.12 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 20 | 0.09 | 0.12 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 20 | 0.79 | 0.96 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 20 | 0.79 | 0.96 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 20 | 0.79 | 0.96 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 20 | 0.77 | 0.94 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 20 | 0.77 | 0.94 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 20 | 0.77 | 0.94 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 20 | 0.74 | 1.37 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 20 | 0.88 | 1.36 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 20 | 1.28 | 2.05 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 20 | 0.09 | 0.11 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 20 | 0.09 | 0.11 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 20 | 0.09 | 0.11 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 20 | 0.08 | 0.13 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 20 | 0.08 | 0.13 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 20 | 0.08 | 0.13 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 20 | 0.57 | 0.83 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 20 | 0.57 | 0.83 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 20 | 0.51 | 0.68 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 20 | 0.51 | 0.68 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 20 | 0.08 | 0.15 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 20 | 0.08 | 0.15 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 20 | 0.08 | 0.15 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 20 | 0.1 | 0.15 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 20 | 0.1 | 0.15 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 20 | 0.1 | 0.15 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 20 | 0.07 | 0.1 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 20 | 0.07 | 0.1 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 20 | 0.07 | 0.1 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 20 | 0.08 | 0.14 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 20 | 0.08 | 0.14 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 20 | 0.08 | 0.14 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 20 | 0.07 | 0.1 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 20 | 0.07 | 0.1 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 20 | 0.07 | 0.1 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 20 | 0.1 | 0.14 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 20 | 0.1 | 0.14 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 20 | 0.1 | 0.14 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 20 | 0.09 | 0.17 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 20 | 0.09 | 0.17 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 20 | 0.09 | 0.17 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 20 | 0.73 | 1.12 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 20 | 0.66 | 0.92 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 20 | 0.41 | 0.44 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 20 | 0.42 | 0.45 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 20 | 0.07 | 0.13 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 20 | 0.07 | 0.13 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 20 | 0.07 | 0.13 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 20 | 0.65 | 1.05 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 20 | 0.65 | 1.05 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 20 | 0.65 | 1.05 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 20 | 0.67 | 0.96 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 20 | 0.67 | 0.96 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 20 | 0.67 | 0.96 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 20 | 0.34 | 0.61 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 20 | 0.08 | 0.14 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 20 | 1.36 | 1.67 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 20 | 1.36 | 1.67 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 20 | 1.36 | 1.67 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 20 | 1.38 | 1.74 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 20 | 1.38 | 1.74 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 20 | 1.38 | 1.74 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 20 | 1.5 | 1.8 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 20 | 1.5 | 1.8 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 20 | 1.5 | 1.8 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 20 | 1.42 | 1.82 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 20 | 1.42 | 1.82 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 20 | 1.42 | 1.82 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 20 | 0.67 | 0.91 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 20 | 0.67 | 0.91 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 20 | 0.67 | 0.91 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 20 | 0.64 | 1.03 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 20 | 0.64 | 1.03 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 20 | 0.64 | 1.03 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 20 | 2.14 | 2.35 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 20 | 2.14 | 2.35 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 20 | 2.14 | 2.35 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 20 | 2.15 | 2.42 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 20 | 2.15 | 2.42 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 20 | 2.15 | 2.42 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 20 | 0.12 | 0.17 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 20 | 0.11 | 0.16 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 20 | 0.06 | 0.14 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 20 | 0.06 | 0.14 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 20 | 0.06 | 0.14 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 20 | 0.06 | 0.11 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 20 | 0.06 | 0.11 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 20 | 0.06 | 0.11 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 20 | 0.1 | 0.21 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 20 | 0.1 | 0.21 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 20 | 0.1 | 0.21 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 20 | 0.81 | 0.95 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 20 | 0.81 | 0.95 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 20 | 0.81 | 0.95 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 20 | 0.78 | 0.85 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 20 | 0.78 | 0.85 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 20 | 0.78 | 0.85 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 20 | 0.06 | 0.15 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 20 | 0.06 | 0.15 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 20 | 0.06 | 0.15 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 20 | 0.07 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 20 | 0.07 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 20 | 0.07 | 0.08 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 20 | 0.07 | 0.13 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 20 | 0.07 | 0.13 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 20 | 0.07 | 0.13 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 20 | 0.06 | 0.09 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 20 | 0.06 | 0.09 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 20 | 0.06 | 0.09 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 20 | 0.1 | 0.13 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 20 | 0.11 | 0.19 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 20 | 0.1 | 0.14 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 20 | 0.93 | 1.13 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 20 | 0.93 | 1.13 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 20 | 0.93 | 1.13 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 20 | 0.81 | 1.17 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 20 | 0.81 | 1.17 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 20 | 0.81 | 1.17 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 20 | 0.08 | 0.13 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 20 | 0.08 | 0.13 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 20 | 0.08 | 0.13 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 20 | 0.38 | 0.51 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 20 | 0.35 | 0.4 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 20 | 0.44 | 0.6 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 20 | 0.54 | 0.66 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 20 | 0.22 | 0.57 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 19 | 0.09 | 0.16 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 19 | 0.1 | 0.17 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 19 | 0.52 | 1.76 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 19 | 0.37 | 0.88 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 19 | 0.37 | 0.88 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 19 | 0.37 | 0.88 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 19 | 0.36 | 0.71 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 19 | 1.4 | 3.22 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 19 | 0.77 | 0.93 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 19 | 0.77 | 0.93 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 19 | 0.77 | 0.93 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 19 | 0.78 | 0.9 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 19 | 0.78 | 0.9 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 19 | 0.5 | 1.02 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 19 | 0.32 | 0.67 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 19 | 0.57 | 1.56 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 19 | 0.5 | 0.77 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 19 | 0.5 | 0.77 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 19 | 0.5 | 0.77 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 19 | 0.67 | 1.36 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 19 | 0.32 | 0.46 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 19 | 1.44 | 3.53 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 19 | 1.38 | 1.79 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 19 | 0.71 | 0.86 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 19 | 0.71 | 0.86 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 19 | 1.19 | 1.51 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 19 | 1.19 | 1.51 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 19 | 1.19 | 1.51 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 19 | 0.37 | 0.81 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 19 | 0.69 | 0.9 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 19 | 0.69 | 0.9 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 19 | 0.69 | 0.9 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 19 | 0.03 | 0.07 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 19 | 1.18 | 1.95 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 19 | 0.05 | 0.08 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 19 | 0.07 | 0.12 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 19 | 0.07 | 0.12 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 19 | 0.07 | 0.12 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 19 | 0.07 | 0.12 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 19 | 0.07 | 0.12 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 19 | 0.07 | 0.12 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 19 | 0.06 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 19 | 0.06 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 19 | 0.06 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 19 | 0.06 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 19 | 0.06 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 19 | 0.06 | 0.09 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 19 | 0.06 | 0.11 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 19 | 0.06 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 19 | 0.06 | 0.11 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 19 | 0.06 | 0.11 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 19 | 0.06 | 0.11 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 19 | 0.06 | 0.11 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 19 | 1.15 | 1.83 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 19 | 1.15 | 1.83 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 19 | 1.15 | 1.83 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 19 | 0.04 | 0.07 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 19 | 0.04 | 0.07 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 19 | 0.04 | 0.07 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 19 | 0.04 | 0.08 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 19 | 0.04 | 0.08 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 19 | 0.04 | 0.08 |
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 19 | 0.05 | 0.12 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 19 | 0.04 | 0.07 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 19 | 0.09 | 0.16 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 19 | 0.09 | 0.16 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 19 | 0.09 | 0.16 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 19 | 0.08 | 0.13 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 19 | 0.08 | 0.13 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 19 | 0.08 | 0.13 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 19 | 0.08 | 0.12 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 19 | 0.08 | 0.12 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 19 | 0.08 | 0.12 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 19 | 0.08 | 0.16 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 19 | 0.08 | 0.16 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 19 | 0.08 | 0.16 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 19 | 0.08 | 0.16 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 19 | 0.08 | 0.16 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 19 | 0.08 | 0.16 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 19 | 0.08 | 0.16 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 19 | 0.08 | 0.16 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 19 | 0.08 | 0.16 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 19 | 0.04 | 0.13 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 19 | 0.04 | 0.13 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 19 | 0.04 | 0.13 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 19 | 0.04 | 0.13 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 19 | 0.04 | 0.13 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 19 | 0.04 | 0.13 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 19 | 1.7 | 2.13 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 19 | 1.41 | 2.22 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 18 | 0.38 | 0.52 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 18 | 0.85 | 1.59 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 18 | 0.5 | 0.84 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 18 | 0.5 | 0.84 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 18 | 0.5 | 0.84 |
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 18 | 0.09 | 0.12 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 18 | 2.55 | 3.2 |
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 18 | 1.38 | 1.71 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 18 | 0.37 | 0.64 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 18 | 0.17 | 0.26 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 18 | 0.25 | 0.27 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 18 | 0.84 | 1.06 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 18 | 1.0 | 1.36 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 18 | 0.02 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 18 | 0.02 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 18 | 0.02 | 0.02 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 18 | 0.08 | 0.13 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 18 | 0.76 | 0.94 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 18 | 0.76 | 0.94 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 18 | 0.76 | 0.94 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 18 | 0.86 | 1.11 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 18 | 0.05 | 0.07 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 18 | 0.83 | 1.01 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 18 | 1.54 | 1.6 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 18 | 0.61 | 0.69 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 18 | 0.83 | 1.11 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 18 | 0.11 | 0.19 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 18 | 0.08 | 0.13 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 18 | 0.08 | 0.13 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 18 | 0.08 | 0.13 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 18 | 0.63 | 1.55 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 18 | 0.62 | 1.45 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 18 | 0.66 | 0.81 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 18 | 0.66 | 0.81 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 18 | 0.66 | 0.81 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 18 | 0.02 | 0.05 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 18 | 0.46 | 1.39 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 18 | 0.46 | 1.39 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 18 | 0.46 | 1.39 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 18 | 0.09 | 0.15 |
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 18 | 0.13 | 0.21 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 18 | 0.13 | 0.21 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 18 | 0.13 | 0.21 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 18 | 0.03 | 0.06 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 18 | 0.03 | 0.06 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 18 | 0.03 | 0.06 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 18 | 0.07 | 0.12 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 18 | 0.07 | 0.12 |
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 18 | 0.07 | 0.12 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 18 | 0.09 | 0.14 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 18 | 0.07 | 0.12 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 18 | 0.07 | 0.12 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 18 | 0.07 | 0.12 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 18 | 0.07 | 0.12 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 18 | 0.07 | 0.12 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 18 | 0.07 | 0.12 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 18 | 0.07 | 0.12 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 18 | 0.07 | 0.12 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 18 | 0.07 | 0.12 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 18 | 0.22 | 0.4 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 18 | 1.16 | 1.92 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 17 | 0.22 | 0.59 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 17 | 1.01 | 1.64 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 17 | 1.01 | 1.64 |
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 17 | 0.58 | 1.52 |
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 17 | 0.58 | 1.52 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 17 | 0.58 | 1.52 |
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 17 | 0.31 | 1.0 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 17 | 0.75 | 0.91 |
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 17 | 0.75 | 0.91 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 17 | 0.75 | 0.91 |
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 17 | 0.26 | 0.62 |
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 17 | 0.8 | 1.04 |
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 17 | 0.48 | 1.48 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 17 | 0.48 | 1.48 |
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 17 | 0.48 | 1.48 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 17 | 0.81 | 1.04 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 17 | 0.69 | 0.95 |
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 17 | 0.69 | 0.95 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 17 | 0.69 | 0.95 |
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 17 | 1.01 | 1.2 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 17 | 0.44 | 0.79 |
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 17 | 2.73 | 3.89 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 17 | 0.04 | 0.07 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 17 | 0.04 | 0.07 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 17 | 0.04 | 0.07 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 17 | 0.31 | 0.73 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 17 | 0.31 | 0.73 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 17 | 0.31 | 0.73 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 17 | 0.05 | 0.08 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 17 | 0.05 | 0.08 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 17 | 0.05 | 0.08 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 17 | 0.4 | 0.69 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 17 | 0.67 | 0.98 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 17 | 0.67 | 0.98 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 17 | 0.67 | 0.98 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 17 | 0.95 | 1.3 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 17 | 0.05 | 0.09 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 17 | 0.05 | 0.09 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 17 | 0.05 | 0.09 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 17 | 0.06 | 0.1 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 17 | 0.06 | 0.1 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 17 | 0.06 | 0.1 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 17 | 0.09 | 0.13 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 17 | 0.09 | 0.13 |
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 17 | 0.09 | 0.13 |
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 17 | 0.04 | 0.1 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 17 | 0.04 | 0.1 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 17 | 0.04 | 0.1 |
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 17 | 0.05 | 0.09 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 16 | 0.53 | 0.79 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 16 | 0.53 | 0.79 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 16 | 0.53 | 0.79 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB2 | 16 | 0.8 | 1.2 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB3 | 16 | 0.8 | 1.2 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG21 | 16 | 0.87 | 1.21 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG22 | 16 | 0.87 | 1.21 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG23 | 16 | 0.87 | 1.21 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD11 | 16 | 0.26 | 0.53 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD12 | 16 | 0.26 | 0.53 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD13 | 16 | 0.26 | 0.53 |
| (1,5057) | 1:B:26:ILE:HG12 | 1:B:27:SER:HG | 16 | 0.97 | 1.2 |
| (1,5056) | 1:B:26:ILE:HG12 | 1:B:27:SER:H | 16 | 0.06 | 0.12 |
| (1,5043) | 1:B:25:VAL:H | 1:B:26:ILE:HG12 | 16 | 0.83 | 1.04 |
| (1,5039) | 1:B:24:GLY:HA2 | 1:B:26:ILE:HG12 | 16 | 1.56 | 1.66 |
| (1,5035) | 1:B:24:GLY:H | 1:B:26:ILE:HG12 | 16 | 0.61 | 0.76 |
| (1,5031) | 1:B:23:THR:HB | 1:B:26:ILE:HG12 | 16 | 0.89 | 1.1 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,4834) | 1:A:39:ASN:HD21 | 1:A:46:THR:HB | 16 | 0.8 | 1.54 |
| (1,4778) | 1:A:28:LYS:HG2 | 1:A:29:PHE:H | 16 | 0.16 | 0.27 |
| (1,4773) | 1:A:28:LYS:HA | 1:A:28:LYS:HD2 | 16 | 0.31 | 1.0 |
| (1,4573) | 1:A:44:ILE:HG12 | 1:A:73:PHE:HE1 | 16 | 0.42 | 0.7 |
| (1,4377) | 1:B:4:PHE:H | 1:B:4:PHE:HE1 | 16 | 0.78 | 1.03 |
| (1,4376) | 1:A:4:PHE:H | 1:A:4:PHE:HE1 | 16 | 0.81 | 1.01 |
| (1,4371) | 1:B:4:PHE:HE1 | 1:B:55:ASN:HA | 16 | 3.05 | 3.87 |
| (1,4370) | 1:A:4:PHE:HE1 | 1:A:55:ASN:HA | 16 | 3.41 | 3.95 |
| (1,4369) | 1:B:4:PHE:HE1 | 1:B:56:THR:HA | 16 | 0.59 | 0.99 |
| (1,4368) | 1:A:4:PHE:HE1 | 1:A:56:THR:HA | 16 | 0.59 | 1.0 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG21 | 16 | 0.56 | 1.13 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG22 | 16 | 0.56 | 1.13 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG23 | 16 | 0.56 | 1.13 |
| (1,4243) | 1:B:15:LYS:HA | 1:B:17:GLY:H | 16 | 0.1 | 0.26 |
| (1,4115) | 1:A:18:MET:HA | 1:A:21:GLN:HB2 | 16 | 0.05 | 0.08 |
| (1,3734) | 1:B:20:ASN:HA | 1:B:22:ILE:HB | 16 | 0.05 | 0.09 |
| (1,3537) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HB2 | 16 | 0.04 | 0.1 |
| (1,3536) | 1:A:64:ASP:HB2 | 1:A:65:LYS:HB2 | 16 | 0.05 | 0.09 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG21 | 16 | 0.85 | 1.72 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG22 | 16 | 0.85 | 1.72 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG23 | 16 | 0.85 | 1.72 |
| (1,3038) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HZ1 | 16 | 0.97 | 1.79 |
| (1,3038) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HZ1 | 16 | 0.97 | 1.79 |
| (1,3038) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HZ1 | 16 | 0.97 | 1.79 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD11 | 16 | 0.3 | 0.6 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD12 | 16 | 0.3 | 0.6 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD13 | 16 | 0.3 | 0.6 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG21 | 16 | 0.04 | 0.07 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG22 | 16 | 0.04 | 0.07 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG23 | 16 | 0.04 | 0.07 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG21 | 16 | 0.04 | 0.1 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG22 | 16 | 0.04 | 0.1 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG23 | 16 | 0.04 | 0.1 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG21 | 16 | 0.04 | 0.1 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG22 | 16 | 0.04 | 0.1 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG23 | 16 | 0.04 | 0.1 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG21 | 16 | 0.04 | 0.1 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG22 | 16 | 0.04 | 0.1 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG23 | 16 | 0.04 | 0.1 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD2 | 16 | 0.04 | 0.08 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD3 | 16 | 0.04 | 0.08 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD2 | 16 | 0.04 | 0.08 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD3 | 16 | 0.04 | 0.08 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD2 | 16 | 0.04 | 0.08 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD3 | 16 | 0.04 | 0.08 |
| (1,1527) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HA | 16 | 0.05 | 0.08 |
| (1,1527) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HA | 16 | 0.05 | 0.08 |
| (1,1527) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HA | 16 | 0.05 | 0.08 |
| (1,1222) | 1:B:69:VAL:H | 1:B:72:VAL:H | 16 | 0.05 | 0.1 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD11 | 15 | 0.03 | 0.05 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD12 | 15 | 0.03 | 0.05 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD13 | 15 | 0.03 | 0.05 |
| (1,4968) | 1:B:8:ILE:H | 1:B:8:ILE:HG12 | 15 | 0.11 | 0.2 |
| (1,4879) | 1:A:55:ASN:HD21 | 1:A:58:LYS:HG3 | 15 | 0.62 | 1.48 |
| (1,4842) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG12 | 15 | 0.97 | 1.96 |
| (1,4760) | 1:A:27:SER:H | 1:A:27:SER:HB2 | 15 | 0.25 | 0.27 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE1 | 15 | 0.01 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE2 | 15 | 0.01 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE3 | 15 | 0.01 | 0.02 |
| (1,4686) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HB2 | 15 | 0.94 | 1.56 |
| (1,4686) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HB2 | 15 | 0.94 | 1.56 |
| (1,4574) | 1:B:44:ILE:HG12 | 1:B:73:PHE:HE1 | 15 | 0.27 | 0.83 |
| (1,4498) | 1:B:13:GLU:H | 1:B:45:PHE:HE1 | 15 | 2.41 | 2.85 |
| (1,4490) | 1:B:18:MET:HB2 | 1:B:45:PHE:HE1 | 15 | 2.81 | 3.4 |
| (1,4488) | 1:B:18:MET:HB3 | 1:B:45:PHE:HE1 | 15 | 1.31 | 1.78 |
| (1,4475) | 1:A:22:ILE:HD11 | 1:A:45:PHE:HE1 | 15 | 0.63 | 1.45 |
| (1,4475) | 1:A:22:ILE:HD12 | 1:A:45:PHE:HE1 | 15 | 0.63 | 1.45 |
| (1,4475) | 1:A:22:ILE:HD13 | 1:A:45:PHE:HE1 | 15 | 0.63 | 1.45 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG21 | 15 | 0.65 | 0.98 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG22 | 15 | 0.65 | 0.98 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG23 | 15 | 0.65 | 0.98 |
| (1,4199) | 1:B:82:GLU:H | 1:B:83:HIS:HB3 | 15 | 0.09 | 0.36 |
| (1,3519) | 1:A:63:MET:HE1 | 1:A:76:GLU:HA | 15 | 0.05 | 0.07 |
| (1,3519) | 1:A:63:MET:HE2 | 1:A:76:GLU:HA | 15 | 0.05 | 0.07 |
| (1,3519) | 1:A:63:MET:HE3 | 1:A:76:GLU:HA | 15 | 0.05 | 0.07 |
| (1,3095) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HZ1 | 15 | 0.37 | 0.98 |
| (1,3095) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HZ1 | 15 | 0.37 | 0.98 |
| (1,3095) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HZ1 | 15 | 0.37 | 0.98 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD11 | 15 | 0.22 | 0.55 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD12 | 15 | 0.22 | 0.55 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD13 | 15 | 0.22 | 0.55 |
| (1,1935) | 1:B:18:MET:HE1 | 1:B:45:PHE:HE1 | 15 | 0.95 | 1.27 |
| (1,1935) | 1:B:18:MET:HE2 | 1:B:45:PHE:HE1 | 15 | 0.95 | 1.27 |
| (1,1935) | 1:B:18:MET:HE3 | 1:B:45:PHE:HE1 | 15 | 0.95 | 1.27 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,1841) | 1:B:13:GLU:HG2 | 1:B:45:PHE:HE1 | 15 | 1.92 | 2.29 |
| (1,1841) | 1:B:13:GLU:HG3 | 1:B:45:PHE:HE1 | 15 | 1.92 | 2.29 |
| (1,1410) | 1:B:15:LYS:H | 1:B:45:PHE:HE1 | 15 | 2.36 | 2.66 |
| (1,5162) | 1:B:53:VAL:HA | 1:B:54:LYS:HB2 | 14 | 0.8 | 1.01 |
| (1,5145) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG12 | 14 | 0.95 | 1.96 |
| (1,5126) | 1:B:37:VAL:HG11 | 1:B:48:ASN:HD21 | 14 | 0.44 | 0.84 |
| (1,5126) | 1:B:37:VAL:HG12 | 1:B:48:ASN:HD21 | 14 | 0.44 | 0.84 |
| (1,5126) | 1:B:37:VAL:HG13 | 1:B:48:ASN:HD21 | 14 | 0.44 | 0.84 |
| (1,5034) | 1:B:23:THR:HG21 | 1:B:27:SER:HB2 | 14 | 0.17 | 0.46 |
| (1,5034) | 1:B:23:THR:HG22 | 1:B:27:SER:HB2 | 14 | 0.17 | 0.46 |
| (1,5034) | 1:B:23:THR:HG23 | 1:B:27:SER:HB2 | 14 | 0.17 | 0.46 |
| (1,5029) | 1:B:20:ASN:HB2 | 1:B:21:GLN:HE21 | 14 | 0.83 | 1.68 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD21 | 14 | 0.37 | 0.8 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD22 | 14 | 0.37 | 0.8 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD23 | 14 | 0.37 | 0.8 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG21 | 14 | 0.9 | 1.21 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG22 | 14 | 0.9 | 1.21 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG23 | 14 | 0.9 | 1.21 |
| (1,4633) | 1:A:4:PHE:H | 1:A:54:LYS:HB2 | 14 | 0.25 | 0.53 |
| (1,4413) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 14 | 0.05 | 0.1 |
| (1,4413) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 14 | 0.05 | 0.1 |
| (1,4392) | 1:A:4:PHE:HZ | 1:A:6:ALA:HA | 14 | 0.02 | 0.04 |
| (1,4217) | 1:B:8:ILE:HA | 1:B:78:LEU:HB2 | 14 | 0.05 | 0.11 |
| (1,3937) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HB3 | 14 | 0.19 | 0.45 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB2 | 14 | 0.04 | 0.1 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB3 | 14 | 0.04 | 0.1 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE1 | 14 | 0.09 | 0.14 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE2 | 14 | 0.09 | 0.14 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE3 | 14 | 0.09 | 0.14 |
| (1,2389) | 1:A:36:ILE:HG21 | 1:A:48:ASN:H | 14 | 0.07 | 0.12 |
| (1,2389) | 1:A:36:ILE:HG22 | 1:A:48:ASN:H | 14 | 0.07 | 0.12 |
| (1,2389) | 1:A:36:ILE:HG23 | 1:A:48:ASN:H | 14 | 0.07 | 0.12 |
| (1,1066) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:H | 14 | 1.08 | 1.85 |
| (1,979) | 1:B:58:LYS:H | 1:B:58:LYS:HG3 | 13 | 0.02 | 0.07 |
| (1,915) | 1:B:51:ILE:HG12 | 1:B:52:PHE:H | 13 | 0.03 | 0.05 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD1 | 13 | 0.05 | 0.1 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD2 | 13 | 0.05 | 0.1 |
| (1,5185) | 1:B:56:THR:HG21 | 1:B:59:LEU:HB2 | 13 | 0.2 | 0.48 |
| (1,5185) | 1:B:56:THR:HG22 | 1:B:59:LEU:HB2 | 13 | 0.2 | 0.48 |
| (1,5185) | 1:B:56:THR:HG23 | 1:B:59:LEU:HB2 | 13 | 0.2 | 0.48 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB2 | 13 | 0.23 | 0.6 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB3 | 13 | 0.23 | 0.6 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,5118) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HA | 13 | 0.95 | 1.09 |
| (1,5019) | 1:B:17:GLY:HA2 | 1:B:21:GLN:HE22 | 13 | 0.24 | 0.4 |
| (1,4862) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HB2 | 13 | 0.26 | 0.47 |
| (1,4862) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HB2 | 13 | 0.26 | 0.47 |
| (1,4862) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HB2 | 13 | 0.26 | 0.47 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE2 | 13 | 0.84 | 1.45 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE3 | 13 | 0.84 | 1.45 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB2 | 13 | 0.9 | 1.13 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB3 | 13 | 0.9 | 1.13 |
| (1,4787) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HD2 | 13 | 0.15 | 0.53 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD11 | 13 | 0.22 | 0.63 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD12 | 13 | 0.22 | 0.63 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD13 | 13 | 0.22 | 0.63 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD11 | 13 | 0.49 | 1.0 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD12 | 13 | 0.49 | 1.0 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD13 | 13 | 0.49 | 1.0 |
| (1,4733) | 1:A:23:THR:HG21 | 1:A:27:SER:HB2 | 13 | 0.22 | 0.81 |
| (1,4733) | 1:A:23:THR:HG22 | 1:A:27:SER:HB2 | 13 | 0.22 | 0.81 |
| (1,4733) | 1:A:23:THR:HG23 | 1:A:27:SER:HB2 | 13 | 0.22 | 0.81 |
| (1,4703) | 1:A:17:GLY:HA2 | 1:A:21:GLN:HE22 | 13 | 0.61 | 1.22 |
| (1,4581) | 1:A:13:GLU:H | 1:A:73:PHE:HE1 | 13 | 1.67 | 1.9 |
| (1,4579) | 1:A:13:GLU:HA | 1:A:73:PHE:HE1 | 13 | 1.8 | 2.09 |
| (1,4577) | 1:A:13:GLU:HG2 | 1:A:73:PHE:HE1 | 13 | 3.1 | 3.23 |
| (1,4577) | 1:A:13:GLU:HG3 | 1:A:73:PHE:HE1 | 13 | 3.1 | 3.23 |
| (1,4575) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HE1 | 13 | 2.34 | 2.42 |
| (1,4538) | 1:B:52:PHE:HD1 | 1:B:53:VAL:H | 13 | 0.04 | 0.07 |
| (1,4538) | 1:B:52:PHE:HD2 | 1:B:53:VAL:H | 13 | 0.04 | 0.07 |
| (1,4497) | 1:A:13:GLU:H | 1:A:45:PHE:HE1 | 13 | 2.41 | 2.79 |
| (1,4489) | 1:A:18:MET:HB3 | 1:A:45:PHE:HE1 | 13 | 1.24 | 1.64 |
| (1,4487) | 1:A:18:MET:HB2 | 1:A:45:PHE:HE1 | 13 | 2.59 | 2.96 |
| (1,4478) | 1:B:19:THR:HG21 | 1:B:45:PHE:HE1 | 13 | 0.29 | 0.64 |
| (1,4478) | 1:B:19:THR:HG22 | 1:B:45:PHE:HE1 | 13 | 0.29 | 0.64 |
| (1,4478) | 1:B:19:THR:HG23 | 1:B:45:PHE:HE1 | 13 | 0.29 | 0.64 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG2 | 13 | 0.03 | 0.05 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG3 | 13 | 0.03 | 0.05 |
| (1,3528) | 1:B:63:MET:HE1 | 1:B:77:ARG:H | 13 | 0.03 | 0.06 |
| (1,3528) | 1:B:63:MET:HE2 | 1:B:77:ARG:H | 13 | 0.03 | 0.06 |
| (1,3528) | 1:B:63:MET:HE3 | 1:B:77:ARG:H | 13 | 0.03 | 0.06 |
| (1,3370) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HB | 13 | 1.08 | 1.43 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD21 | 13 | 0.03 | 0.06 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD22 | 13 | 0.03 | 0.06 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD23 | 13 | 0.03 | 0.06 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,2390) | 1:B:36:ILE:HG21 | 1:B:48:ASN:H | 13 | 0.08 | 0.11 |
| (1,2390) | 1:B:36:ILE:HG22 | 1:B:48:ASN:H | 13 | 0.08 | 0.11 |
| (1,2390) | 1:B:36:ILE:HG23 | 1:B:48:ASN:H | 13 | 0.08 | 0.11 |
| (1,2268) | 1:B:29:PHE:HD1 | 1:B:31:THR:HB | 13 | 0.04 | 0.08 |
| (1,2268) | 1:B:29:PHE:HD2 | 1:B:31:THR:HB | 13 | 0.04 | 0.08 |
| (1,2267) | 1:A:29:PHE:HD1 | 1:A:31:THR:HB | 13 | 0.05 | 0.09 |
| (1,2267) | 1:A:29:PHE:HD2 | 1:A:31:THR:HB | 13 | 0.05 | 0.09 |
| (1,2172) | 1:B:25:VAL:HG11 | 1:B:27:SER:H | 13 | 0.02 | 0.04 |
| (1,2172) | 1:B:25:VAL:HG12 | 1:B:27:SER:H | 13 | 0.02 | 0.04 |
| (1,2172) | 1:B:25:VAL:HG13 | 1:B:27:SER:H | 13 | 0.02 | 0.04 |
| (1,1934) | 1:A:18:MET:HE1 | 1:A:45:PHE:HE1 | 13 | 1.04 | 1.46 |
| (1,1934) | 1:A:18:MET:HE2 | 1:A:45:PHE:HE1 | 13 | 1.04 | 1.46 |
| (1,1934) | 1:A:18:MET:HE3 | 1:A:45:PHE:HE1 | 13 | 1.04 | 1.46 |
| (1,1840) | 1:A:13:GLU:HG2 | 1:A:45:PHE:HE1 | 13 | 1.96 | 2.39 |
| (1,1840) | 1:A:13:GLU:HG3 | 1:A:45:PHE:HE1 | 13 | 1.96 | 2.39 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG11 | 13 | 0.06 | 0.14 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG12 | 13 | 0.06 | 0.14 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG13 | 13 | 0.06 | 0.14 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG11 | 13 | 0.06 | 0.14 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG12 | 13 | 0.06 | 0.14 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG13 | 13 | 0.06 | 0.14 |
| (1,1818) | 1:A:13:GLU:HB2 | 1:A:73:PHE:HE1 | 13 | 3.2 | 3.33 |
| (1,1803) | 1:B:13:GLU:HB3 | 1:B:71:GLY:HA3 | 13 | 0.14 | 0.34 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG21 | 13 | 0.04 | 0.1 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG22 | 13 | 0.04 | 0.1 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG23 | 13 | 0.04 | 0.1 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG21 | 13 | 0.04 | 0.1 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG22 | 13 | 0.04 | 0.1 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG23 | 13 | 0.04 | 0.1 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG21 | 13 | 0.04 | 0.1 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG22 | 13 | 0.04 | 0.1 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG23 | 13 | 0.04 | 0.1 |
| (1,1409) | 1:A:15:LYS:H | 1:A:45:PHE:HE1 | 13 | 2.49 | 3.04 |
| (1,1129) | 1:A:62:LEU:HD11 | 1:A:65:LYS:H | 13 | 0.02 | 0.03 |
| (1,1129) | 1:A:62:LEU:HD12 | 1:A:65:LYS:H | 13 | 0.02 | 0.03 |
| (1,1129) | 1:A:62:LEU:HD13 | 1:A:65:LYS:H | 13 | 0.02 | 0.03 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD1 | 12 | 0.04 | 0.06 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD2 | 12 | 0.04 | 0.06 |
| (1,561) | 1:A:29:PHE:HD1 | 1:A:31:THR:H | 12 | 0.07 | 0.18 |
| (1,561) | 1:A:29:PHE:HD2 | 1:A:31:THR:H | 12 | 0.07 | 0.18 |
| (1,5262) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HA | 12 | 0.38 | 0.86 |
| (1,5182) | 1:B:55:ASN:HD21 | 1:B:58:LYS:HG3 | 12 | 0.48 | 1.43 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,5165) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HB2 | 12 | 0.2 | 0.4 |
| (1,5165) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HB2 | 12 | 0.2 | 0.4 |
| (1,5165) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HB2 | 12 | 0.2 | 0.4 |
| (1,5008) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD21 | 12 | 0.51 | 0.9 |
| (1,5008) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD21 | 12 | 0.51 | 0.9 |
| (1,5007) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HB2 | 12 | 0.75 | 1.48 |
| (1,5007) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HB2 | 12 | 0.75 | 1.48 |
| (1,4882) | 1:A:56:THR:HG21 | 1:A:59:LEU:HB2 | 12 | 0.19 | 0.43 |
| (1,4882) | 1:A:56:THR:HG22 | 1:A:59:LEU:HB2 | 12 | 0.19 | 0.43 |
| (1,4882) | 1:A:56:THR:HG23 | 1:A:59:LEU:HB2 | 12 | 0.19 | 0.43 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB2 | 12 | 0.27 | 0.53 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB3 | 12 | 0.27 | 0.53 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD2 | 12 | 0.59 | 1.27 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD3 | 12 | 0.59 | 1.27 |
| (1,4814) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HA | 12 | 0.92 | 1.09 |
| (1,4812) | 1:A:36:ILE:HG21 | 1:A:48:ASN:HB2 | 12 | 0.12 | 0.28 |
| (1,4812) | 1:A:36:ILE:HG22 | 1:A:48:ASN:HB2 | 12 | 0.12 | 0.28 |
| (1,4812) | 1:A:36:ILE:HG23 | 1:A:48:ASN:HB2 | 12 | 0.12 | 0.28 |
| (1,4774) | 1:A:28:LYS:HB2 | 1:A:28:LYS:HD2 | 12 | 0.44 | 0.95 |
| (1,4724) | 1:A:20:ASN:HB2 | 1:A:21:GLN:HE21 | 12 | 0.58 | 1.73 |
| (1,4690) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD21 | 12 | 0.39 | 0.88 |
| (1,4690) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD21 | 12 | 0.39 | 0.88 |
| (1,4477) | 1:A:19:THR:HG21 | 1:A:45:PHE:HE1 | 12 | 0.35 | 0.7 |
| (1,4477) | 1:A:19:THR:HG22 | 1:A:45:PHE:HE1 | 12 | 0.35 | 0.7 |
| (1,4477) | 1:A:19:THR:HG23 | 1:A:45:PHE:HE1 | 12 | 0.35 | 0.7 |
| (1,4393) | 1:B:4:PHE:HZ | 1:B:6:ALA:HA | 12 | 0.02 | 0.05 |
| (1,4363) | 1:B:29:PHE:HE1 | 1:B:66:LEU:HG | 12 | 0.25 | 0.92 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD21 | 12 | 1.03 | 2.72 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD22 | 12 | 1.03 | 2.72 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD23 | 12 | 1.03 | 2.72 |
| (1,4350) | 1:A:4:PHE:HD1 | 1:A:5:LEU:H | 12 | 0.02 | 0.04 |
| (1,4350) | 1:A:4:PHE:HD2 | 1:A:5:LEU:H | 12 | 0.02 | 0.04 |
| (1,4198) | 1:A:82:GLU:H | 1:A:83:HIS:HB3 | 12 | 0.08 | 0.15 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD11 | 12 | 0.03 | 0.07 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD12 | 12 | 0.03 | 0.07 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD13 | 12 | 0.03 | 0.07 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD11 | 12 | 0.04 | 0.1 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD12 | 12 | 0.04 | 0.1 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD13 | 12 | 0.04 | 0.1 |
| (1,397) | 1:B:22:ILE:H | 1:B:23:THR:HG1 | 12 | 0.02 | 0.04 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG11 | 12 | 0.03 | 0.07 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG12 | 12 | 0.03 | 0.07 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG13 | 12 | 0.03 | 0.07 |
| (1,2753) | 1:A:23:THR:HG1 | 1:A:47:CYS:HB3 | 12 | 0.03 | 0.06 |
| (1,1819) | 1:B:13:GLU:HB2 | 1:B:73:PHE:HE1 | 12 | 2.9 | 3.35 |
| (1,1132) | 1:B:62:LEU:HD11 | 1:B:66:LEU:H | 12 | 0.02 | 0.05 |
| (1,1132) | 1:B:62:LEU:HD12 | 1:B:66:LEU:H | 12 | 0.02 | 0.05 |
| (1,1132) | 1:B:62:LEU:HD13 | 1:B:66:LEU:H | 12 | 0.02 | 0.05 |
| (1,1130) | 1:B:62:LEU:HD11 | 1:B:65:LYS:H | 12 | 0.03 | 0.07 |
| (1,1130) | 1:B:62:LEU:HD12 | 1:B:65:LYS:H | 12 | 0.03 | 0.07 |
| (1,1130) | 1:B:62:LEU:HD13 | 1:B:65:LYS:H | 12 | 0.03 | 0.07 |
| (1,5206) | 1:B:62:LEU:HA | 1:B:65:LYS:HG2 | 11 | 0.12 | 0.27 |
| (1,5176) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD21 | 11 | 0.53 | 0.73 |
| (1,5176) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD21 | 11 | 0.53 | 0.73 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD11 | 11 | 0.23 | 0.62 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD12 | 11 | 0.23 | 0.62 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD13 | 11 | 0.23 | 0.62 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD2 | 11 | 0.92 | 1.52 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD3 | 11 | 0.92 | 1.52 |
| (1,5099) | 1:B:32:ASN:HD21 | 1:B:33:ILE:HB | 11 | 0.33 | 1.0 |
| (1,5072) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HD2 | 11 | 0.44 | 0.52 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE2 | 11 | 0.57 | 0.95 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE3 | 11 | 0.57 | 0.95 |
| (1,5000) | 1:B:15:LYS:HA | 1:B:16:ASN:HB2 | 11 | 0.24 | 0.39 |
| (1,4956) | 1:B:4:PHE:H | 1:B:54:LYS:HB2 | 11 | 0.28 | 0.63 |
| (1,4948) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HA | 11 | 0.38 | 0.83 |
| (1,4801) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG2 | 11 | 0.85 | 1.56 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG21 | 11 | 0.34 | 0.67 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG22 | 11 | 0.34 | 0.67 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG23 | 11 | 0.34 | 0.67 |
| (1,4582) | 1:B:13:GLU:H | 1:B:73:PHE:HE1 | 11 | 1.59 | 1.77 |
| (1,4580) | 1:B:13:GLU:HA | 1:B:73:PHE:HE1 | 11 | 1.63 | 1.88 |
| (1,4578) | 1:B:13:GLU:HG2 | 1:B:73:PHE:HE1 | 11 | 3.08 | 3.22 |
| (1,4578) | 1:B:13:GLU:HG3 | 1:B:73:PHE:HE1 | 11 | 3.08 | 3.22 |
| (1,4576) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HE1 | 11 | 2.35 | 2.42 |
| (1,4537) | 1:A:52:PHE:HD1 | 1:A:53:VAL:H | 11 | 0.03 | 0.06 |
| (1,4537) | 1:A:52:PHE:HD2 | 1:A:53:VAL:H | 11 | 0.03 | 0.06 |
| (1,4496) | 1:B:12:GLY:H | 1:B:45:PHE:HE1 | 11 | 0.08 | 0.2 |
| (1,4412) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 11 | 0.03 | 0.06 |
| (1,4412) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 11 | 0.03 | 0.06 |
| (1,4351) | 1:B:4:PHE:HD1 | 1:B:5:LEU:H | 11 | 0.02 | 0.04 |
| (1,4351) | 1:B:4:PHE:HD2 | 1:B:5:LEU:H | 11 | 0.02 | 0.04 |
| (1,4259) | 1:B:41:LYS:HG2 | 1:B:42:ASP:HA | 11 | 0.07 | 0.13 |
| (1,4259) | 1:B:41:LYS:HG3 | 1:B:42:ASP:HA | 11 | 0.07 | 0.13 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,4216) | 1:A:8:ILE:HA | 1:A:78:LEU:HB2 | 11 | 0.03 | 0.07 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD11 | 11 | 0.04 | 0.08 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD12 | 11 | 0.04 | 0.08 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD13 | 11 | 0.04 | 0.08 |
| (1,4074) | 1:A:82:GLU:HA | 1:A:83:HIS:HB2 | 11 | 0.04 | 0.1 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE2 | 11 | 0.19 | 0.33 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE3 | 11 | 0.19 | 0.33 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB2 | 11 | 0.05 | 0.15 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB3 | 11 | 0.05 | 0.15 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE1 | 11 | 0.08 | 0.14 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE2 | 11 | 0.08 | 0.14 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE3 | 11 | 0.08 | 0.14 |
| (1,3094) | 1:A:53:VAL:HG11 | 1:A:58:LYS:HZ1 | 11 | 0.23 | 0.92 |
| (1,3094) | 1:A:53:VAL:HG12 | 1:A:58:LYS:HZ1 | 11 | 0.23 | 0.92 |
| (1,3094) | 1:A:53:VAL:HG13 | 1:A:58:LYS:HZ1 | 11 | 0.23 | 0.92 |
| (1,2571) | 1:A:40:ALA:HA | 1:A:45:PHE:HA | 11 | 0.03 | 0.08 |
| (1,2473) | 1:A:37:VAL:HG21 | 1:A:38:LEU:H | 11 | 0.02 | 0.04 |
| (1,2473) | 1:A:37:VAL:HG22 | 1:A:38:LEU:H | 11 | 0.02 | 0.04 |
| (1,2473) | 1:A:37:VAL:HG23 | 1:A:38:LEU:H | 11 | 0.02 | 0.04 |
| (1,1802) | 1:A:13:GLU:HB3 | 1:A:71:GLY:HA3 | 11 | 0.27 | 0.4 |
| (1,1131) | 1:A:62:LEU:HD11 | 1:A:66:LEU:H | 11 | 0.04 | 0.07 |
| (1,1131) | 1:A:62:LEU:HD12 | 1:A:66:LEU:H | 11 | 0.04 | 0.07 |
| (1,1131) | 1:A:62:LEU:HD13 | 1:A:66:LEU:H | 11 | 0.04 | 0.07 |
| (1,978) | 1:A:58:LYS:H | 1:A:58:LYS:HG3 | 10 | 0.03 | 0.06 |
| (1,579) | 1:A:32:ASN:HD21 | 1:A:33:ILE:HB | 10 | 0.05 | 0.12 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD11 | 10 | 0.4 | 0.77 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD12 | 10 | 0.4 | 0.77 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD13 | 10 | 0.4 | 0.77 |
| (1,5173) | 1:B:54:LYS:HG2 | 1:B:55:ASN:HD21 | 10 | 0.95 | 1.44 |
| (1,5166) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HG2 | 10 | 0.69 | 1.24 |
| (1,5166) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HG2 | 10 | 0.69 | 1.24 |
| (1,5166) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HG2 | 10 | 0.69 | 1.24 |
| (1,5086) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HD2 | 10 | 0.2 | 0.55 |
| (1,5067) | 1:B:28:LYS:H | 1:B:28:LYS:HG2 | 10 | 0.08 | 0.17 |
| (1,5009) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD21 | 10 | 0.45 | 0.78 |
| (1,5009) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD21 | 10 | 0.45 | 0.78 |
| (1,4871) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HB2 | 10 | 0.6 | 1.31 |
| (1,4871) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HB2 | 10 | 0.6 | 1.31 |
| (1,4802) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG3 | 10 | 0.66 | 1.26 |
| (1,4720) | 1:A:20:ASN:H | 1:B:32:ASN:HB2 | 10 | 0.54 | 1.35 |
| (1,4682) | 1:A:15:LYS:HB2 | 1:A:16:ASN:HB2 | 10 | 1.71 | 2.21 |
| (1,4672) | 1:A:14:ASP:HB2 | 1:A:43:GLY:HA2 | 10 | 0.3 | 0.57 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,4671) | 1:A:14:ASP:HB2 | 1:A:43:GLY:H | 10 | 0.36 | 0.77 |
| (1,4628) | 1:A:3:ASP:HB2 | 1:A:4:PHE:H | 10 | 0.41 | 0.77 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG21 | 10 | 0.04 | 0.08 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG22 | 10 | 0.04 | 0.08 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG23 | 10 | 0.04 | 0.08 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG21 | 10 | 0.03 | 0.06 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG22 | 10 | 0.03 | 0.06 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG23 | 10 | 0.03 | 0.06 |
| (1,4325) | 1:B:80:ASN:HA | 1:B:81:LEU:HG | 10 | 0.04 | 0.07 |
| (1,4106) | 1:B:15:LYS:HB3 | 1:B:18:MET:HB3 | 10 | 0.07 | 0.14 |
| (1,3936) | 1:A:7:GLY:HA2 | 1:A:78:LEU:HB3 | 10 | 0.09 | 0.19 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG21 | 10 | 0.03 | 0.05 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG22 | 10 | 0.03 | 0.05 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG23 | 10 | 0.03 | 0.05 |
| (1,3735) | 1:A:66:LEU:HA | 1:A:69:VAL:HB | 10 | 0.03 | 0.07 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG21 | 10 | 0.29 | 0.66 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG22 | 10 | 0.29 | 0.66 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG23 | 10 | 0.29 | 0.66 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG21 | 10 | 0.03 | 0.05 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG22 | 10 | 0.03 | 0.05 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG23 | 10 | 0.03 | 0.05 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG21 | 10 | 0.03 | 0.06 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG22 | 10 | 0.03 | 0.06 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG23 | 10 | 0.03 | 0.06 |
| (1,2669) | 1:A:44:ILE:HD11 | 1:A:46:THR:HB | 10 | 0.03 | 0.06 |
| (1,2669) | 1:A:44:ILE:HD12 | 1:A:46:THR:HB | 10 | 0.03 | 0.06 |
| (1,2669) | 1:A:44:ILE:HD13 | 1:A:46:THR:HB | 10 | 0.03 | 0.06 |
| (1,2510) | 1:B:38:LEU:HD11 | 1:B:39:ASN:H | 10 | 0.03 | 0.07 |
| (1,2510) | 1:B:38:LEU:HD12 | 1:B:39:ASN:H | 10 | 0.03 | 0.07 |
| (1,2510) | 1:B:38:LEU:HD13 | 1:B:39:ASN:H | 10 | 0.03 | 0.07 |
| (1,2171) | 1:A:25:VAL:HG11 | 1:A:27:SER:H | 10 | 0.02 | 0.04 |
| (1,2171) | 1:A:25:VAL:HG12 | 1:A:27:SER:H | 10 | 0.02 | 0.04 |
| (1,2171) | 1:A:25:VAL:HG13 | 1:A:27:SER:H | 10 | 0.02 | 0.04 |
| (1,216) | 1:B:16:ASN:HA | 1:B:17:GLY:H | 10 | 0.05 | 0.07 |
| (1,215) | 1:A:16:ASN:HA | 1:A:17:GLY:H | 10 | 0.05 | 0.07 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG11 | 10 | 0.04 | 0.09 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG12 | 10 | 0.04 | 0.09 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG13 | 10 | 0.04 | 0.09 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG11 | 10 | 0.04 | 0.09 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG12 | 10 | 0.04 | 0.09 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG13 | 10 | 0.04 | 0.09 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD11 | 10 | 0.02 | 0.04 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD12 | 10 | 0.02 | 0.04 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD13 | 10 | 0.02 | 0.04 |
| (1,914) | 1:A:51:ILE:HG12 | 1:A:52:PHE:H | 9 | 0.03 | 0.05 |
| (1,735) | 1:B:41:LYS:H | 1:B:46:THR:H | 9 | 0.05 | 0.08 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD11 | 9 | 0.04 | 0.07 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD12 | 9 | 0.04 | 0.07 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD13 | 9 | 0.04 | 0.07 |
| (1,562) | 1:B:29:PHE:HD1 | 1:B:31:THR:H | 9 | 0.03 | 0.1 |
| (1,562) | 1:B:29:PHE:HD2 | 1:B:31:THR:H | 9 | 0.03 | 0.1 |
| (1,5248) | 1:B:76:GLU:HB2 | 1:B:77:ARG:H | 9 | 0.14 | 0.34 |
| (1,5175) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HD21 | 9 | 0.26 | 0.64 |
| (1,5175) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HD21 | 9 | 0.26 | 0.64 |
| (1,5130) | 1:B:38:LEU:HD21 | 1:B:39:ASN:HD21 | 9 | 0.27 | 0.37 |
| (1,5130) | 1:B:38:LEU:HD22 | 1:B:39:ASN:HD21 | 9 | 0.27 | 0.37 |
| (1,5130) | 1:B:38:LEU:HD23 | 1:B:39:ASN:HD21 | 9 | 0.27 | 0.37 |
| (1,5116) | 1:B:36:ILE:HG21 | 1:B:48:ASN:HB2 | 9 | 0.32 | 1.21 |
| (1,5116) | 1:B:36:ILE:HG22 | 1:B:48:ASN:HB2 | 9 | 0.32 | 1.21 |
| (1,5116) | 1:B:36:ILE:HG23 | 1:B:48:ASN:HB2 | 9 | 0.32 | 1.21 |
| (1,5108) | 1:B:34:ARG:HB2 | 1:B:51:ILE:H | 9 | 0.41 | 0.81 |
| (1,5107) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG3 | 9 | 0.89 | 1.21 |
| (1,5106) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG2 | 9 | 1.15 | 1.52 |
| (1,5013) | 1:B:16:ASN:HB2 | 1:B:18:MET:H | 9 | 0.34 | 0.56 |
| (1,5012) | 1:B:16:ASN:HB2 | 1:B:17:GLY:H | 9 | 0.38 | 0.47 |
| (1,4999) | 1:B:15:LYS:H | 1:B:18:MET:HG2 | 9 | 0.34 | 0.77 |
| (1,4952) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HB2 | 9 | 0.66 | 1.82 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD11 | 9 | 0.44 | 0.74 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD12 | 9 | 0.44 | 0.74 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD13 | 9 | 0.44 | 0.74 |
| (1,4870) | 1:A:54:LYS:HG2 | 1:A:55:ASN:HD21 | 9 | 0.92 | 1.7 |
| (1,4822) | 1:A:37:VAL:HG11 | 1:A:48:ASN:HD21 | 9 | 0.48 | 0.84 |
| (1,4822) | 1:A:37:VAL:HG12 | 1:A:48:ASN:HD21 | 9 | 0.48 | 0.84 |
| (1,4822) | 1:A:37:VAL:HG13 | 1:A:48:ASN:HD21 | 9 | 0.48 | 0.84 |
| (1,4820) | 1:A:37:VAL:HG11 | 1:A:39:ASN:HD21 | 9 | 0.95 | 1.23 |
| (1,4820) | 1:A:37:VAL:HG12 | 1:A:39:ASN:HD21 | 9 | 0.95 | 1.23 |
| (1,4820) | 1:A:37:VAL:HG13 | 1:A:39:ASN:HD21 | 9 | 0.95 | 1.23 |
| (1,4809) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 9 | 0.02 | 0.04 |
| (1,4803) | 1:A:34:ARG:HB2 | 1:A:51:ILE:H | 9 | 0.28 | 0.72 |
| (1,4795) | 1:A:32:ASN:HB2 | 1:B:20:ASN:H | 9 | 0.34 | 0.99 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE2 | 9 | 0.79 | 0.96 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE3 | 9 | 0.79 | 0.96 |
| (1,4689) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HB2 | 9 | 0.66 | 1.35 |
| (1,4689) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HB2 | 9 | 0.66 | 1.35 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,4679) | 1:A:15:LYS:HA | 1:A:16:ASN:HB2 | 9 | 0.23 | 0.3 |
| (1,4678) | 1:A:15:LYS:H | 1:A:18:MET:HG2 | 9 | 0.42 | 0.67 |
| (1,4665) | 1:A:13:GLU:HG2 | 1:A:15:LYS:HB2 | 9 | 0.34 | 0.62 |
| (1,4665) | 1:A:13:GLU:HG3 | 1:A:15:LYS:HB2 | 9 | 0.34 | 0.62 |
| (1,4627) | 1:A:3:ASP:HA | 1:A:54:LYS:HB2 | 9 | 0.18 | 0.48 |
| (1,4609) | 1:A:81:LEU:HB3 | 1:A:83:HIS:HD2 | 9 | 0.03 | 0.07 |
| (1,4607) | 1:A:5:LEU:HG | 1:A:83:HIS:HD2 | 9 | 0.02 | 0.06 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG21 | 9 | 1.78 | 1.85 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG22 | 9 | 1.78 | 1.85 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG23 | 9 | 1.78 | 1.85 |
| (1,4568) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HE1 | 9 | 0.36 | 0.64 |
| (1,4568) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HE1 | 9 | 0.36 | 0.64 |
| (1,4568) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HE1 | 9 | 0.36 | 0.64 |
| (1,4566) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HE1 | 9 | 1.13 | 1.6 |
| (1,4566) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HE1 | 9 | 1.13 | 1.6 |
| (1,4566) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HE1 | 9 | 1.13 | 1.6 |
| (1,4242) | 1:A:15:LYS:HA | 1:A:17:GLY:H | 9 | 0.13 | 0.33 |
| (1,396) | 1:A:22:ILE:H | 1:A:23:THR:HG1 | 9 | 0.02 | 0.03 |
| (1,3527) | 1:A:63:MET:HE1 | 1:A:77:ARG:H | 9 | 0.03 | 0.05 |
| (1,3527) | 1:A:63:MET:HE2 | 1:A:77:ARG:H | 9 | 0.03 | 0.05 |
| (1,3527) | 1:A:63:MET:HE3 | 1:A:77:ARG:H | 9 | 0.03 | 0.05 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD2 | 9 | 0.04 | 0.07 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD3 | 9 | 0.04 | 0.07 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD11 | 9 | 0.04 | 0.06 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD12 | 9 | 0.04 | 0.06 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD13 | 9 | 0.04 | 0.06 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG21 | 9 | 0.02 | 0.03 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG22 | 9 | 0.02 | 0.03 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG23 | 9 | 0.02 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD21 | 9 | 0.03 | 0.07 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD22 | 9 | 0.03 | 0.07 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD23 | 9 | 0.03 | 0.07 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD21 | 9 | 0.03 | 0.07 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD22 | 9 | 0.03 | 0.07 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD23 | 9 | 0.03 | 0.07 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD21 | 9 | 0.03 | 0.07 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD22 | 9 | 0.03 | 0.07 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD23 | 9 | 0.03 | 0.07 |
| (1,2725) | 1:A:46:THR:HG21 | 1:A:47:CYS:H | 9 | 0.02 | 0.04 |
| (1,2725) | 1:A:46:THR:HG22 | 1:A:47:CYS:H | 9 | 0.02 | 0.04 |
| (1,2725) | 1:A:46:THR:HG23 | 1:A:47:CYS:H | 9 | 0.02 | 0.04 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG21 | 9 | 0.02 | 0.04 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG22 | 9 | 0.02 | 0.04 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG23 | 9 | 0.02 | 0.04 |
| (1,2465) | 1:A:37:VAL:HG21 | 1:A:48:ASN:HD22 | 9 | 0.02 | 0.03 |
| (1,2465) | 1:A:37:VAL:HG22 | 1:A:48:ASN:HD22 | 9 | 0.02 | 0.03 |
| (1,2465) | 1:A:37:VAL:HG23 | 1:A:48:ASN:HD22 | 9 | 0.02 | 0.03 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD11 | 9 | 0.15 | 0.18 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD12 | 9 | 0.15 | 0.18 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD13 | 9 | 0.15 | 0.18 |
| (1,2343) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 9 | 0.02 | 0.04 |
| (1,2016) | 1:A:21:GLN:HE21 | 1:A:22:ILE:HA | 9 | 0.02 | 0.04 |
| (1,1779) | 1:B:11:VAL:HG11 | 1:B:73:PHE:HE1 | 9 | 0.49 | 0.7 |
| (1,1779) | 1:B:11:VAL:HG12 | 1:B:73:PHE:HE1 | 9 | 0.49 | 0.7 |
| (1,1779) | 1:B:11:VAL:HG13 | 1:B:73:PHE:HE1 | 9 | 0.49 | 0.7 |
| (1,1753) | 1:B:11:VAL:HG21 | 1:B:45:PHE:HE1 | 9 | 0.91 | 1.58 |
| (1,1753) | 1:B:11:VAL:HG22 | 1:B:45:PHE:HE1 | 9 | 0.91 | 1.58 |
| (1,1753) | 1:B:11:VAL:HG23 | 1:B:45:PHE:HE1 | 9 | 0.91 | 1.58 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD11 | 9 | 0.04 | 0.06 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD12 | 9 | 0.04 | 0.06 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD13 | 9 | 0.04 | 0.06 |
| (1,848) | 1:A:47:CYS:HG | 1:A:48:ASN:H | 8 | 0.02 | 0.03 |
| (1,5246) | 1:B:76:GLU:H | 1:B:76:GLU:HB2 | 8 | 0.19 | 0.26 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD21 | 8 | 0.41 | 0.76 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD22 | 8 | 0.41 | 0.76 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD23 | 8 | 0.41 | 0.76 |
| (1,5174) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HB2 | 8 | 0.86 | 1.33 |
| (1,5174) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HB2 | 8 | 0.86 | 1.33 |
| (1,5051) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HD2 | 8 | 0.24 | 0.49 |
| (1,5051) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HD2 | 8 | 0.24 | 0.49 |
| (1,5051) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HD2 | 8 | 0.24 | 0.49 |
| (1,4981) | 1:B:9:ARG:H | 1:B:76:GLU:HB2 | 8 | 0.17 | 0.38 |
| (1,4951) | 1:B:3:ASP:HB2 | 1:B:4:PHE:H | 8 | 0.39 | 0.64 |
| (1,4950) | 1:B:3:ASP:HA | 1:B:54:LYS:HB2 | 8 | 0.35 | 0.72 |
| (1,4910) | 1:A:64:ASP:HA | 1:A:67:ARG:HG2 | 8 | 0.15 | 0.28 |
| (1,4872) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HD21 | 8 | 0.41 | 1.23 |
| (1,4872) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HD21 | 8 | 0.41 | 1.23 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD11 | 8 | 0.19 | 0.63 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD12 | 8 | 0.19 | 0.63 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD13 | 8 | 0.19 | 0.63 |
| (1,4728) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HG12 | 8 | 0.37 | 0.83 |
| (1,4691) | 1:A:15:LYS:HE2 | 1:A:16:ASN:HD21 | 8 | 0.58 | 0.78 |
| (1,4691) | 1:A:15:LYS:HE3 | 1:A:16:ASN:HD21 | 8 | 0.58 | 0.78 |
| (1,4661) | 1:A:9:ARG:HD2 | 1:A:48:ASN:HD21 | 8 | 0.44 | 0.85 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,4661) | 1:A:9:ARG:HD3 | 1:A:48:ASN:HD21 | 8 | 0.44 | 0.85 |
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD1 | 8 | 0.02 | 0.05 |
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD2 | 8 | 0.02 | 0.05 |
| (1,4473) | 1:A:38:LEU:HD11 | 1:A:45:PHE:HE1 | 8 | 1.41 | 1.87 |
| (1,4473) | 1:A:38:LEU:HD12 | 1:A:45:PHE:HE1 | 8 | 1.41 | 1.87 |
| (1,4473) | 1:A:38:LEU:HD13 | 1:A:45:PHE:HE1 | 8 | 1.41 | 1.87 |
| (1,4362) | 1:A:29:PHE:HE1 | 1:A:66:LEU:HG | 8 | 0.3 | 0.58 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD21 | 8 | 1.25 | 2.59 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD22 | 8 | 1.25 | 2.59 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD23 | 8 | 1.25 | 2.59 |
| (1,4324) | 1:A:80:ASN:HA | 1:A:81:LEU:HG | 8 | 0.04 | 0.1 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD11 | 8 | 0.03 | 0.05 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD12 | 8 | 0.03 | 0.05 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD13 | 8 | 0.03 | 0.05 |
| (1,3702) | 1:B:15:LYS:HE2 | 1:B:18:MET:H | 8 | 0.03 | 0.06 |
| (1,3702) | 1:B:15:LYS:HE3 | 1:B:18:MET:H | 8 | 0.03 | 0.06 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE2 | 8 | 0.21 | 0.29 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE3 | 8 | 0.21 | 0.29 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD11 | 8 | 0.02 | 0.04 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD12 | 8 | 0.02 | 0.04 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD13 | 8 | 0.02 | 0.04 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD11 | 8 | 0.02 | 0.04 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD12 | 8 | 0.02 | 0.04 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD13 | 8 | 0.02 | 0.04 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD11 | 8 | 0.02 | 0.04 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD12 | 8 | 0.02 | 0.04 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD13 | 8 | 0.02 | 0.04 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD11 | 8 | 0.03 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD12 | 8 | 0.03 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD13 | 8 | 0.03 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD11 | 8 | 0.03 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD12 | 8 | 0.03 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD13 | 8 | 0.03 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD11 | 8 | 0.03 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD12 | 8 | 0.03 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD13 | 8 | 0.03 | 0.05 |
| (1,292) | 1:B:20:ASN:H | 1:B:20:ASN:HD22 | 8 | 0.13 | 0.18 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD11 | 8 | 0.01 | 0.02 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD12 | 8 | 0.01 | 0.02 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD13 | 8 | 0.01 | 0.02 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD11 | 8 | 0.01 | 0.02 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD12 | 8 | 0.01 | 0.02 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD13 | 8 | 0.01 | 0.02 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD11 | 8 | 0.01 | 0.02 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD12 | 8 | 0.01 | 0.02 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD13 | 8 | 0.01 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD21 | 8 | 0.02 | 0.04 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD22 | 8 | 0.02 | 0.04 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD23 | 8 | 0.02 | 0.04 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD21 | 8 | 0.02 | 0.04 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD22 | 8 | 0.02 | 0.04 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD23 | 8 | 0.02 | 0.04 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD21 | 8 | 0.02 | 0.04 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD22 | 8 | 0.02 | 0.04 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD23 | 8 | 0.02 | 0.04 |
| (1,2754) | 1:B:23:THR:HG1 | 1:B:47:CYS:HB3 | 8 | 0.04 | 0.06 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG21 | 8 | 0.03 | 0.05 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG22 | 8 | 0.03 | 0.05 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG23 | 8 | 0.03 | 0.05 |
| (1,2572) | 1:B:40:ALA:HA | 1:B:45:PHE:HA | 8 | 0.03 | 0.04 |
| (1,2549) | 1:A:38:LEU:HD21 | 1:A:45:PHE:HE1 | 8 | 0.71 | 1.38 |
| (1,2549) | 1:A:38:LEU:HD22 | 1:A:45:PHE:HE1 | 8 | 0.71 | 1.38 |
| (1,2549) | 1:A:38:LEU:HD23 | 1:A:45:PHE:HE1 | 8 | 0.71 | 1.38 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD21 | 8 | 0.03 | 0.04 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD22 | 8 | 0.03 | 0.04 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD23 | 8 | 0.03 | 0.04 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD11 | 8 | 0.16 | 0.19 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD12 | 8 | 0.16 | 0.19 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD13 | 8 | 0.16 | 0.19 |
| (1,1752) | 1:A:11:VAL:HG21 | 1:A:45:PHE:HE1 | 8 | 1.2 | 1.6 |
| (1,1752) | 1:A:11:VAL:HG22 | 1:A:45:PHE:HE1 | 8 | 1.2 | 1.6 |
| (1,1752) | 1:A:11:VAL:HG23 | 1:A:45:PHE:HE1 | 8 | 1.2 | 1.6 |
| (1,1242) | 1:B:69:VAL:HG11 | 1:B:71:GLY:H | 8 | 0.03 | 0.08 |
| (1,1242) | 1:B:69:VAL:HG12 | 1:B:71:GLY:H | 8 | 0.03 | 0.08 |
| (1,1242) | 1:B:69:VAL:HG13 | 1:B:71:GLY:H | 8 | 0.03 | 0.08 |
| (1,840) | 1:A:45:PHE:HE1 | 1:A:47:CYS:H | 7 | 1.54 | 1.62 |
| (1,5245) | 1:B:69:VAL:HG11 | 1:B:70:GLN:HE21 | 7 | 0.3 | 0.54 |
| (1,5245) | 1:B:69:VAL:HG12 | 1:B:70:GLN:HE21 | 7 | 0.3 | 0.54 |
| (1,5245) | 1:B:69:VAL:HG13 | 1:B:70:GLN:HE21 | 7 | 0.3 | 0.54 |
| (1,5242) | 1:B:68:LYS:HA | 1:B:68:LYS:HG2 | 7 | 0.02 | 0.04 |
| (1,5223) | 1:B:65:LYS:H | 1:B:65:LYS:HD2 | 7 | 0.04 | 0.08 |
| (1,5222) | 1:B:65:LYS:H | 1:B:65:LYS:HG2 | 7 | 0.14 | 0.43 |
| (1,5192) | 1:B:58:LYS:HE2 | 1:B:59:LEU:HA | 7 | 0.23 | 0.81 |
| (1,5172) | 1:B:54:LYS:HG2 | 1:B:55:ASN:H | 7 | 0.29 | 0.34 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,5124) | 1:B:37:VAL:HG11 | 1:B:39:ASN:HD21 | 7 | 0.85 | 0.92 |
| (1,5124) | 1:B:37:VAL:HG12 | 1:B:39:ASN:HD21 | 7 | 0.85 | 0.92 |
| (1,5124) | 1:B:37:VAL:HG13 | 1:B:39:ASN:HD21 | 7 | 0.85 | 0.92 |
| (1,5114) | 1:B:35:THR:HB | 1:B:50:MET:HB2 | 7 | 0.03 | 0.05 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD11 | 7 | 0.29 | 0.69 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD12 | 7 | 0.29 | 0.69 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD13 | 7 | 0.29 | 0.69 |
| (1,5005) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HD21 | 7 | 0.39 | 0.85 |
| (1,5005) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HD21 | 7 | 0.39 | 0.85 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG21 | 7 | 0.36 | 0.5 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG22 | 7 | 0.36 | 0.5 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG23 | 7 | 0.36 | 0.5 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG11 | 7 | 0.91 | 1.07 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG12 | 7 | 0.91 | 1.07 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG13 | 7 | 0.91 | 1.07 |
| (1,4925) | 1:A:67:ARG:HG2 | 1:A:75:VAL:H | 7 | 1.51 | 1.86 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG11 | 7 | 0.28 | 0.59 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG12 | 7 | 0.28 | 0.59 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG13 | 7 | 0.28 | 0.59 |
| (1,4920) | 1:A:67:ARG:H | 1:A:67:ARG:HG2 | 7 | 0.53 | 0.55 |
| (1,4912) | 1:A:65:LYS:H | 1:A:65:LYS:HD2 | 7 | 0.05 | 0.11 |
| (1,4873) | 1:A:54:LYS:HE2 | 1:A:55:ASN:HD21 | 7 | 0.56 | 0.85 |
| (1,4873) | 1:A:54:LYS:HE3 | 1:A:55:ASN:HD21 | 7 | 0.56 | 0.85 |
| (1,4863) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HG2 | 7 | 0.61 | 1.12 |
| (1,4863) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HG2 | 7 | 0.61 | 1.12 |
| (1,4863) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HG2 | 7 | 0.61 | 1.12 |
| (1,4769) | 1:A:28:LYS:H | 1:A:28:LYS:HG2 | 7 | 0.1 | 0.25 |
| (1,4695) | 1:A:16:ASN:HB2 | 1:A:17:GLY:H | 7 | 0.26 | 0.46 |
| (1,4694) | 1:A:16:ASN:HB2 | 1:A:16:ASN:HD21 | 7 | 0.34 | 0.36 |
| (1,4608) | 1:B:5:LEU:HG | 1:B:83:HIS:HD2 | 7 | 0.03 | 0.05 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG21 | 7 | 1.73 | 1.83 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG22 | 7 | 1.73 | 1.83 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG23 | 7 | 1.73 | 1.83 |
| (1,4567) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HE1 | 7 | 0.31 | 0.52 |
| (1,4567) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HE1 | 7 | 0.31 | 0.52 |
| (1,4567) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HE1 | 7 | 0.31 | 0.52 |
| (1,4565) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HE1 | 7 | 1.18 | 1.58 |
| (1,4565) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HE1 | 7 | 1.18 | 1.58 |
| (1,4565) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HE1 | 7 | 1.18 | 1.58 |
| (1,4491) | 1:A:45:PHE:HE1 | 1:A:47:CYS:HB2 | 7 | 2.3 | 2.59 |
| (1,4485) | 1:A:10:ILE:HB | 1:A:45:PHE:HE1 | 7 | 2.82 | 3.02 |
| (1,4481) | 1:A:10:ILE:HG21 | 1:A:45:PHE:HE1 | 7 | 1.33 | 1.6 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,4481) | 1:A:10:ILE:HG22 | 1:A:45:PHE:HE1 | 7 | 1.33 | 1.6 |
| (1,4481) | 1:A:10:ILE:HG23 | 1:A:45:PHE:HE1 | 7 | 1.33 | 1.6 |
| (1,4471) | 1:A:22:ILE:HG21 | 1:A:45:PHE:HE1 | 7 | 1.93 | 2.09 |
| (1,4471) | 1:A:22:ILE:HG22 | 1:A:45:PHE:HE1 | 7 | 1.93 | 2.09 |
| (1,4471) | 1:A:22:ILE:HG23 | 1:A:45:PHE:HE1 | 7 | 1.93 | 2.09 |
| (1,4075) | 1:B:82:GLU:HA | 1:B:83:HIS:HB2 | 7 | 0.04 | 0.09 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD21 | 7 | 0.02 | 0.03 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD22 | 7 | 0.02 | 0.03 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD23 | 7 | 0.02 | 0.03 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD21 | 7 | 0.02 | 0.03 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD22 | 7 | 0.02 | 0.03 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD23 | 7 | 0.02 | 0.03 |
| (1,3921) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HD2 | 7 | 0.05 | 0.08 |
| (1,3921) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HD3 | 7 | 0.05 | 0.08 |
| (1,3921) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HD2 | 7 | 0.05 | 0.08 |
| (1,3921) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HD3 | 7 | 0.05 | 0.08 |
| (1,3921) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HD2 | 7 | 0.05 | 0.08 |
| (1,3921) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HD3 | 7 | 0.05 | 0.08 |
| (1,3897) | 1:B:74:THR:HA | 1:B:76:GLU:HG2 | 7 | 0.04 | 0.09 |
| (1,3897) | 1:B:74:THR:HA | 1:B:76:GLU:HG3 | 7 | 0.04 | 0.09 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG21 | 7 | 0.02 | 0.05 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG22 | 7 | 0.02 | 0.05 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG23 | 7 | 0.02 | 0.05 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG11 | 7 | 0.03 | 0.05 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG12 | 7 | 0.03 | 0.05 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG13 | 7 | 0.03 | 0.05 |
| (1,3756) | 1:B:69:VAL:H | 1:B:70:GLN:HB2 | 7 | 0.03 | 0.07 |
| (1,3756) | 1:B:69:VAL:H | 1:B:70:GLN:HB3 | 7 | 0.03 | 0.07 |
| (1,3755) | 1:A:69:VAL:H | 1:A:70:GLN:HB2 | 7 | 0.06 | 0.14 |
| (1,3755) | 1:A:69:VAL:H | 1:A:70:GLN:HB3 | 7 | 0.06 | 0.14 |
| (1,3701) | 1:A:15:LYS:HE2 | 1:A:18:MET:H | 7 | 0.04 | 0.08 |
| (1,3701) | 1:A:15:LYS:HE3 | 1:A:18:MET:H | 7 | 0.04 | 0.08 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE1 | 7 | 0.03 | 0.07 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE2 | 7 | 0.03 | 0.07 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE3 | 7 | 0.03 | 0.07 |
| (1,3517) | 1:A:63:MET:HE1 | 1:A:77:ARG:HA | 7 | 0.06 | 0.13 |
| (1,3517) | 1:A:63:MET:HE2 | 1:A:77:ARG:HA | 7 | 0.06 | 0.13 |
| (1,3517) | 1:A:63:MET:HE3 | 1:A:77:ARG:HA | 7 | 0.06 | 0.13 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD21 | 7 | 0.02 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD22 | 7 | 0.02 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD23 | 7 | 0.02 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD21 | 7 | 0.02 | 0.03 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD22 | 7 | 0.02 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD23 | 7 | 0.02 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD21 | 7 | 0.02 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD22 | 7 | 0.02 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD23 | 7 | 0.02 | 0.03 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD21 | 7 | 0.02 | 0.04 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD22 | 7 | 0.02 | 0.04 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD23 | 7 | 0.02 | 0.04 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD21 | 7 | 0.02 | 0.04 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD22 | 7 | 0.02 | 0.04 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD23 | 7 | 0.02 | 0.04 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD21 | 7 | 0.02 | 0.04 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD22 | 7 | 0.02 | 0.04 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD23 | 7 | 0.02 | 0.04 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG21 | 7 | 0.02 | 0.02 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG22 | 7 | 0.02 | 0.02 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG23 | 7 | 0.02 | 0.02 |
| (1,2757) | 1:A:45:PHE:HE1 | 1:A:47:CYS:HB3 | 7 | 1.91 | 2.0 |
| (1,2638) | 1:B:44:ILE:HG13 | 1:B:45:PHE:H | 7 | 0.03 | 0.05 |
| (1,2550) | 1:B:38:LEU:HD21 | 1:B:45:PHE:HE1 | 7 | 0.46 | 0.71 |
| (1,2550) | 1:B:38:LEU:HD22 | 1:B:45:PHE:HE1 | 7 | 0.46 | 0.71 |
| (1,2550) | 1:B:38:LEU:HD23 | 1:B:45:PHE:HE1 | 7 | 0.46 | 0.71 |
| (1,2368) | 1:B:36:ILE:HG21 | 1:B:37:VAL:HB | 7 | 0.02 | 0.04 |
| (1,2368) | 1:B:36:ILE:HG22 | 1:B:37:VAL:HB | 7 | 0.02 | 0.04 |
| (1,2368) | 1:B:36:ILE:HG23 | 1:B:37:VAL:HB | 7 | 0.02 | 0.04 |
| (1,2344) | 1:B:35:THR:HB | 1:B:50:MET:HB2 | 7 | 0.03 | 0.05 |
| (1,2033) | 1:A:22:ILE:HB | 1:A:45:PHE:HE1 | 7 | 0.25 | 0.36 |
| (1,2017) | 1:B:21:GLN:HE21 | 1:B:22:ILE:HA | 7 | 0.01 | 0.02 |
| (1,1778) | 1:A:11:VAL:HG11 | 1:A:73:PHE:HE1 | 7 | 0.43 | 0.7 |
| (1,1778) | 1:A:11:VAL:HG12 | 1:A:73:PHE:HE1 | 7 | 0.43 | 0.7 |
| (1,1778) | 1:A:11:VAL:HG13 | 1:A:73:PHE:HE1 | 7 | 0.43 | 0.7 |
| (1,1714) | 1:A:10:ILE:HD11 | 1:A:45:PHE:HE1 | 7 | 2.36 | 2.55 |
| (1,1714) | 1:A:10:ILE:HD12 | 1:A:45:PHE:HE1 | 7 | 2.36 | 2.55 |
| (1,1714) | 1:A:10:ILE:HD13 | 1:A:45:PHE:HE1 | 7 | 2.36 | 2.55 |
| (1,1662) | 1:A:10:ILE:HG13 | 1:A:45:PHE:HE1 | 7 | 3.14 | 3.31 |
| (1,5218) | 1:B:64:ASP:HA | 1:B:67:ARG:HG2 | 6 | 0.17 | 0.5 |
| (1,5093) | 1:B:32:ASN:HB2 | 1:B:32:ASN:HD21 | 6 | 0.29 | 0.31 |
| (1,5065) | 1:B:27:SER:HG | 1:B:28:LYS:HD2 | 6 | 0.46 | 0.63 |
| (1,5028) | 1:B:20:ASN:HB2 | 1:B:21:GLN:H | 6 | 0.06 | 0.1 |
| (1,5011) | 1:B:16:ASN:HB2 | 1:B:16:ASN:HD21 | 6 | 0.34 | 0.36 |
| (1,4994) | 1:B:14:ASP:HB2 | 1:B:43:GLY:HA2 | 6 | 0.24 | 0.44 |
| (1,4985) | 1:B:9:ARG:HD2 | 1:B:48:ASN:HD21 | 6 | 0.51 | 1.27 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,4985) | 1:B:9:ARG:HD3 | 1:B:48:ASN:HD21 | 6 | 0.51 | 1.27 |
| (1,4943) | 1:A:80:ASN:HB2 | 1:A:80:ASN:HD21 | 6 | 0.34 | 0.38 |
| (1,4889) | 1:A:58:LYS:HE2 | 1:A:59:LEU:HA | 6 | 0.37 | 0.81 |
| (1,4868) | 1:A:54:LYS:HB2 | 1:A:55:ASN:HD21 | 6 | 0.71 | 1.23 |
| (1,4856) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HE2 | 6 | 0.67 | 1.09 |
| (1,4856) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HE2 | 6 | 0.67 | 1.09 |
| (1,4856) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HE2 | 6 | 0.67 | 1.09 |
| (1,4767) | 1:A:27:SER:HG | 1:A:28:LYS:HD2 | 6 | 0.95 | 1.55 |
| (1,4752) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HD2 | 6 | 0.42 | 0.69 |
| (1,4752) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HD2 | 6 | 0.42 | 0.69 |
| (1,4752) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HD2 | 6 | 0.42 | 0.69 |
| (1,4696) | 1:A:16:ASN:HB2 | 1:A:18:MET:H | 6 | 0.25 | 0.5 |
| (1,4684) | 1:A:15:LYS:HB2 | 1:A:18:MET:HB2 | 6 | 0.9 | 1.18 |
| (1,4629) | 1:A:3:ASP:HB2 | 1:A:52:PHE:HB2 | 6 | 1.18 | 1.8 |
| (1,4344) | 1:A:4:PHE:HD1 | 1:A:54:LYS:HA | 6 | 0.02 | 0.04 |
| (1,4344) | 1:A:4:PHE:HD2 | 1:A:54:LYS:HA | 6 | 0.02 | 0.04 |
| (1,4335) | 1:B:83:HIS:HA | 1:B:83:HIS:HD2 | 6 | 0.03 | 0.05 |
| (1,4318) | 1:A:77:ARG:HG3 | 1:A:79:SER:HA | 6 | 0.02 | 0.04 |
| (1,4296) | 1:A:73:PHE:HA | 1:A:73:PHE:HD1 | 6 | 0.02 | 0.02 |
| (1,4296) | 1:A:73:PHE:HA | 1:A:73:PHE:HD2 | 6 | 0.02 | 0.02 |
| (1,4193) | 1:B:5:LEU:HB2 | 1:B:83:HIS:HB3 | 6 | 0.09 | 0.14 |
| (1,4192) | 1:A:5:LEU:HB2 | 1:A:83:HIS:HB3 | 6 | 0.03 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD11 | 6 | 0.03 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD12 | 6 | 0.03 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD13 | 6 | 0.03 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD11 | 6 | 0.03 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD12 | 6 | 0.03 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD13 | 6 | 0.03 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD11 | 6 | 0.03 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD12 | 6 | 0.03 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD13 | 6 | 0.03 | 0.04 |
| (1,4147) | 1:B:61:THR:HG21 | 1:B:65:LYS:HB3 | 6 | 0.03 | 0.06 |
| (1,4147) | 1:B:61:THR:HG22 | 1:B:65:LYS:HB3 | 6 | 0.03 | 0.06 |
| (1,4147) | 1:B:61:THR:HG23 | 1:B:65:LYS:HB3 | 6 | 0.03 | 0.06 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD21 | 6 | 0.02 | 0.04 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD22 | 6 | 0.02 | 0.04 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD23 | 6 | 0.02 | 0.04 |
| (1,3916) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HD2 | 6 | 0.02 | 0.03 |
| (1,3916) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HD3 | 6 | 0.02 | 0.03 |
| (1,3916) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HD2 | 6 | 0.02 | 0.03 |
| (1,3916) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HD3 | 6 | 0.02 | 0.03 |
| (1,3916) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HD2 | 6 | 0.02 | 0.03 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,3916) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HD3 | 6 | 0.02 | 0.03 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG21 | 6 | 0.02 | 0.03 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG22 | 6 | 0.02 | 0.03 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG23 | 6 | 0.02 | 0.03 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG21 | 6 | 0.02 | 0.03 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG22 | 6 | 0.02 | 0.03 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG23 | 6 | 0.02 | 0.03 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG21 | 6 | 0.02 | 0.05 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG22 | 6 | 0.02 | 0.05 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG23 | 6 | 0.02 | 0.05 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG21 | 6 | 0.02 | 0.05 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG22 | 6 | 0.02 | 0.05 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG23 | 6 | 0.02 | 0.05 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG21 | 6 | 0.02 | 0.05 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG22 | 6 | 0.02 | 0.05 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG23 | 6 | 0.02 | 0.05 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG11 | 6 | 0.11 | 0.26 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG12 | 6 | 0.11 | 0.26 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG13 | 6 | 0.11 | 0.26 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG11 | 6 | 0.11 | 0.26 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG12 | 6 | 0.11 | 0.26 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG13 | 6 | 0.11 | 0.26 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE1 | 6 | 0.05 | 0.07 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE2 | 6 | 0.05 | 0.07 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE3 | 6 | 0.05 | 0.07 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE1 | 6 | 0.05 | 0.07 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE2 | 6 | 0.05 | 0.07 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE3 | 6 | 0.05 | 0.07 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE1 | 6 | 0.05 | 0.07 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE2 | 6 | 0.05 | 0.07 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE3 | 6 | 0.05 | 0.07 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG21 | 6 | 0.04 | 0.06 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG22 | 6 | 0.04 | 0.06 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG23 | 6 | 0.04 | 0.06 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG21 | 6 | 0.04 | 0.06 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG22 | 6 | 0.04 | 0.06 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG23 | 6 | 0.04 | 0.06 |
| (1,3192) | 1:A:54:LYS:HA | 1:A:54:LYS:HE2 | 6 | 0.23 | 0.34 |
| (1,3192) | 1:A:54:LYS:HA | 1:A:54:LYS:HE3 | 6 | 0.23 | 0.34 |
| (1,3182) | 1:A:54:LYS:HA | 1:A:54:LYS:HD2 | 6 | 0.03 | 0.07 |
| (1,3182) | 1:A:54:LYS:HA | 1:A:54:LYS:HD3 | 6 | 0.03 | 0.07 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG11 | 6 | 0.03 | 0.04 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG12 | 6 | 0.03 | 0.04 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG13 | 6 | 0.03 | 0.04 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD11 | 6 | 0.05 | 0.07 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD12 | 6 | 0.05 | 0.07 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD13 | 6 | 0.05 | 0.07 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD11 | 6 | 0.05 | 0.07 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD12 | 6 | 0.05 | 0.07 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD13 | 6 | 0.05 | 0.07 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD11 | 6 | 0.02 | 0.03 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD12 | 6 | 0.02 | 0.03 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD13 | 6 | 0.02 | 0.03 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD11 | 6 | 0.02 | 0.03 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD12 | 6 | 0.02 | 0.03 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD13 | 6 | 0.02 | 0.03 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD11 | 6 | 0.02 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD12 | 6 | 0.02 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD13 | 6 | 0.02 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD11 | 6 | 0.02 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD12 | 6 | 0.02 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD13 | 6 | 0.02 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD11 | 6 | 0.02 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD12 | 6 | 0.02 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD13 | 6 | 0.02 | 0.02 |
| (1,2726) | 1:B:46:THR:HG21 | 1:B:47:CYS:H | 6 | 0.02 | 0.03 |
| (1,2726) | 1:B:46:THR:HG22 | 1:B:47:CYS:H | 6 | 0.02 | 0.03 |
| (1,2726) | 1:B:46:THR:HG23 | 1:B:47:CYS:H | 6 | 0.02 | 0.03 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD11 | 6 | 0.02 | 0.04 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD12 | 6 | 0.02 | 0.04 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD13 | 6 | 0.02 | 0.04 |
| (1,2474) | 1:B:37:VAL:HG21 | 1:B:38:LEU:H | 6 | 0.02 | 0.03 |
| (1,2474) | 1:B:37:VAL:HG22 | 1:B:38:LEU:H | 6 | 0.02 | 0.03 |
| (1,2474) | 1:B:37:VAL:HG23 | 1:B:38:LEU:H | 6 | 0.02 | 0.03 |
| (1,227) | 1:B:18:MET:H | 1:B:18:MET:HG3 | 6 | 0.02 | 0.03 |
| (1,1898) | 1:B:16:ASN:HB3 | 1:B:17:GLY:H | 6 | 0.06 | 0.08 |
| (1,1875) | 1:B:11:VAL:HG21 | 1:B:41:LYS:HE2 | 6 | 0.06 | 0.14 |
| (1,1875) | 1:B:11:VAL:HG21 | 1:B:41:LYS:HE3 | 6 | 0.06 | 0.14 |
| (1,1875) | 1:B:11:VAL:HG22 | 1:B:41:LYS:HE2 | 6 | 0.06 | 0.14 |
| (1,1875) | 1:B:11:VAL:HG22 | 1:B:41:LYS:HE3 | 6 | 0.06 | 0.14 |
| (1,1875) | 1:B:11:VAL:HG23 | 1:B:41:LYS:HE2 | 6 | 0.06 | 0.14 |
| (1,1875) | 1:B:11:VAL:HG23 | 1:B:41:LYS:HE3 | 6 | 0.06 | 0.14 |
| (1,1762) | 1:A:11:VAL:HG11 | 1:A:73:PHE:HB2 | 6 | 0.02 | 0.03 |
| (1,1762) | 1:A:11:VAL:HG12 | 1:A:73:PHE:HB2 | 6 | 0.02 | 0.03 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,1762) | 1:A:11:VAL:HG13 | 1:A:73:PHE:HB2 | 6 | 0.02 | 0.03 |
| (1,1630) | 1:A:9:ARG:HD2 | 1:A:11:VAL:HB | 6 | 0.02 | 0.03 |
| (1,1630) | 1:A:9:ARG:HD3 | 1:A:11:VAL:HB | 6 | 0.02 | 0.03 |
| (1,1606) | 1:B:8:ILE:HD11 | 1:B:77:ARG:HA | 6 | 0.03 | 0.04 |
| (1,1606) | 1:B:8:ILE:HD12 | 1:B:77:ARG:HA | 6 | 0.03 | 0.04 |
| (1,1606) | 1:B:8:ILE:HD13 | 1:B:77:ARG:HA | 6 | 0.03 | 0.04 |
| (1,1420) | 1:B:40:ALA:H | 1:B:41:LYS:HD2 | 6 | 0.05 | 0.15 |
| (1,1420) | 1:B:40:ALA:H | 1:B:41:LYS:HD3 | 6 | 0.05 | 0.15 |
| (1,1226) | 1:B:69:VAL:H | 1:B:70:GLN:H | 6 | 0.02 | 0.05 |
| (1,1176) | 1:B:67:ARG:HE | 1:B:75:VAL:HB | 6 | 0.04 | 0.07 |
| (1,849) | 1:B:47:CYS:HG | 1:B:48:ASN:H | 5 | 0.02 | 0.04 |
| (1,841) | 1:B:45:PHE:HE1 | 1:B:47:CYS:H | 5 | 1.49 | 1.54 |
| (1,631) | 1:B:35:THR:H | 1:B:83:HIS:HE1 | 5 | 0.03 | 0.05 |
| (1,5257) | 1:B:80:ASN:HB2 | 1:B:80:ASN:HD21 | 5 | 0.33 | 0.34 |
| (1,5220) | 1:B:64:ASP:HB3 | 1:B:65:LYS:HG2 | 5 | 0.15 | 0.57 |
| (1,5159) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HE2 | 5 | 0.59 | 1.19 |
| (1,5159) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HE2 | 5 | 0.59 | 1.19 |
| (1,5159) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HE2 | 5 | 0.59 | 1.19 |
| (1,5128) | 1:B:37:VAL:HG21 | 1:B:48:ASN:HD21 | 5 | 0.48 | 0.55 |
| (1,5128) | 1:B:37:VAL:HG22 | 1:B:48:ASN:HD21 | 5 | 0.48 | 0.55 |
| (1,5128) | 1:B:37:VAL:HG23 | 1:B:48:ASN:HD21 | 5 | 0.48 | 0.55 |
| (1,5123) | 1:B:37:VAL:HB | 1:B:48:ASN:HD21 | 5 | 0.13 | 0.21 |
| (1,5073) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HE2 | 5 | 0.13 | 0.22 |
| (1,5073) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HE3 | 5 | 0.13 | 0.22 |
| (1,4993) | 1:B:14:ASP:HB2 | 1:B:43:GLY:H | 5 | 0.37 | 0.6 |
| (1,4949) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HD2 | 5 | 0.68 | 0.84 |
| (1,4930) | 1:A:68:LYS:HA | 1:A:68:LYS:HG2 | 5 | 0.03 | 0.07 |
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD21 | 5 | 0.47 | 0.76 |
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD22 | 5 | 0.47 | 0.76 |
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD23 | 5 | 0.47 | 0.76 |
| (1,4888) | 1:A:58:LYS:HG2 | 1:A:58:LYS:HE2 | 5 | 0.09 | 0.16 |
| (1,4869) | 1:A:54:LYS:HG2 | 1:A:55:ASN:H | 5 | 0.25 | 0.52 |
| (1,4813) | 1:A:36:ILE:HG12 | 1:A:37:VAL:H | 5 | 0.04 | 0.08 |
| (1,4734) | 1:A:23:THR:HG21 | 1:B:27:SER:HB2 | 5 | 0.27 | 0.65 |
| (1,4734) | 1:A:23:THR:HG22 | 1:B:27:SER:HB2 | 5 | 0.27 | 0.65 |
| (1,4734) | 1:A:23:THR:HG23 | 1:B:27:SER:HB2 | 5 | 0.27 | 0.65 |
| (1,4727) | 1:A:20:ASN:HD21 | 1:B:33:ILE:HG12 | 5 | 0.28 | 0.71 |
| (1,4693) | 1:A:16:ASN:HA | 1:B:32:ASN:HD21 | 5 | 0.56 | 1.16 |
| (1,4687) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HD21 | 5 | 0.34 | 0.89 |
| (1,4687) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HD21 | 5 | 0.34 | 0.89 |
| (1,4495) | 1:A:12:GLY:H | 1:A:45:PHE:HE1 | 5 | 0.12 | 0.18 |
| (1,4492) | 1:B:45:PHE:HE1 | 1:B:47:CYS:HB2 | 5 | 2.16 | 2.26 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,4486) | 1:B:10:ILE:HB | 1:B:45:PHE:HE1 | 5 | 2.92 | 3.05 |
| (1,4482) | 1:B:10:ILE:HG21 | 1:B:45:PHE:HE1 | 5 | 1.4 | 1.6 |
| (1,4482) | 1:B:10:ILE:HG22 | 1:B:45:PHE:HE1 | 5 | 1.4 | 1.6 |
| (1,4482) | 1:B:10:ILE:HG23 | 1:B:45:PHE:HE1 | 5 | 1.4 | 1.6 |
| (1,4474) | 1:B:38:LEU:HD11 | 1:B:45:PHE:HE1 | 5 | 1.45 | 1.64 |
| (1,4474) | 1:B:38:LEU:HD12 | 1:B:45:PHE:HE1 | 5 | 1.45 | 1.64 |
| (1,4474) | 1:B:38:LEU:HD13 | 1:B:45:PHE:HE1 | 5 | 1.45 | 1.64 |
| (1,4472) | 1:B:22:ILE:HG21 | 1:B:45:PHE:HE1 | 5 | 1.89 | 1.98 |
| (1,4472) | 1:B:22:ILE:HG22 | 1:B:45:PHE:HE1 | 5 | 1.89 | 1.98 |
| (1,4472) | 1:B:22:ILE:HG23 | 1:B:45:PHE:HE1 | 5 | 1.89 | 1.98 |
| (1,4379) | 1:B:4:PHE:HE1 | 1:B:7:GLY:H | 5 | 3.63 | 3.7 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB1 | 5 | 2.1 | 2.16 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB2 | 5 | 2.1 | 2.16 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB3 | 5 | 2.1 | 2.16 |
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD21 | 5 | 0.02 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD22 | 5 | 0.02 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD23 | 5 | 0.02 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD21 | 5 | 0.02 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD22 | 5 | 0.02 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD23 | 5 | 0.02 | 0.02 |
| (1,4258) | 1:A:41:LYS:HG2 | 1:A:42:ASP:HA | 5 | 0.05 | 0.1 |
| (1,4258) | 1:A:41:LYS:HG3 | 1:A:42:ASP:HA | 5 | 0.05 | 0.1 |
| (1,4255) | 1:B:41:LYS:HA | 1:B:41:LYS:HD2 | 5 | 0.02 | 0.03 |
| (1,4255) | 1:B:41:LYS:HA | 1:B:41:LYS:HD3 | 5 | 0.02 | 0.03 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD11 | 5 | 0.05 | 0.07 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD12 | 5 | 0.05 | 0.07 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD13 | 5 | 0.05 | 0.07 |
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD11 | 5 | 0.05 | 0.07 |
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD12 | 5 | 0.05 | 0.07 |
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD13 | 5 | 0.05 | 0.07 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD11 | 5 | 0.05 | 0.07 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD12 | 5 | 0.05 | 0.07 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD13 | 5 | 0.05 | 0.07 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD21 | 5 | 0.11 | 0.2 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD22 | 5 | 0.11 | 0.2 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD23 | 5 | 0.11 | 0.2 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD21 | 5 | 0.03 | 0.05 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD22 | 5 | 0.03 | 0.05 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD23 | 5 | 0.03 | 0.05 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD21 | 5 | 0.03 | 0.05 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD22 | 5 | 0.03 | 0.05 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD23 | 5 | 0.03 | 0.05 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD21 | 5 | 0.02 | 0.03 |
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD22 | 5 | 0.02 | 0.03 |
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD23 | 5 | 0.02 | 0.03 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD21 | 5 | 0.02 | 0.03 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD22 | 5 | 0.02 | 0.03 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD23 | 5 | 0.02 | 0.03 |
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD11 | 5 | 0.05 | 0.09 |
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD12 | 5 | 0.05 | 0.09 |
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD13 | 5 | 0.05 | 0.09 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD11 | 5 | 0.05 | 0.09 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD12 | 5 | 0.05 | 0.09 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD13 | 5 | 0.05 | 0.09 |
| (1,3952) | 1:A:78:LEU:HB2 | 1:A:80:ASN:H | 5 | 0.03 | 0.06 |
| (1,3929) | 1:B:4:PHE:HE1 | 1:B:77:ARG:HD2 | 5 | 2.05 | 2.46 |
| (1,3929) | 1:B:4:PHE:HE1 | 1:B:77:ARG:HD3 | 5 | 2.05 | 2.46 |
| (1,3917) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HD2 | 5 | 0.04 | 0.06 |
| (1,3917) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HD3 | 5 | 0.04 | 0.06 |
| (1,3917) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HD2 | 5 | 0.04 | 0.06 |
| (1,3917) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HD3 | 5 | 0.04 | 0.06 |
| (1,3917) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HD2 | 5 | 0.04 | 0.06 |
| (1,3917) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HD3 | 5 | 0.04 | 0.06 |
| (1,3896) | 1:A:74:THR:HA | 1:A:76:GLU:HG2 | 5 | 0.05 | 0.07 |
| (1,3896) | 1:A:74:THR:HA | 1:A:76:GLU:HG3 | 5 | 0.05 | 0.07 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG11 | 5 | 0.13 | 0.18 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG12 | 5 | 0.13 | 0.18 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG13 | 5 | 0.13 | 0.18 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG11 | 5 | 0.13 | 0.18 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG12 | 5 | 0.13 | 0.18 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG13 | 5 | 0.13 | 0.18 |
| (1,3699) | 1:A:15:LYS:HE2 | 1:A:16:ASN:HD21 | 5 | 0.07 | 0.12 |
| (1,3699) | 1:A:15:LYS:HE3 | 1:A:16:ASN:HD21 | 5 | 0.07 | 0.12 |
| (1,3386) | 1:A:61:THR:HG21 | 1:A:65:LYS:HE2 | 5 | 0.03 | 0.06 |
| (1,3386) | 1:A:61:THR:HG21 | 1:A:65:LYS:HE3 | 5 | 0.03 | 0.06 |
| (1,3386) | 1:A:61:THR:HG22 | 1:A:65:LYS:HE2 | 5 | 0.03 | 0.06 |
| (1,3386) | 1:A:61:THR:HG22 | 1:A:65:LYS:HE3 | 5 | 0.03 | 0.06 |
| (1,3386) | 1:A:61:THR:HG23 | 1:A:65:LYS:HE2 | 5 | 0.03 | 0.06 |
| (1,3386) | 1:A:61:THR:HG23 | 1:A:65:LYS:HE3 | 5 | 0.03 | 0.06 |
| (1,3231) | 1:B:57:ASP:HB2 | 1:B:58:LYS:HG3 | 5 | 0.06 | 0.21 |
| (1,3231) | 1:B:57:ASP:HB3 | 1:B:58:LYS:HG3 | 5 | 0.06 | 0.21 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG11 | 5 | 0.02 | 0.05 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG12 | 5 | 0.02 | 0.05 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG13 | 5 | 0.02 | 0.05 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD11 | 5 | 0.05 | 0.08 |
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD12 | 5 | 0.05 | 0.08 |
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD13 | 5 | 0.05 | 0.08 |
| (1,2879) | 1:B:8:ILE:H | 1:B:50:MET:HG3 | 5 | 0.03 | 0.06 |
| (1,2758) | 1:B:45:PHE:HE1 | 1:B:47:CYS:HB3 | 5 | 1.84 | 1.98 |
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD11 | 5 | 0.02 | 0.03 |
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD12 | 5 | 0.02 | 0.03 |
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD13 | 5 | 0.02 | 0.03 |
| (1,2670) | 1:B:44:ILE:HD11 | 1:B:46:THR:HB | 5 | 0.03 | 0.04 |
| (1,2670) | 1:B:44:ILE:HD12 | 1:B:46:THR:HB | 5 | 0.03 | 0.04 |
| (1,2670) | 1:B:44:ILE:HD13 | 1:B:46:THR:HB | 5 | 0.03 | 0.04 |
| (1,2466) | 1:B:37:VAL:HG21 | 1:B:48:ASN:HD22 | 5 | 0.02 | 0.04 |
| (1,2466) | 1:B:37:VAL:HG22 | 1:B:48:ASN:HD22 | 5 | 0.02 | 0.04 |
| (1,2466) | 1:B:37:VAL:HG23 | 1:B:48:ASN:HD22 | 5 | 0.02 | 0.04 |
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD11 | 5 | 0.02 | 0.03 |
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD12 | 5 | 0.02 | 0.03 |
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD13 | 5 | 0.02 | 0.03 |
| (1,2034) | 1:B:22:ILE:HB | 1:B:45:PHE:HE1 | 5 | 0.2 | 0.27 |
| (1,181) | 1:A:15:LYS:H | 1:A:18:MET:HG2 | 5 | 0.07 | 0.14 |
| (1,1796) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HG2 | 5 | 0.02 | 0.02 |
| (1,1796) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HG3 | 5 | 0.02 | 0.02 |
| (1,1715) | 1:B:10:ILE:HD11 | 1:B:45:PHE:HE1 | 5 | 2.43 | 2.6 |
| (1,1715) | 1:B:10:ILE:HD12 | 1:B:45:PHE:HE1 | 5 | 2.43 | 2.6 |
| (1,1715) | 1:B:10:ILE:HD13 | 1:B:45:PHE:HE1 | 5 | 2.43 | 2.6 |
| (1,1663) | 1:B:10:ILE:HG13 | 1:B:45:PHE:HE1 | 5 | 3.24 | 3.4 |
| (1,1631) | 1:B:9:ARG:HD2 | 1:B:11:VAL:HB | 5 | 0.02 | 0.04 |
| (1,1631) | 1:B:9:ARG:HD3 | 1:B:11:VAL:HB | 5 | 0.02 | 0.04 |
| (1,1456) | 1:B:3:ASP:HB2 | 1:B:53:VAL:H | 5 | 0.05 | 0.08 |
| (1,1455) | 1:A:3:ASP:HB2 | 1:A:53:VAL:H | 5 | 0.07 | 0.11 |
| (1,924) | 1:A:3:ASP:HB3 | 1:A:53:VAL:H | 4 | 0.04 | 0.06 |
| (1,777) | 1:B:43:GLY:H | 1:B:44:ILE:H | 4 | 0.03 | 0.05 |
| (1,734) | 1:A:41:LYS:H | 1:A:46:THR:H | 4 | 0.06 | 0.11 |
| (1,5263) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HD2 | 4 | 0.8 | 0.84 |
| (1,5260) | 1:B:82:GLU:H | 1:B:82:GLU:HG2 | 4 | 0.09 | 0.26 |
| (1,5239) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG21 | 4 | 0.18 | 0.35 |
| (1,5239) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG22 | 4 | 0.18 | 0.35 |
| (1,5239) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG23 | 4 | 0.18 | 0.35 |
| (1,5238) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG11 | 4 | 0.88 | 1.09 |
| (1,5238) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG12 | 4 | 0.88 | 1.09 |
| (1,5238) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG13 | 4 | 0.88 | 1.09 |
| (1,5237) | 1:B:67:ARG:HG2 | 1:B:75:VAL:H | 4 | 1.39 | 1.85 |
| (1,5232) | 1:B:67:ARG:H | 1:B:67:ARG:HG2 | 4 | 0.54 | 0.6 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,5216) | 1:B:63:MET:HE1 | 1:B:77:ARG:HB2 | 4 | 0.07 | 0.2 |
| (1,5216) | 1:B:63:MET:HE2 | 1:B:77:ARG:HB2 | 4 | 0.07 | 0.2 |
| (1,5216) | 1:B:63:MET:HE3 | 1:B:77:ARG:HB2 | 4 | 0.07 | 0.2 |
| (1,5171) | 1:B:54:LYS:HB2 | 1:B:55:ASN:HD21 | 4 | 0.42 | 0.64 |
| (1,5167) | 1:B:53:VAL:HG21 | 1:B:58:LYS:HB2 | 4 | 0.06 | 0.18 |
| (1,5167) | 1:B:53:VAL:HG22 | 1:B:58:LYS:HB2 | 4 | 0.06 | 0.18 |
| (1,5167) | 1:B:53:VAL:HG23 | 1:B:58:LYS:HB2 | 4 | 0.06 | 0.18 |
| (1,5146) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG13 | 4 | 0.21 | 0.29 |
| (1,5063) | 1:B:27:SER:HB2 | 1:B:28:LYS:H | 4 | 0.03 | 0.05 |
| (1,4932) | 1:A:68:LYS:HD2 | 1:A:69:VAL:H | 4 | 0.33 | 0.4 |
| (1,4931) | 1:A:68:LYS:HA | 1:A:68:LYS:HD2 | 4 | 0.58 | 0.62 |
| (1,4902) | 1:A:62:LEU:H | 1:A:65:LYS:HD2 | 4 | 0.08 | 0.16 |
| (1,4826) | 1:A:38:LEU:HD21 | 1:A:39:ASN:HD21 | 4 | 0.22 | 0.35 |
| (1,4826) | 1:A:38:LEU:HD22 | 1:A:39:ASN:HD21 | 4 | 0.22 | 0.35 |
| (1,4826) | 1:A:38:LEU:HD23 | 1:A:39:ASN:HD21 | 4 | 0.22 | 0.35 |
| (1,4792) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG13 | 4 | 0.4 | 0.82 |
| (1,4723) | 1:A:20:ASN:HB2 | 1:A:21:GLN:H | 4 | 0.04 | 0.09 |
| (1,4705) | 1:A:18:MET:H | 1:B:32:ASN:HD21 | 4 | 0.34 | 0.61 |
| (1,4667) | 1:A:14:ASP:HA | 1:A:15:LYS:HB2 | 4 | 0.04 | 0.07 |
| (1,4630) | 1:A:3:ASP:HB2 | 1:A:52:PHE:HD1 | 4 | 0.69 | 1.28 |
| (1,4630) | 1:A:3:ASP:HB2 | 1:A:52:PHE:HD2 | 4 | 0.69 | 1.28 |
| (1,4620) | 1:B:82:GLU:HA | 1:B:83:HIS:HD2 | 4 | 0.07 | 0.15 |
| (1,4614) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HD2 | 4 | 0.07 | 0.11 |
| (1,4613) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HD2 | 4 | 0.08 | 0.11 |
| (1,4610) | 1:B:81:LEU:HB3 | 1:B:83:HIS:HD2 | 4 | 0.02 | 0.04 |
| (1,4378) | 1:A:4:PHE:HE1 | 1:A:7:GLY:H | 4 | 3.59 | 3.63 |
| (1,4358) | 1:A:4:PHE:HE1 | 1:A:6:ALA:HB1 | 4 | 2.07 | 2.19 |
| (1,4358) | 1:A:4:PHE:HE1 | 1:A:6:ALA:HB2 | 4 | 2.07 | 2.19 |
| (1,4358) | 1:A:4:PHE:HE1 | 1:A:6:ALA:HB3 | 4 | 2.07 | 2.19 |
| (1,4334) | 1:A:83:HIS:HA | 1:A:83:HIS:HD2 | 4 | 0.02 | 0.06 |
| (1,432) | 1:A:24:GLY:H | 1:A:27:SER:HG | 4 | 0.01 | 0.02 |
| (1,4170) | 1:A:72:VAL:HG21 | 1:A:73:PHE:HB3 | 4 | 0.01 | 0.01 |
| (1,4170) | 1:A:72:VAL:HG22 | 1:A:73:PHE:HB3 | 4 | 0.01 | 0.01 |
| (1,4170) | 1:A:72:VAL:HG23 | 1:A:73:PHE:HB3 | 4 | 0.01 | 0.01 |
| (1,4079) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 4 | 0.15 | 0.15 |
| (1,4078) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 4 | 0.14 | 0.14 |
| (1,4073) | 1:B:8:ILE:H | 1:B:81:LEU:HD21 | 4 | 0.02 | 0.03 |
| (1,4073) | 1:B:8:ILE:H | 1:B:81:LEU:HD22 | 4 | 0.02 | 0.03 |
| (1,4073) | 1:B:8:ILE:H | 1:B:81:LEU:HD23 | 4 | 0.02 | 0.03 |
| (1,3928) | 1:A:4:PHE:HE1 | 1:A:77:ARG:HD2 | 4 | 1.99 | 2.4 |
| (1,3928) | 1:A:4:PHE:HE1 | 1:A:77:ARG:HD3 | 4 | 1.99 | 2.4 |
| (1,3920) | 1:A:6:ALA:HB1 | 1:A:77:ARG:HD2 | 4 | 0.01 | 0.02 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,3920) | 1:A:6:ALA:HB1 | 1:A:77:ARG:HD3 | 4 | 0.01 | 0.02 |
| (1,3920) | 1:A:6:ALA:HB2 | 1:A:77:ARG:HD2 | 4 | 0.01 | 0.02 |
| (1,3920) | 1:A:6:ALA:HB2 | 1:A:77:ARG:HD3 | 4 | 0.01 | 0.02 |
| (1,3920) | 1:A:6:ALA:HB3 | 1:A:77:ARG:HD2 | 4 | 0.01 | 0.02 |
| (1,3920) | 1:A:6:ALA:HB3 | 1:A:77:ARG:HD3 | 4 | 0.01 | 0.02 |
| (1,3736) | 1:B:66:LEU:HA | 1:B:69:VAL:HB | 4 | 0.03 | 0.04 |
| (1,3700) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD21 | 4 | 0.07 | 0.12 |
| (1,3700) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD21 | 4 | 0.07 | 0.12 |
| (1,3620) | 1:A:41:LYS:HE2 | 1:A:44:ILE:H | 4 | 0.05 | 0.11 |
| (1,3620) | 1:A:41:LYS:HE3 | 1:A:44:ILE:H | 4 | 0.05 | 0.11 |
| (1,3440) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD11 | 4 | 0.03 | 0.05 |
| (1,3440) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD12 | 4 | 0.03 | 0.05 |
| (1,3440) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD13 | 4 | 0.03 | 0.05 |
| (1,3436) | 1:B:62:LEU:HD11 | 1:B:66:LEU:HG | 4 | 0.01 | 0.02 |
| (1,3436) | 1:B:62:LEU:HD12 | 1:B:66:LEU:HG | 4 | 0.01 | 0.02 |
| (1,3436) | 1:B:62:LEU:HD13 | 1:B:66:LEU:HG | 4 | 0.01 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD11 | 4 | 0.02 | 0.04 |
| (1,3311) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD12 | 4 | 0.02 | 0.04 |
| (1,3311) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD13 | 4 | 0.02 | 0.04 |
| (1,3311) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD11 | 4 | 0.02 | 0.04 |
| (1,3311) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD12 | 4 | 0.02 | 0.04 |
| (1,3311) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD13 | 4 | 0.02 | 0.04 |
| (1,3311) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD11 | 4 | 0.02 | 0.04 |
| (1,3311) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD12 | 4 | 0.02 | 0.04 |
| (1,3311) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD13 | 4 | 0.02 | 0.04 |
| (1,3275) | 1:B:30:ASP:HB2 | 1:B:58:LYS:HD2 | 4 | 0.06 | 0.09 |
| (1,3275) | 1:B:30:ASP:HB2 | 1:B:58:LYS:HD3 | 4 | 0.06 | 0.09 |
| (1,3275) | 1:B:30:ASP:HB3 | 1:B:58:LYS:HD2 | 4 | 0.06 | 0.09 |
| (1,3275) | 1:B:30:ASP:HB3 | 1:B:58:LYS:HD3 | 4 | 0.06 | 0.09 |
| (1,3274) | 1:A:30:ASP:HB2 | 1:A:58:LYS:HD2 | 4 | 0.05 | 0.08 |
| (1,3274) | 1:A:30:ASP:HB2 | 1:A:58:LYS:HD3 | 4 | 0.05 | 0.08 |
| (1,3274) | 1:A:30:ASP:HB3 | 1:A:58:LYS:HD2 | 4 | 0.05 | 0.08 |
| (1,3274) | 1:A:30:ASP:HB3 | 1:A:58:LYS:HD3 | 4 | 0.05 | 0.08 |
| (1,3220) | 1:A:4:PHE:HD1 | 1:A:56:THR:HG21 | 4 | 0.04 | 0.12 |
| (1,3220) | 1:A:4:PHE:HD1 | 1:A:56:THR:HG22 | 4 | 0.04 | 0.12 |
| (1,3220) | 1:A:4:PHE:HD1 | 1:A:56:THR:HG23 | 4 | 0.04 | 0.12 |
| (1,3220) | 1:A:4:PHE:HD2 | 1:A:56:THR:HG21 | 4 | 0.04 | 0.12 |
| (1,3220) | 1:A:4:PHE:HD2 | 1:A:56:THR:HG22 | 4 | 0.04 | 0.12 |
| (1,3220) | 1:A:4:PHE:HD2 | 1:A:56:THR:HG23 | 4 | 0.04 | 0.12 |
| (1,3190) | 1:A:54:LYS:H | 1:A:54:LYS:HD2 | 4 | 0.08 | 0.15 |
| (1,3190) | 1:A:54:LYS:H | 1:A:54:LYS:HD3 | 4 | 0.08 | 0.15 |
| (1,3184) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD22 | 4 | 0.05 | 0.09 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,3184) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD22 | 4 | 0.05 | 0.09 |
| (1,3013) | 1:B:51:ILE:HD11 | 1:B:62:LEU:HD21 | 4 | 0.04 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD11 | 1:B:62:LEU:HD22 | 4 | 0.04 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD11 | 1:B:62:LEU:HD23 | 4 | 0.04 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD12 | 1:B:62:LEU:HD21 | 4 | 0.04 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD12 | 1:B:62:LEU:HD22 | 4 | 0.04 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD12 | 1:B:62:LEU:HD23 | 4 | 0.04 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD13 | 1:B:62:LEU:HD21 | 4 | 0.04 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD13 | 1:B:62:LEU:HD22 | 4 | 0.04 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD13 | 1:B:62:LEU:HD23 | 4 | 0.04 | 0.05 |
| (1,291) | 1:A:20:ASN:H | 1:A:20:ASN:HD22 | 4 | 0.16 | 0.19 |
| (1,2716) | 1:B:9:ARG:HE | 1:B:46:THR:HG21 | 4 | 0.13 | 0.18 |
| (1,2716) | 1:B:9:ARG:HE | 1:B:46:THR:HG22 | 4 | 0.13 | 0.18 |
| (1,2716) | 1:B:9:ARG:HE | 1:B:46:THR:HG23 | 4 | 0.13 | 0.18 |
| (1,2704) | 1:B:9:ARG:HD2 | 1:B:46:THR:HG21 | 4 | 0.04 | 0.07 |
| (1,2704) | 1:B:9:ARG:HD2 | 1:B:46:THR:HG22 | 4 | 0.04 | 0.07 |
| (1,2704) | 1:B:9:ARG:HD2 | 1:B:46:THR:HG23 | 4 | 0.04 | 0.07 |
| (1,2704) | 1:B:9:ARG:HD3 | 1:B:46:THR:HG21 | 4 | 0.04 | 0.07 |
| (1,2704) | 1:B:9:ARG:HD3 | 1:B:46:THR:HG22 | 4 | 0.04 | 0.07 |
| (1,2704) | 1:B:9:ARG:HD3 | 1:B:46:THR:HG23 | 4 | 0.04 | 0.07 |
| (1,2637) | 1:A:44:ILE:HG13 | 1:A:45:PHE:H | 4 | 0.02 | 0.06 |
| (1,2518) | 1:A:38:LEU:HD21 | 1:B:35:THR:HG21 | 4 | 0.02 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD21 | 1:B:35:THR:HG22 | 4 | 0.02 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD21 | 1:B:35:THR:HG23 | 4 | 0.02 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD22 | 1:B:35:THR:HG21 | 4 | 0.02 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD22 | 1:B:35:THR:HG22 | 4 | 0.02 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD22 | 1:B:35:THR:HG23 | 4 | 0.02 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD23 | 1:B:35:THR:HG21 | 4 | 0.02 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD23 | 1:B:35:THR:HG22 | 4 | 0.02 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD23 | 1:B:35:THR:HG23 | 4 | 0.02 | 0.03 |
| (1,2509) | 1:A:38:LEU:HD11 | 1:A:39:ASN:H | 4 | 0.04 | 0.06 |
| (1,2509) | 1:A:38:LEU:HD12 | 1:A:39:ASN:H | 4 | 0.04 | 0.06 |
| (1,2509) | 1:A:38:LEU:HD13 | 1:A:39:ASN:H | 4 | 0.04 | 0.06 |
| (1,245) | 1:B:15:LYS:HG2 | 1:B:19:THR:H | 4 | 0.02 | 0.03 |
| (1,245) | 1:B:15:LYS:HG3 | 1:B:19:THR:H | 4 | 0.02 | 0.03 |
| (1,244) | 1:A:15:LYS:HG2 | 1:A:19:THR:H | 4 | 0.04 | 0.09 |
| (1,244) | 1:A:15:LYS:HG3 | 1:A:19:THR:H | 4 | 0.04 | 0.09 |
| (1,2259) | 1:A:68:LYS:HA | 1:A:68:LYS:HD2 | 4 | 0.09 | 0.13 |
| (1,206) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD22 | 4 | 0.04 | 0.06 |
| (1,206) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD22 | 4 | 0.04 | 0.06 |
| (1,2025) | 1:B:22:ILE:HB | 1:B:47:CYS:HG | 4 | 0.01 | 0.02 |
| (1,2009) | 1:B:21:GLN:HG3 | 1:B:25:VAL:H | 4 | 0.02 | 0.03 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,1897) | 1:A:16:ASN:HB3 | 1:A:17:GLY:H | 4 | 0.05 | 0.07 |
| (1,1881) | 1:B:68:LYS:HE2 | 1:B:69:VAL:HG21 | 4 | 0.11 | 0.17 |
| (1,1881) | 1:B:68:LYS:HE2 | 1:B:69:VAL:HG22 | 4 | 0.11 | 0.17 |
| (1,1881) | 1:B:68:LYS:HE2 | 1:B:69:VAL:HG23 | 4 | 0.11 | 0.17 |
| (1,1881) | 1:B:68:LYS:HE3 | 1:B:69:VAL:HG21 | 4 | 0.11 | 0.17 |
| (1,1881) | 1:B:68:LYS:HE3 | 1:B:69:VAL:HG22 | 4 | 0.11 | 0.17 |
| (1,1881) | 1:B:68:LYS:HE3 | 1:B:69:VAL:HG23 | 4 | 0.11 | 0.17 |
| (1,1880) | 1:A:68:LYS:HE2 | 1:A:69:VAL:HG21 | 4 | 0.06 | 0.16 |
| (1,1880) | 1:A:68:LYS:HE2 | 1:A:69:VAL:HG22 | 4 | 0.06 | 0.16 |
| (1,1880) | 1:A:68:LYS:HE2 | 1:A:69:VAL:HG23 | 4 | 0.06 | 0.16 |
| (1,1880) | 1:A:68:LYS:HE3 | 1:A:69:VAL:HG21 | 4 | 0.06 | 0.16 |
| (1,1880) | 1:A:68:LYS:HE3 | 1:A:69:VAL:HG22 | 4 | 0.06 | 0.16 |
| (1,1880) | 1:A:68:LYS:HE3 | 1:A:69:VAL:HG23 | 4 | 0.06 | 0.16 |
| (1,187) | 1:A:15:LYS:H | 1:A:44:ILE:HA | 4 | 0.02 | 0.03 |
| (1,1612) | 1:B:24:GLY:H | 1:B:26:ILE:HD11 | 4 | 0.03 | 0.06 |
| (1,1612) | 1:B:24:GLY:H | 1:B:26:ILE:HD12 | 4 | 0.03 | 0.06 |
| (1,1612) | 1:B:24:GLY:H | 1:B:26:ILE:HD13 | 4 | 0.03 | 0.06 |
| (1,1542) | 1:B:6:ALA:HB1 | 1:B:7:GLY:HA3 | 4 | 0.04 | 0.06 |
| (1,1542) | 1:B:6:ALA:HB2 | 1:B:7:GLY:HA3 | 4 | 0.04 | 0.06 |
| (1,1542) | 1:B:6:ALA:HB3 | 1:B:7:GLY:HA3 | 4 | 0.04 | 0.06 |
| (1,1541) | 1:A:6:ALA:HB1 | 1:A:7:GLY:HA3 | 4 | 0.04 | 0.06 |
| (1,1541) | 1:A:6:ALA:HB2 | 1:A:7:GLY:HA3 | 4 | 0.04 | 0.06 |
| (1,1541) | 1:A:6:ALA:HB3 | 1:A:7:GLY:HA3 | 4 | 0.04 | 0.06 |
| (1,1225) | 1:A:69:VAL:H | 1:A:70:GLN:H | 4 | 0.03 | 0.06 |
| (1,957) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD22 | 3 | 0.03 | 0.04 |
| (1,957) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD22 | 3 | 0.03 | 0.04 |
| (1,925) | 1:B:3:ASP:HB3 | 1:B:53:VAL:H | 3 | 0.04 | 0.06 |
| (1,85) | 1:B:9:ARG:HE | 1:B:11:VAL:HG21 | 3 | 0.04 | 0.08 |
| (1,85) | 1:B:9:ARG:HE | 1:B:11:VAL:HG22 | 3 | 0.04 | 0.08 |
| (1,85) | 1:B:9:ARG:HE | 1:B:11:VAL:HG23 | 3 | 0.04 | 0.08 |
| (1,581) | 1:B:32:ASN:HA | 1:B:32:ASN:HD21 | 3 | 0.01 | 0.02 |
| (1,557) | 1:A:30:ASP:HA | 1:A:31:THR:H | 3 | 0.02 | 0.04 |
| (1,5243) | 1:B:68:LYS:HA | 1:B:68:LYS:HD2 | 3 | 0.41 | 0.63 |
| (1,5164) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HE2 | 3 | 0.14 | 0.4 |
| (1,5164) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HE2 | 3 | 0.14 | 0.4 |
| (1,5164) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HE2 | 3 | 0.14 | 0.4 |
| (1,5117) | 1:B:36:ILE:HG12 | 1:B:37:VAL:H | 3 | 0.16 | 0.24 |
| (1,5111) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HD1 | 3 | 0.16 | 0.18 |
| (1,5111) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HD2 | 3 | 0.16 | 0.18 |
| (1,5092) | 1:B:32:ASN:HA | 1:B:32:ASN:HD21 | 3 | 0.01 | 0.02 |
| (1,5074) | 1:B:28:LYS:HB2 | 1:B:29:PHE:H | 3 | 0.26 | 0.27 |
| (1,5070) | 1:B:28:LYS:HA | 1:B:28:LYS:HG2 | 3 | 0.49 | 0.77 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,5066) | 1:B:28:LYS:H | 1:B:28:LYS:HB2 | 3 | 0.44 | 0.47 |
| (1,5060) | 1:B:27:SER:H | 1:B:28:LYS:HB2 | 3 | 0.7 | 0.75 |
| (1,5046) | 1:B:25:VAL:HA | 1:B:28:LYS:HB2 | 3 | 0.62 | 0.74 |
| (1,5045) | 1:B:25:VAL:H | 1:B:28:LYS:HD2 | 3 | 0.59 | 0.82 |
| (1,5006) | 1:B:15:LYS:HG2 | 1:B:18:MET:HG2 | 3 | 0.18 | 0.43 |
| (1,5006) | 1:B:15:LYS:HG3 | 1:B:18:MET:HG2 | 3 | 0.18 | 0.43 |
| (1,4996) | 1:B:14:ASP:HB2 | 1:B:44:ILE:HG21 | 3 | 0.24 | 0.41 |
| (1,4996) | 1:B:14:ASP:HB2 | 1:B:44:ILE:HG22 | 3 | 0.24 | 0.41 |
| (1,4996) | 1:B:14:ASP:HB2 | 1:B:44:ILE:HG23 | 3 | 0.24 | 0.41 |
| (1,4984) | 1:B:9:ARG:HG2 | 1:B:76:GLU:H | 3 | 0.48 | 0.53 |
| (1,4983) | 1:B:9:ARG:HG2 | 1:B:47:CYS:H | 3 | 0.41 | 0.7 |
| (1,4982) | 1:B:9:ARG:HG2 | 1:B:11:VAL:HG21 | 3 | 0.6 | 0.8 |
| (1,4982) | 1:B:9:ARG:HG2 | 1:B:11:VAL:HG22 | 3 | 0.6 | 0.8 |
| (1,4982) | 1:B:9:ARG:HG2 | 1:B:11:VAL:HG23 | 3 | 0.6 | 0.8 |
| (1,4964) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HG2 | 3 | 0.66 | 0.96 |
| (1,4964) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HG2 | 3 | 0.66 | 0.96 |
| (1,4964) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HG2 | 3 | 0.66 | 0.96 |
| (1,4953) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HD1 | 3 | 0.53 | 1.37 |
| (1,4953) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HD2 | 3 | 0.53 | 1.37 |
| (1,4946) | 1:A:82:GLU:H | 1:A:82:GLU:HG2 | 3 | 0.06 | 0.1 |
| (1,4934) | 1:A:76:GLU:HA | 1:A:77:ARG:HB2 | 3 | 0.07 | 0.12 |
| (1,4933) | 1:A:69:VAL:HG11 | 1:A:70:GLN:HE21 | 3 | 0.15 | 0.35 |
| (1,4933) | 1:A:69:VAL:HG12 | 1:A:70:GLN:HE21 | 3 | 0.15 | 0.35 |
| (1,4933) | 1:A:69:VAL:HG13 | 1:A:70:GLN:HE21 | 3 | 0.15 | 0.35 |
| (1,4915) | 1:A:65:LYS:HA | 1:A:68:LYS:HD2 | 3 | 0.11 | 0.17 |
| (1,4898) | 1:A:59:LEU:HD21 | 1:A:77:ARG:HG2 | 3 | 0.1 | 0.11 |
| (1,4898) | 1:A:59:LEU:HD22 | 1:A:77:ARG:HG2 | 3 | 0.1 | 0.11 |
| (1,4898) | 1:A:59:LEU:HD23 | 1:A:77:ARG:HG2 | 3 | 0.1 | 0.11 |
| (1,4867) | 1:A:54:LYS:HB2 | 1:A:55:ASN:HB2 | 3 | 0.34 | 0.81 |
| (1,4866) | 1:A:54:LYS:HB2 | 1:A:54:LYS:HE2 | 3 | 0.15 | 0.23 |
| (1,4866) | 1:A:54:LYS:HB2 | 1:A:54:LYS:HE3 | 3 | 0.15 | 0.23 |
| (1,4865) | 1:A:54:LYS:H | 1:A:54:LYS:HG2 | 3 | 0.23 | 0.44 |
| (1,4864) | 1:A:53:VAL:HG21 | 1:A:58:LYS:HB2 | 3 | 0.26 | 0.66 |
| (1,4864) | 1:A:53:VAL:HG22 | 1:A:58:LYS:HB2 | 3 | 0.26 | 0.66 |
| (1,4864) | 1:A:53:VAL:HG23 | 1:A:58:LYS:HB2 | 3 | 0.26 | 0.66 |
| (1,4861) | 1:A:53:VAL:HG11 | 1:A:58:LYS:HE2 | 3 | 0.25 | 0.35 |
| (1,4861) | 1:A:53:VAL:HG12 | 1:A:58:LYS:HE2 | 3 | 0.25 | 0.35 |
| (1,4861) | 1:A:53:VAL:HG13 | 1:A:58:LYS:HE2 | 3 | 0.25 | 0.35 |
| (1,4848) | 1:A:46:THR:HG1 | 1:A:48:ASN:HD21 | 3 | 0.75 | 0.82 |
| (1,4843) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG13 | 3 | 0.18 | 0.22 |
| (1,4824) | 1:A:37:VAL:HG21 | 1:A:48:ASN:HD21 | 3 | 0.47 | 0.51 |
| (1,4824) | 1:A:37:VAL:HG22 | 1:A:48:ASN:HD21 | 3 | 0.47 | 0.51 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,4824) | 1:A:37:VAL:HG23 | 1:A:48:ASN:HD21 | 3 | 0.47 | 0.51 |
| (1,4819) | 1:A:37:VAL:HB | 1:A:48:ASN:HD21 | 3 | 0.1 | 0.13 |
| (1,4806) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HD1 | 3 | 0.82 | 1.53 |
| (1,4806) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HD2 | 3 | 0.82 | 1.53 |
| (1,4762) | 1:A:27:SER:HB2 | 1:A:28:LYS:H | 3 | 0.01 | 0.02 |
| (1,4746) | 1:A:25:VAL:H | 1:A:28:LYS:HD2 | 3 | 0.36 | 0.55 |
| (1,4726) | 1:A:20:ASN:HB2 | 1:B:33:ILE:HD11 | 3 | 0.12 | 0.17 |
| (1,4726) | 1:A:20:ASN:HB2 | 1:B:33:ILE:HD12 | 3 | 0.12 | 0.17 |
| (1,4726) | 1:A:20:ASN:HB2 | 1:B:33:ILE:HD13 | 3 | 0.12 | 0.17 |
| (1,4697) | 1:A:17:GLY:H | 1:A:18:MET:HG2 | 3 | 0.69 | 0.86 |
| (1,4685) | 1:A:15:LYS:HB2 | 1:A:18:MET:HG2 | 3 | 0.99 | 1.18 |
| (1,4562) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HE2 | 3 | 0.06 | 0.12 |
| (1,4562) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HE3 | 3 | 0.06 | 0.12 |
| (1,4526) | 1:B:5:LEU:HA | 1:B:52:PHE:HD1 | 3 | 0.02 | 0.03 |
| (1,4526) | 1:B:5:LEU:HA | 1:B:52:PHE:HD2 | 3 | 0.02 | 0.03 |
| (1,4444) | 1:A:45:PHE:HD1 | 1:A:47:CYS:HG | 3 | 0.04 | 0.06 |
| (1,4444) | 1:A:45:PHE:HD2 | 1:A:47:CYS:HG | 3 | 0.04 | 0.06 |
| (1,4419) | 1:B:29:PHE:H | 1:B:29:PHE:HD1 | 3 | 0.03 | 0.06 |
| (1,4419) | 1:B:29:PHE:H | 1:B:29:PHE:HD2 | 3 | 0.03 | 0.06 |
| (1,4417) | 1:B:29:PHE:HA | 1:B:29:PHE:HD1 | 3 | 0.07 | 0.11 |
| (1,4417) | 1:B:29:PHE:HA | 1:B:29:PHE:HD2 | 3 | 0.07 | 0.11 |
| (1,4416) | 1:A:29:PHE:HA | 1:A:29:PHE:HD1 | 3 | 0.03 | 0.05 |
| (1,4416) | 1:A:29:PHE:HA | 1:A:29:PHE:HD2 | 3 | 0.03 | 0.05 |
| (1,4366) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HA | 3 | 0.06 | 0.12 |
| (1,4339) | 1:B:4:PHE:HD1 | 1:B:59:LEU:HD21 | 3 | 0.02 | 0.03 |
| (1,4339) | 1:B:4:PHE:HD1 | 1:B:59:LEU:HD22 | 3 | 0.02 | 0.03 |
| (1,4339) | 1:B:4:PHE:HD1 | 1:B:59:LEU:HD23 | 3 | 0.02 | 0.03 |
| (1,4339) | 1:B:4:PHE:HD2 | 1:B:59:LEU:HD21 | 3 | 0.02 | 0.03 |
| (1,4339) | 1:B:4:PHE:HD2 | 1:B:59:LEU:HD22 | 3 | 0.02 | 0.03 |
| (1,4339) | 1:B:4:PHE:HD2 | 1:B:59:LEU:HD23 | 3 | 0.02 | 0.03 |
| (1,4319) | 1:B:77:ARG:HG3 | 1:B:79:SER:HA | 3 | 0.02 | 0.03 |
| (1,4317) | 1:B:79:SER:HA | 1:B:81:LEU:HG | 3 | 0.03 | 0.04 |
| (1,4191) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HB3 | 3 | 0.07 | 0.08 |
| (1,4191) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HB3 | 3 | 0.07 | 0.08 |
| (1,4191) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HB3 | 3 | 0.07 | 0.08 |
| (1,4146) | 1:A:61:THR:HG21 | 1:A:65:LYS:HB3 | 3 | 0.03 | 0.05 |
| (1,4146) | 1:A:61:THR:HG22 | 1:A:65:LYS:HB3 | 3 | 0.03 | 0.05 |
| (1,4146) | 1:A:61:THR:HG23 | 1:A:65:LYS:HB3 | 3 | 0.03 | 0.05 |
| (1,4110) | 1:B:18:MET:HE1 | 1:B:72:VAL:HG21 | 3 | 0.02 | 0.03 |
| (1,4110) | 1:B:18:MET:HE1 | 1:B:72:VAL:HG22 | 3 | 0.02 | 0.03 |
| (1,4110) | 1:B:18:MET:HE1 | 1:B:72:VAL:HG23 | 3 | 0.02 | 0.03 |
| (1,4110) | 1:B:18:MET:HE2 | 1:B:72:VAL:HG21 | 3 | 0.02 | 0.03 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,4110) | 1:B:18:MET:HE2 | 1:B:72:VAL:HG22 | 3 | 0.02 | 0.03 |
| (1,4110) | 1:B:18:MET:HE2 | 1:B:72:VAL:HG23 | 3 | 0.02 | 0.03 |
| (1,4110) | 1:B:18:MET:HE3 | 1:B:72:VAL:HG21 | 3 | 0.02 | 0.03 |
| (1,4110) | 1:B:18:MET:HE3 | 1:B:72:VAL:HG22 | 3 | 0.02 | 0.03 |
| (1,4110) | 1:B:18:MET:HE3 | 1:B:72:VAL:HG23 | 3 | 0.02 | 0.03 |
| (1,4087) | 1:B:82:GLU:H | 1:B:82:GLU:HG3 | 3 | 0.01 | 0.02 |
| (1,4082) | 1:A:82:GLU:HA | 1:A:82:GLU:HG3 | 3 | 0.14 | 0.15 |
| (1,4019) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 3 | 0.02 | 0.03 |
| (1,4019) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 3 | 0.02 | 0.03 |
| (1,4019) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 3 | 0.02 | 0.03 |
| (1,3927) | 1:B:4:PHE:HZ | 1:B:77:ARG:HD2 | 3 | 0.03 | 0.04 |
| (1,3927) | 1:B:4:PHE:HZ | 1:B:77:ARG:HD3 | 3 | 0.03 | 0.04 |
| (1,3846) | 1:B:10:ILE:HA | 1:B:74:THR:HB | 3 | 0.02 | 0.02 |
| (1,3768) | 1:B:69:VAL:HA | 1:B:70:GLN:HG2 | 3 | 0.16 | 0.25 |
| (1,3768) | 1:B:69:VAL:HA | 1:B:70:GLN:HG3 | 3 | 0.16 | 0.25 |
| (1,3621) | 1:B:41:LYS:HE2 | 1:B:44:ILE:H | 3 | 0.11 | 0.19 |
| (1,3621) | 1:B:41:LYS:HE3 | 1:B:44:ILE:H | 3 | 0.11 | 0.19 |
| (1,3530) | 1:B:9:ARG:H | 1:B:63:MET:HE1 | 3 | 0.05 | 0.08 |
| (1,3530) | 1:B:9:ARG:H | 1:B:63:MET:HE2 | 3 | 0.05 | 0.08 |
| (1,3530) | 1:B:9:ARG:H | 1:B:63:MET:HE3 | 3 | 0.05 | 0.08 |
| (1,3518) | 1:B:63:MET:HE1 | 1:B:77:ARG:HA | 3 | 0.06 | 0.07 |
| (1,3518) | 1:B:63:MET:HE2 | 1:B:77:ARG:HA | 3 | 0.06 | 0.07 |
| (1,3518) | 1:B:63:MET:HE3 | 1:B:77:ARG:HA | 3 | 0.06 | 0.07 |
| (1,3435) | 1:A:62:LEU:HD11 | 1:A:66:LEU:HG | 3 | 0.01 | 0.02 |
| (1,3435) | 1:A:62:LEU:HD12 | 1:A:66:LEU:HG | 3 | 0.01 | 0.02 |
| (1,3435) | 1:A:62:LEU:HD13 | 1:A:66:LEU:HG | 3 | 0.01 | 0.02 |
| (1,3387) | 1:B:61:THR:HG21 | 1:B:65:LYS:HE2 | 3 | 0.02 | 0.02 |
| (1,3387) | 1:B:61:THR:HG21 | 1:B:65:LYS:HE3 | 3 | 0.02 | 0.02 |
| (1,3387) | 1:B:61:THR:HG22 | 1:B:65:LYS:HE2 | 3 | 0.02 | 0.02 |
| (1,3387) | 1:B:61:THR:HG22 | 1:B:65:LYS:HE3 | 3 | 0.02 | 0.02 |
| (1,3387) | 1:B:61:THR:HG23 | 1:B:65:LYS:HE2 | 3 | 0.02 | 0.02 |
| (1,3387) | 1:B:61:THR:HG23 | 1:B:65:LYS:HE3 | 3 | 0.02 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD21 | 3 | 0.03 | 0.04 |
| (1,3323) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD22 | 3 | 0.03 | 0.04 |
| (1,3323) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD23 | 3 | 0.03 | 0.04 |
| (1,3323) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD21 | 3 | 0.03 | 0.04 |
| (1,3323) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD22 | 3 | 0.03 | 0.04 |
| (1,3323) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD23 | 3 | 0.03 | 0.04 |
| (1,3323) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD21 | 3 | 0.03 | 0.04 |
| (1,3323) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD22 | 3 | 0.03 | 0.04 |
| (1,3323) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD23 | 3 | 0.03 | 0.04 |
| (1,3285) | 1:B:58:LYS:H | 1:B:58:LYS:HD2 | 3 | 0.05 | 0.06 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,3285) | 1:B:58:LYS:H | 1:B:58:LYS:HD3 | 3 | 0.05 | 0.06 |
| (1,3284) | 1:A:58:LYS:H | 1:A:58:LYS:HD2 | 3 | 0.03 | 0.04 |
| (1,3284) | 1:A:58:LYS:H | 1:A:58:LYS:HD3 | 3 | 0.03 | 0.04 |
| (1,3260) | 1:A:58:LYS:HG2 | 1:A:62:LEU:HD11 | 3 | 0.01 | 0.02 |
| (1,3260) | 1:A:58:LYS:HG2 | 1:A:62:LEU:HD12 | 3 | 0.01 | 0.02 |
| (1,3260) | 1:A:58:LYS:HG2 | 1:A:62:LEU:HD13 | 3 | 0.01 | 0.02 |
| (1,3249) | 1:B:31:THR:HG21 | 1:B:58:LYS:HG3 | 3 | 0.03 | 0.03 |
| (1,3249) | 1:B:31:THR:HG22 | 1:B:58:LYS:HG3 | 3 | 0.03 | 0.03 |
| (1,3249) | 1:B:31:THR:HG23 | 1:B:58:LYS:HG3 | 3 | 0.03 | 0.03 |
| (1,3195) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD21 | 3 | 0.08 | 0.09 |
| (1,3195) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD21 | 3 | 0.08 | 0.09 |
| (1,3194) | 1:A:54:LYS:HE2 | 1:A:55:ASN:HD21 | 3 | 0.16 | 0.21 |
| (1,3194) | 1:A:54:LYS:HE3 | 1:A:55:ASN:HD21 | 3 | 0.16 | 0.21 |
| (1,3189) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD21 | 3 | 0.08 | 0.12 |
| (1,3189) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD21 | 3 | 0.08 | 0.12 |
| (1,2991) | 1:A:51:ILE:HG21 | 1:B:20:ASN:HD22 | 3 | 0.04 | 0.06 |
| (1,2991) | 1:A:51:ILE:HG22 | 1:B:20:ASN:HD22 | 3 | 0.04 | 0.06 |
| (1,2991) | 1:A:51:ILE:HG23 | 1:B:20:ASN:HD22 | 3 | 0.04 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG21 | 1:B:62:LEU:HD11 | 3 | 0.04 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG21 | 1:B:62:LEU:HD12 | 3 | 0.04 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG21 | 1:B:62:LEU:HD13 | 3 | 0.04 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG22 | 1:B:62:LEU:HD11 | 3 | 0.04 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG22 | 1:B:62:LEU:HD12 | 3 | 0.04 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG22 | 1:B:62:LEU:HD13 | 3 | 0.04 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG23 | 1:B:62:LEU:HD11 | 3 | 0.04 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG23 | 1:B:62:LEU:HD12 | 3 | 0.04 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG23 | 1:B:62:LEU:HD13 | 3 | 0.04 | 0.06 |
| (1,2878) | 1:A:8:ILE:H | 1:A:50:MET:HG3 | 3 | 0.04 | 0.07 |
| (1,2703) | 1:A:9:ARG:HD2 | 1:A:46:THR:HG21 | 3 | 0.02 | 0.02 |
| (1,2703) | 1:A:9:ARG:HD2 | 1:A:46:THR:HG22 | 3 | 0.02 | 0.02 |
| (1,2703) | 1:A:9:ARG:HD2 | 1:A:46:THR:HG23 | 3 | 0.02 | 0.02 |
| (1,2703) | 1:A:9:ARG:HD3 | 1:A:46:THR:HG21 | 3 | 0.02 | 0.02 |
| (1,2703) | 1:A:9:ARG:HD3 | 1:A:46:THR:HG22 | 3 | 0.02 | 0.02 |
| (1,2703) | 1:A:9:ARG:HD3 | 1:A:46:THR:HG23 | 3 | 0.02 | 0.02 |
| (1,2681) | 1:A:44:ILE:H | 1:A:44:ILE:HD11 | 3 | 0.02 | 0.04 |
| (1,2681) | 1:A:44:ILE:H | 1:A:44:ILE:HD12 | 3 | 0.02 | 0.04 |
| (1,2681) | 1:A:44:ILE:H | 1:A:44:ILE:HD13 | 3 | 0.02 | 0.04 |
| (1,2676) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HD1 | 3 | 0.02 | 0.04 |
| (1,2676) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HD2 | 3 | 0.02 | 0.04 |
| (1,2676) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HD1 | 3 | 0.02 | 0.04 |
| (1,2676) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HD2 | 3 | 0.02 | 0.04 |
| (1,2676) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HD1 | 3 | 0.02 | 0.04 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,2676) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HD2 | 3 | 0.02 | 0.04 |
| (1,2675) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HD1 | 3 | 0.01 | 0.02 |
| (1,2675) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HD2 | 3 | 0.01 | 0.02 |
| (1,2675) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HD1 | 3 | 0.01 | 0.02 |
| (1,2675) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HD2 | 3 | 0.01 | 0.02 |
| (1,2675) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HD1 | 3 | 0.01 | 0.02 |
| (1,2675) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HD2 | 3 | 0.01 | 0.02 |
| (1,2672) | 1:B:13:GLU:HA | 1:B:44:ILE:HD11 | 3 | 0.03 | 0.04 |
| (1,2672) | 1:B:13:GLU:HA | 1:B:44:ILE:HD12 | 3 | 0.03 | 0.04 |
| (1,2672) | 1:B:13:GLU:HA | 1:B:44:ILE:HD13 | 3 | 0.03 | 0.04 |
| (1,2662) | 1:B:44:ILE:HG21 | 1:B:45:PHE:H | 3 | 0.03 | 0.05 |
| (1,2662) | 1:B:44:ILE:HG22 | 1:B:45:PHE:H | 3 | 0.03 | 0.05 |
| (1,2662) | 1:B:44:ILE:HG23 | 1:B:45:PHE:H | 3 | 0.03 | 0.05 |
| (1,2661) | 1:A:44:ILE:HG21 | 1:A:45:PHE:H | 3 | 0.04 | 0.06 |
| (1,2661) | 1:A:44:ILE:HG22 | 1:A:45:PHE:H | 3 | 0.04 | 0.06 |
| (1,2661) | 1:A:44:ILE:HG23 | 1:A:45:PHE:H | 3 | 0.04 | 0.06 |
| (1,2612) | 1:B:13:GLU:HA | 1:B:44:ILE:HB | 3 | 0.01 | 0.02 |
| (1,2611) | 1:A:13:GLU:HA | 1:A:44:ILE:HB | 3 | 0.02 | 0.03 |
| (1,2587) | 1:A:15:LYS:H | 1:A:40:ALA:HB1 | 3 | 0.04 | 0.05 |
| (1,2587) | 1:A:15:LYS:H | 1:A:40:ALA:HB2 | 3 | 0.04 | 0.05 |
| (1,2587) | 1:A:15:LYS:H | 1:A:40:ALA:HB3 | 3 | 0.04 | 0.05 |
| (1,2534) | 1:B:23:THR:HG1 | 1:B:38:LEU:HD21 | 3 | 0.03 | 0.05 |
| (1,2534) | 1:B:23:THR:HG1 | 1:B:38:LEU:HD22 | 3 | 0.03 | 0.05 |
| (1,2534) | 1:B:23:THR:HG1 | 1:B:38:LEU:HD23 | 3 | 0.03 | 0.05 |
| (1,2503) | 1:A:38:LEU:HD11 | 1:A:45:PHE:HZ | 3 | 0.01 | 0.02 |
| (1,2503) | 1:A:38:LEU:HD12 | 1:A:45:PHE:HZ | 3 | 0.01 | 0.02 |
| (1,2503) | 1:A:38:LEU:HD13 | 1:A:45:PHE:HZ | 3 | 0.01 | 0.02 |
| (1,2367) | 1:A:36:ILE:HG21 | 1:A:37:VAL:HB | 3 | 0.02 | 0.03 |
| (1,2367) | 1:A:36:ILE:HG22 | 1:A:37:VAL:HB | 3 | 0.02 | 0.03 |
| (1,2367) | 1:A:36:ILE:HG23 | 1:A:37:VAL:HB | 3 | 0.02 | 0.03 |
| (1,2334) | 1:B:33:ILE:HD11 | 1:B:34:ARG:H | 3 | 0.03 | 0.05 |
| (1,2334) | 1:B:33:ILE:HD12 | 1:B:34:ARG:H | 3 | 0.03 | 0.05 |
| (1,2334) | 1:B:33:ILE:HD13 | 1:B:34:ARG:H | 3 | 0.03 | 0.05 |
| (1,2261) | 1:A:25:VAL:HA | 1:A:28:LYS:HE2 | 3 | 0.02 | 0.03 |
| (1,2261) | 1:A:25:VAL:HA | 1:A:28:LYS:HE3 | 3 | 0.02 | 0.03 |
| (1,2104) | 1:B:22:ILE:HA | 1:B:22:ILE:HD11 | 3 | 0.01 | 0.01 |
| (1,2104) | 1:B:22:ILE:HA | 1:B:22:ILE:HD12 | 3 | 0.01 | 0.01 |
| (1,2104) | 1:B:22:ILE:HA | 1:B:22:ILE:HD13 | 3 | 0.01 | 0.01 |
| (1,2055) | 1:B:20:ASN:H | 1:B:22:ILE:HG13 | 3 | 0.01 | 0.01 |
| (1,2054) | 1:A:20:ASN:H | 1:A:22:ILE:HG13 | 3 | 0.02 | 0.03 |
| (1,1879) | 1:B:25:VAL:HG21 | 1:B:65:LYS:HE2 | 3 | 0.08 | 0.12 |
| (1,1879) | 1:B:25:VAL:HG21 | 1:B:65:LYS:HE3 | 3 | 0.08 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,1879) | 1:B:25:VAL:HG22 | 1:B:65:LYS:HE2 | 3 | 0.08 | 0.12 |
| (1,1879) | 1:B:25:VAL:HG22 | 1:B:65:LYS:HE3 | 3 | 0.08 | 0.12 |
| (1,1879) | 1:B:25:VAL:HG23 | 1:B:65:LYS:HE2 | 3 | 0.08 | 0.12 |
| (1,1879) | 1:B:25:VAL:HG23 | 1:B:65:LYS:HE3 | 3 | 0.08 | 0.12 |
| (1,1878) | 1:A:25:VAL:HG21 | 1:A:65:LYS:HE2 | 3 | 0.04 | 0.07 |
| (1,1878) | 1:A:25:VAL:HG21 | 1:A:65:LYS:HE3 | 3 | 0.04 | 0.07 |
| (1,1878) | 1:A:25:VAL:HG22 | 1:A:65:LYS:HE2 | 3 | 0.04 | 0.07 |
| (1,1878) | 1:A:25:VAL:HG22 | 1:A:65:LYS:HE3 | 3 | 0.04 | 0.07 |
| (1,1878) | 1:A:25:VAL:HG23 | 1:A:65:LYS:HE2 | 3 | 0.04 | 0.07 |
| (1,1878) | 1:A:25:VAL:HG23 | 1:A:65:LYS:HE3 | 3 | 0.04 | 0.07 |
| (1,1861) | 1:B:15:LYS:HG2 | 1:B:18:MET:HE1 | 3 | 0.03 | 0.04 |
| (1,1861) | 1:B:15:LYS:HG2 | 1:B:18:MET:HE2 | 3 | 0.03 | 0.04 |
| (1,1861) | 1:B:15:LYS:HG2 | 1:B:18:MET:HE3 | 3 | 0.03 | 0.04 |
| (1,1861) | 1:B:15:LYS:HG3 | 1:B:18:MET:HE1 | 3 | 0.03 | 0.04 |
| (1,1861) | 1:B:15:LYS:HG3 | 1:B:18:MET:HE2 | 3 | 0.03 | 0.04 |
| (1,1861) | 1:B:15:LYS:HG3 | 1:B:18:MET:HE3 | 3 | 0.03 | 0.04 |
| (1,1799) | 1:B:13:GLU:HB3 | 1:B:15:LYS:HD2 | 3 | 0.03 | 0.06 |
| (1,1799) | 1:B:13:GLU:HB3 | 1:B:15:LYS:HD3 | 3 | 0.03 | 0.06 |
| (1,1798) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HD2 | 3 | 0.02 | 0.04 |
| (1,1798) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HD3 | 3 | 0.02 | 0.04 |
| (1,176) | 1:B:13:GLU:HG2 | 1:B:15:LYS:H | 3 | 0.02 | 0.04 |
| (1,176) | 1:B:13:GLU:HG3 | 1:B:15:LYS:H | 3 | 0.02 | 0.04 |
| (1,175) | 1:A:13:GLU:HG2 | 1:A:15:LYS:H | 3 | 0.02 | 0.03 |
| (1,175) | 1:A:13:GLU:HG3 | 1:A:15:LYS:H | 3 | 0.02 | 0.03 |
| (1,171) | 1:A:15:LYS:H | 1:A:18:MET:HE1 | 3 | 0.02 | 0.03 |
| (1,171) | 1:A:15:LYS:H | 1:A:18:MET:HE2 | 3 | 0.02 | 0.03 |
| (1,171) | 1:A:15:LYS:H | 1:A:18:MET:HE3 | 3 | 0.02 | 0.03 |
| (1,1370) | 1:B:78:LEU:HD21 | 1:B:79:SER:H | 3 | 0.06 | 0.1 |
| (1,1370) | 1:B:78:LEU:HD22 | 1:B:79:SER:H | 3 | 0.06 | 0.1 |
| (1,1370) | 1:B:78:LEU:HD23 | 1:B:79:SER:H | 3 | 0.06 | 0.1 |
| (1,1241) | 1:A:69:VAL:HG11 | 1:A:71:GLY:H | 3 | 0.02 | 0.03 |
| (1,1241) | 1:A:69:VAL:HG12 | 1:A:71:GLY:H | 3 | 0.02 | 0.03 |
| (1,1241) | 1:A:69:VAL:HG13 | 1:A:71:GLY:H | 3 | 0.02 | 0.03 |
| (1,1150) | 1:B:67:ARG:H | 1:B:69:VAL:HG21 | 3 | 0.02 | 0.02 |
| (1,1150) | 1:B:67:ARG:H | 1:B:69:VAL:HG22 | 3 | 0.02 | 0.02 |
| (1,1150) | 1:B:67:ARG:H | 1:B:69:VAL:HG23 | 3 | 0.02 | 0.02 |
| (1,1091) | 1:B:64:ASP:H | 1:B:75:VAL:HG11 | 3 | 0.03 | 0.06 |
| (1,1091) | 1:B:64:ASP:H | 1:B:75:VAL:HG12 | 3 | 0.03 | 0.06 |
| (1,1091) | 1:B:64:ASP:H | 1:B:75:VAL:HG13 | 3 | 0.03 | 0.06 |
| (1,855) | 1:B:48:ASN:HD21 | 1:B:78:LEU:HD21 | 2 | 0.03 | 0.03 |
| (1,855) | 1:B:48:ASN:HD21 | 1:B:78:LEU:HD22 | 2 | 0.03 | 0.03 |
| (1,855) | 1:B:48:ASN:HD21 | 1:B:78:LEU:HD23 | 2 | 0.03 | 0.03 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,854) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD21 | 2 | 0.03 | 0.03 |
| (1,854) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD22 | 2 | 0.03 | 0.03 |
| (1,854) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD23 | 2 | 0.03 | 0.03 |
| (1,845) | 1:B:36:ILE:HD11 | 1:B:48:ASN:H | 2 | 0.01 | 0.01 |
| (1,845) | 1:B:36:ILE:HD12 | 1:B:48:ASN:H | 2 | 0.01 | 0.01 |
| (1,845) | 1:B:36:ILE:HD13 | 1:B:48:ASN:H | 2 | 0.01 | 0.01 |
| (1,84) | 1:A:9:ARG:HE | 1:A:11:VAL:HG21 | 2 | 0.08 | 0.12 |
| (1,84) | 1:A:9:ARG:HE | 1:A:11:VAL:HG22 | 2 | 0.08 | 0.12 |
| (1,84) | 1:A:9:ARG:HE | 1:A:11:VAL:HG23 | 2 | 0.08 | 0.12 |
| (1,760) | 1:A:44:ILE:H | 1:A:44:ILE:HG21 | 2 | 0.01 | 0.02 |
| (1,760) | 1:A:44:ILE:H | 1:A:44:ILE:HG22 | 2 | 0.01 | 0.02 |
| (1,760) | 1:A:44:ILE:H | 1:A:44:ILE:HG23 | 2 | 0.01 | 0.02 |
| (1,742) | 1:A:41:LYS:HB2 | 1:A:42:ASP:H | 2 | 0.04 | 0.06 |
| (1,742) | 1:A:41:LYS:HB3 | 1:A:42:ASP:H | 2 | 0.04 | 0.06 |
| (1,684) | 1:A:39:ASN:H | 1:A:48:ASN:H | 2 | 0.05 | 0.07 |
| (1,630) | 1:A:35:THR:H | 1:A:83:HIS:HE1 | 2 | 0.04 | 0.06 |
| (1,584) | 1:A:20:ASN:H | 1:B:32:ASN:HD21 | 2 | 0.07 | 0.07 |
| (1,558) | 1:B:30:ASP:HA | 1:B:31:THR:H | 2 | 0.02 | 0.03 |
| (1,5256) | 1:B:77:ARG:HG2 | 1:B:79:SER:HA | 2 | 0.8 | 0.87 |
| (1,5255) | 1:B:77:ARG:HG2 | 1:B:78:LEU:HB2 | 2 | 0.71 | 0.81 |
| (1,5253) | 1:B:77:ARG:HG2 | 1:B:78:LEU:H | 2 | 0.74 | 0.76 |
| (1,5249) | 1:B:77:ARG:H | 1:B:77:ARG:HB2 | 2 | 0.53 | 0.54 |
| (1,5247) | 1:B:76:GLU:HA | 1:B:77:ARG:HB2 | 2 | 1.0 | 1.07 |
| (1,5244) | 1:B:68:LYS:HD2 | 1:B:69:VAL:H | 2 | 0.3 | 0.4 |
| (1,5236) | 1:B:67:ARG:HG2 | 1:B:72:VAL:HG11 | 2 | 0.41 | 0.52 |
| (1,5236) | 1:B:67:ARG:HG2 | 1:B:72:VAL:HG12 | 2 | 0.41 | 0.52 |
| (1,5236) | 1:B:67:ARG:HG2 | 1:B:72:VAL:HG13 | 2 | 0.41 | 0.52 |
| (1,5205) | 1:B:62:LEU:H | 1:B:65:LYS:HD2 | 2 | 0.1 | 0.19 |
| (1,5191) | 1:B:58:LYS:HG2 | 1:B:58:LYS:HE2 | 2 | 0.1 | 0.15 |
| (1,5170) | 1:B:54:LYS:HB2 | 1:B:55:ASN:HB2 | 2 | 0.04 | 0.07 |
| (1,5168) | 1:B:54:LYS:H | 1:B:54:LYS:HG2 | 2 | 0.56 | 0.65 |
| (1,5151) | 1:B:46:THR:HG1 | 1:B:48:ASN:HD21 | 2 | 0.15 | 0.26 |
| (1,5122) | 1:B:37:VAL:HB | 1:B:48:ASN:HB2 | 2 | 0.01 | 0.01 |
| (1,5098) | 1:B:32:ASN:HD21 | 1:B:33:ILE:H | 2 | 0.48 | 0.49 |
| (1,5061) | 1:B:27:SER:H | 1:B:33:ILE:HG12 | 2 | 0.41 | 0.73 |
| (1,5041) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HG2 | 2 | 0.1 | 0.18 |
| (1,5001) | 1:B:15:LYS:HA | 1:B:16:ASN:HD21 | 2 | 0.17 | 0.3 |
| (1,4998) | 1:B:14:ASP:HB2 | 1:B:45:PHE:HD1 | 2 | 0.22 | 0.4 |
| (1,4998) | 1:B:14:ASP:HB2 | 1:B:45:PHE:HD2 | 2 | 0.22 | 0.4 |
| (1,4992) | 1:B:14:ASP:HB2 | 1:B:40:ALA:HB1 | 2 | 0.24 | 0.29 |
| (1,4992) | 1:B:14:ASP:HB2 | 1:B:40:ALA:HB2 | 2 | 0.24 | 0.29 |
| (1,4992) | 1:B:14:ASP:HB2 | 1:B:40:ALA:HB3 | 2 | 0.24 | 0.29 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,4990) | 1:B:14:ASP:H | 1:B:14:ASP:HB2 | 2 | 0.03 | 0.03 |
| (1,4986) | 1:B:9:ARG:HD2 | 1:B:76:GLU:HB2 | 2 | 0.15 | 0.25 |
| (1,4986) | 1:B:9:ARG:HD3 | 1:B:76:GLU:HB2 | 2 | 0.15 | 0.25 |
| (1,4965) | 1:B:7:GLY:H | 1:B:77:ARG:HG2 | 2 | 1.16 | 1.45 |
| (1,4954) | 1:B:3:ASP:HB2 | 1:B:54:LYS:HA | 2 | 0.07 | 0.11 |
| (1,4923) | 1:A:67:ARG:HG2 | 1:A:68:LYS:H | 2 | 0.01 | 0.01 |
| (1,4894) | 1:A:59:LEU:HB2 | 1:A:60:THR:HG21 | 2 | 0.23 | 0.23 |
| (1,4894) | 1:A:59:LEU:HB2 | 1:A:60:THR:HG22 | 2 | 0.23 | 0.23 |
| (1,4894) | 1:A:59:LEU:HB2 | 1:A:60:THR:HG23 | 2 | 0.23 | 0.23 |
| (1,478) | 1:B:25:VAL:HB | 1:B:27:SER:H | 2 | 0.01 | 0.01 |
| (1,4777) | 1:A:28:LYS:HG2 | 1:A:28:LYS:HE2 | 2 | 0.13 | 0.13 |
| (1,4777) | 1:A:28:LYS:HG2 | 1:A:28:LYS:HE3 | 2 | 0.13 | 0.13 |
| (1,4776) | 1:A:28:LYS:HB2 | 1:A:29:PHE:H | 2 | 0.24 | 0.31 |
| (1,4772) | 1:A:28:LYS:HA | 1:A:28:LYS:HG2 | 2 | 0.28 | 0.33 |
| (1,4768) | 1:A:28:LYS:H | 1:A:28:LYS:HB2 | 2 | 0.4 | 0.47 |
| (1,4766) | 1:A:27:SER:HB2 | 1:B:24:GLY:H | 2 | 0.09 | 0.16 |
| (1,4761) | 1:A:27:SER:H | 1:A:28:LYS:HB2 | 2 | 0.69 | 0.7 |
| (1,476) | 1:A:27:SER:H | 1:A:33:ILE:HG12 | 2 | 0.02 | 0.02 |
| (1,4747) | 1:A:25:VAL:HA | 1:A:28:LYS:HB2 | 2 | 0.46 | 0.49 |
| (1,4721) | 1:A:20:ASN:H | 1:B:32:ASN:HD21 | 2 | 0.88 | 0.88 |
| (1,4710) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG12 | 2 | 0.06 | 0.1 |
| (1,4702) | 1:A:17:GLY:HA2 | 1:A:21:GLN:HE21 | 2 | 0.49 | 0.89 |
| (1,4680) | 1:A:15:LYS:HA | 1:A:16:ASN:HD21 | 2 | 0.27 | 0.33 |
| (1,4659) | 1:A:9:ARG:HG2 | 1:A:47:CYS:H | 2 | 0.59 | 0.97 |
| (1,4641) | 1:A:6:ALA:HB1 | 1:A:77:ARG:HG2 | 2 | 0.18 | 0.28 |
| (1,4641) | 1:A:6:ALA:HB2 | 1:A:77:ARG:HG2 | 2 | 0.18 | 0.28 |
| (1,4641) | 1:A:6:ALA:HB3 | 1:A:77:ARG:HG2 | 2 | 0.18 | 0.28 |
| (1,4636) | 1:A:5:LEU:HD11 | 1:A:34:ARG:HG2 | 2 | 0.32 | 0.33 |
| (1,4636) | 1:A:5:LEU:HD12 | 1:A:34:ARG:HG2 | 2 | 0.32 | 0.33 |
| (1,4636) | 1:A:5:LEU:HD13 | 1:A:34:ARG:HG2 | 2 | 0.32 | 0.33 |
| (1,4601) | 1:A:5:LEU:HD21 | 1:A:83:HIS:HD2 | 2 | 0.01 | 0.01 |
| (1,4601) | 1:A:5:LEU:HD22 | 1:A:83:HIS:HD2 | 2 | 0.01 | 0.01 |
| (1,4601) | 1:A:5:LEU:HD23 | 1:A:83:HIS:HD2 | 2 | 0.01 | 0.01 |
| (1,4561) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HE2 | 2 | 0.02 | 0.02 |
| (1,4561) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HE3 | 2 | 0.02 | 0.02 |
| (1,4554) | 1:B:5:LEU:H | 1:B:52:PHE:HE1 | 2 | 2.05 | 2.07 |
| (1,4552) | 1:B:4:PHE:HA | 1:B:52:PHE:HE1 | 2 | 3.1 | 3.18 |
| (1,4548) | 1:B:5:LEU:HB3 | 1:B:52:PHE:HE1 | 2 | 1.16 | 1.23 |
| (1,4546) | 1:B:5:LEU:HB2 | 1:B:52:PHE:HE1 | 2 | 0.45 | 0.5 |
| (1,4425) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HZ | 2 | 0.02 | 0.02 |
| (1,4425) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HZ | 2 | 0.02 | 0.02 |
| (1,4425) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HZ | 2 | 0.02 | 0.02 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,4353) | 1:B:4:PHE:H | 1:B:4:PHE:HD1 | 2 | 0.03 | 0.03 |
| (1,4353) | 1:B:4:PHE:H | 1:B:4:PHE:HD2 | 2 | 0.03 | 0.03 |
| (1,4333) | 1:B:83:HIS:HA | 1:B:83:HIS:HB3 | 2 | 0.07 | 0.12 |
| (1,4316) | 1:A:79:SER:HA | 1:A:81:LEU:HG | 2 | 0.04 | 0.04 |
| (1,4314) | 1:A:79:SER:HA | 1:A:81:LEU:HD21 | 2 | 0.02 | 0.03 |
| (1,4314) | 1:A:79:SER:HA | 1:A:81:LEU:HD22 | 2 | 0.02 | 0.03 |
| (1,4314) | 1:A:79:SER:HA | 1:A:81:LEU:HD23 | 2 | 0.02 | 0.03 |
| (1,4297) | 1:B:73:PHE:HA | 1:B:73:PHE:HD1 | 2 | 0.01 | 0.02 |
| (1,4297) | 1:B:73:PHE:HA | 1:B:73:PHE:HD2 | 2 | 0.01 | 0.02 |
| (1,4292) | 1:A:73:PHE:HA | 1:A:75:VAL:HG21 | 2 | 0.02 | 0.03 |
| (1,4292) | 1:A:73:PHE:HA | 1:A:75:VAL:HG22 | 2 | 0.02 | 0.03 |
| (1,4292) | 1:A:73:PHE:HA | 1:A:75:VAL:HG23 | 2 | 0.02 | 0.03 |
| (1,4278) | 1:A:60:THR:HB | 1:A:61:THR:H | 2 | 0.1 | 0.1 |
| (1,4256) | 1:A:41:LYS:HA | 1:A:42:ASP:H | 2 | 0.24 | 0.4 |
| (1,4254) | 1:A:41:LYS:HA | 1:A:41:LYS:HD2 | 2 | 0.01 | 0.02 |
| (1,4254) | 1:A:41:LYS:HA | 1:A:41:LYS:HD3 | 2 | 0.01 | 0.02 |
| (1,4123) | 1:B:23:THR:H | 1:B:26:ILE:HD11 | 2 | 0.03 | 0.04 |
| (1,4123) | 1:B:23:THR:H | 1:B:26:ILE:HD12 | 2 | 0.03 | 0.04 |
| (1,4123) | 1:B:23:THR:H | 1:B:26:ILE:HD13 | 2 | 0.03 | 0.04 |
| (1,4111) | 1:A:18:MET:HE1 | 1:A:21:GLN:HE21 | 2 | 0.04 | 0.07 |
| (1,4111) | 1:A:18:MET:HE2 | 1:A:21:GLN:HE21 | 2 | 0.04 | 0.07 |
| (1,4111) | 1:A:18:MET:HE3 | 1:A:21:GLN:HE21 | 2 | 0.04 | 0.07 |
| (1,4107) | 1:A:18:MET:HE1 | 1:A:69:VAL:HG11 | 2 | 0.01 | 0.01 |
| (1,4107) | 1:A:18:MET:HE1 | 1:A:69:VAL:HG12 | 2 | 0.01 | 0.01 |
| (1,4107) | 1:A:18:MET:HE1 | 1:A:69:VAL:HG13 | 2 | 0.01 | 0.01 |
| (1,4107) | 1:A:18:MET:HE2 | 1:A:69:VAL:HG11 | 2 | 0.01 | 0.01 |
| (1,4107) | 1:A:18:MET:HE2 | 1:A:69:VAL:HG12 | 2 | 0.01 | 0.01 |
| (1,4107) | 1:A:18:MET:HE2 | 1:A:69:VAL:HG13 | 2 | 0.01 | 0.01 |
| (1,4107) | 1:A:18:MET:HE3 | 1:A:69:VAL:HG11 | 2 | 0.01 | 0.01 |
| (1,4107) | 1:A:18:MET:HE3 | 1:A:69:VAL:HG12 | 2 | 0.01 | 0.01 |
| (1,4107) | 1:A:18:MET:HE3 | 1:A:69:VAL:HG13 | 2 | 0.01 | 0.01 |
| (1,4059) | 1:B:50:MET:HG3 | 1:B:81:LEU:HD21 | 2 | 0.01 | 0.02 |
| (1,4059) | 1:B:50:MET:HG3 | 1:B:81:LEU:HD22 | 2 | 0.01 | 0.02 |
| (1,4059) | 1:B:50:MET:HG3 | 1:B:81:LEU:HD23 | 2 | 0.01 | 0.02 |
| (1,4023) | 1:B:80:ASN:HB3 | 1:B:81:LEU:HD21 | 2 | 0.04 | 0.08 |
| (1,4023) | 1:B:80:ASN:HB3 | 1:B:81:LEU:HD22 | 2 | 0.04 | 0.08 |
| (1,4023) | 1:B:80:ASN:HB3 | 1:B:81:LEU:HD23 | 2 | 0.04 | 0.08 |
| (1,4016) | 1:A:78:LEU:H | 1:A:79:SER:HB2 | 2 | 0.09 | 0.1 |
| (1,4016) | 1:A:78:LEU:H | 1:A:79:SER:HB3 | 2 | 0.09 | 0.1 |
| (1,4014) | 1:A:78:LEU:HB3 | 1:A:79:SER:HB2 | 2 | 0.03 | 0.04 |
| (1,4014) | 1:A:78:LEU:HB3 | 1:A:79:SER:HB3 | 2 | 0.03 | 0.04 |
| (1,3986) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD11 | 2 | 0.03 | 0.03 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,3986) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD12 | 2 | 0.03 | 0.03 |
| (1,3986) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD13 | 2 | 0.03 | 0.03 |
| (1,3972) | 1:A:9:ARG:HD2 | 1:A:78:LEU:HD11 | 2 | 0.03 | 0.04 |
| (1,3972) | 1:A:9:ARG:HD2 | 1:A:78:LEU:HD12 | 2 | 0.03 | 0.04 |
| (1,3972) | 1:A:9:ARG:HD2 | 1:A:78:LEU:HD13 | 2 | 0.03 | 0.04 |
| (1,3972) | 1:A:9:ARG:HD3 | 1:A:78:LEU:HD11 | 2 | 0.03 | 0.04 |
| (1,3972) | 1:A:9:ARG:HD3 | 1:A:78:LEU:HD12 | 2 | 0.03 | 0.04 |
| (1,3972) | 1:A:9:ARG:HD3 | 1:A:78:LEU:HD13 | 2 | 0.03 | 0.04 |
| (1,3967) | 1:B:50:MET:HE1 | 1:B:78:LEU:HD11 | 2 | 0.04 | 0.04 |
| (1,3967) | 1:B:50:MET:HE1 | 1:B:78:LEU:HD12 | 2 | 0.04 | 0.04 |
| (1,3967) | 1:B:50:MET:HE1 | 1:B:78:LEU:HD13 | 2 | 0.04 | 0.04 |
| (1,3967) | 1:B:50:MET:HE2 | 1:B:78:LEU:HD11 | 2 | 0.04 | 0.04 |
| (1,3967) | 1:B:50:MET:HE2 | 1:B:78:LEU:HD12 | 2 | 0.04 | 0.04 |
| (1,3967) | 1:B:50:MET:HE2 | 1:B:78:LEU:HD13 | 2 | 0.04 | 0.04 |
| (1,3967) | 1:B:50:MET:HE3 | 1:B:78:LEU:HD11 | 2 | 0.04 | 0.04 |
| (1,3967) | 1:B:50:MET:HE3 | 1:B:78:LEU:HD12 | 2 | 0.04 | 0.04 |
| (1,3967) | 1:B:50:MET:HE3 | 1:B:78:LEU:HD13 | 2 | 0.04 | 0.04 |
| (1,3953) | 1:B:78:LEU:HB2 | 1:B:80:ASN:H | 2 | 0.03 | 0.03 |
| (1,3945) | 1:B:9:ARG:H | 1:B:78:LEU:HB3 | 2 | 0.01 | 0.02 |
| (1,3931) | 1:B:77:ARG:HD2 | 1:B:78:LEU:H | 2 | 0.01 | 0.02 |
| (1,3931) | 1:B:77:ARG:HD3 | 1:B:78:LEU:H | 2 | 0.01 | 0.02 |
| (1,3901) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 2 | 0.03 | 0.04 |
| (1,3901) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 2 | 0.03 | 0.04 |
| (1,3901) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 2 | 0.03 | 0.04 |
| (1,3895) | 1:B:9:ARG:HB2 | 1:B:76:GLU:HG2 | 2 | 0.02 | 0.02 |
| (1,3895) | 1:B:9:ARG:HB2 | 1:B:76:GLU:HG3 | 2 | 0.02 | 0.02 |
| (1,3895) | 1:B:9:ARG:HB3 | 1:B:76:GLU:HG2 | 2 | 0.02 | 0.02 |
| (1,3895) | 1:B:9:ARG:HB3 | 1:B:76:GLU:HG3 | 2 | 0.02 | 0.02 |
| (1,3848) | 1:B:74:THR:HB | 1:B:75:VAL:H | 2 | 0.02 | 0.03 |
| (1,3748) | 1:B:69:VAL:HG11 | 1:B:70:GLN:HB2 | 2 | 0.07 | 0.13 |
| (1,3748) | 1:B:69:VAL:HG11 | 1:B:70:GLN:HB3 | 2 | 0.07 | 0.13 |
| (1,3748) | 1:B:69:VAL:HG12 | 1:B:70:GLN:HB2 | 2 | 0.07 | 0.13 |
| (1,3748) | 1:B:69:VAL:HG12 | 1:B:70:GLN:HB3 | 2 | 0.07 | 0.13 |
| (1,3748) | 1:B:69:VAL:HG13 | 1:B:70:GLN:HB2 | 2 | 0.07 | 0.13 |
| (1,3748) | 1:B:69:VAL:HG13 | 1:B:70:GLN:HB3 | 2 | 0.07 | 0.13 |
| (1,3705) | 1:A:68:LYS:HB3 | 1:A:69:VAL:HA | 2 | 0.01 | 0.02 |
| (1,3667) | 1:B:68:LYS:HA | 1:B:68:LYS:HG3 | 2 | 0.01 | 0.01 |
| (1,3653) | 1:B:67:ARG:HD2 | 1:B:75:VAL:HG11 | 2 | 0.03 | 0.04 |
| (1,3653) | 1:B:67:ARG:HD2 | 1:B:75:VAL:HG12 | 2 | 0.03 | 0.04 |
| (1,3653) | 1:B:67:ARG:HD2 | 1:B:75:VAL:HG13 | 2 | 0.03 | 0.04 |
| (1,3653) | 1:B:67:ARG:HD3 | 1:B:75:VAL:HG11 | 2 | 0.03 | 0.04 |
| (1,3653) | 1:B:67:ARG:HD3 | 1:B:75:VAL:HG12 | 2 | 0.03 | 0.04 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|------|--------|--------|--------|----------|---------|
| (1,3653) | 1:B:67:ARG:HD3 | 1:B:75:VAL:HG13 | 2 | 0.03 | 0.04 |
| (1,365) | 1:B:18:MET:HE1 | 1:B:21:GLN:HE22 | 2 | 0.01 | 0.02 |
| (1,365) | 1:B:18:MET:HE2 | 1:B:21:GLN:HE22 | 2 | 0.01 | 0.02 |
| (1,365) | 1:B:18:MET:HE3 | 1:B:21:GLN:HE22 | 2 | 0.01 | 0.02 |
| (1,3546) | 1:B:61:THR:HA | 1:B:64:ASP:HB3 | 2 | 0.07 | 0.12 |
| (1,3544) | 1:B:64:ASP:HB3 | 1:B:65:LYS:HB2 | 2 | 0.1 | 0.12 |
| (1,3532) | 1:B:61:THR:HG21 | 1:B:64:ASP:HB2 | 2 | 0.01 | 0.01 |
| (1,3532) | 1:B:61:THR:HG22 | 1:B:64:ASP:HB2 | 2 | 0.01 | 0.01 |
| (1,3532) | 1:B:61:THR:HG23 | 1:B:64:ASP:HB2 | 2 | 0.01 | 0.01 |
| (1,3503) | 1:A:60:THR:HG21 | 1:A:63:MET:HE1 | 2 | 0.19 | 0.22 |
| (1,3503) | 1:A:60:THR:HG21 | 1:A:63:MET:HE2 | 2 | 0.19 | 0.22 |
| (1,3503) | 1:A:60:THR:HG21 | 1:A:63:MET:HE3 | 2 | 0.19 | 0.22 |
| (1,3503) | 1:A:60:THR:HG22 | 1:A:63:MET:HE1 | 2 | 0.19 | 0.22 |
| (1,3503) | 1:A:60:THR:HG22 | 1:A:63:MET:HE2 | 2 | 0.19 | 0.22 |
| (1,3503) | 1:A:60:THR:HG22 | 1:A:63:MET:HE3 | 2 | 0.19 | 0.22 |
| (1,3503) | 1:A:60:THR:HG23 | 1:A:63:MET:HE1 | 2 | 0.19 | 0.22 |
| (1,3503) | 1:A:60:THR:HG23 | 1:A:63:MET:HE2 | 2 | 0.19 | 0.22 |
| (1,3503) | 1:A:60:THR:HG23 | 1:A:63:MET:HE3 | 2 | 0.19 | 0.22 |
| (1,3465) | 1:A:30:ASP:H | 1:A:62:LEU:HD11 | 2 | 0.08 | 0.08 |
| (1,3465) | 1:A:30:ASP:H | 1:A:62:LEU:HD12 | 2 | 0.08 | 0.08 |
| (1,3465) | 1:A:30:ASP:H | 1:A:62:LEU:HD13 | 2 | 0.08 | 0.08 |
| (1,3460) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:HD11 | 2 | 0.13 | 0.24 |
| (1,3460) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:HD12 | 2 | 0.13 | 0.24 |
| (1,3460) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:HD13 | 2 | 0.13 | 0.24 |
| (1,3356) | 1:A:60:THR:HA | 1:A:60:THR:HG21 | 2 | 0.05 | 0.05 |
| (1,3356) | 1:A:60:THR:HA | 1:A:60:THR:HG22 | 2 | 0.05 | 0.05 |
| (1,3356) | 1:A:60:THR:HA | 1:A:60:THR:HG23 | 2 | 0.05 | 0.05 |
| (1,3261) | 1:B:58:LYS:HG2 | 1:B:62:LEU:HD11 | 2 | 0.01 | 0.02 |
| (1,3261) | 1:B:58:LYS:HG2 | 1:B:62:LEU:HD12 | 2 | 0.01 | 0.02 |
| (1,3261) | 1:B:58:LYS:HG2 | 1:B:62:LEU:HD13 | 2 | 0.01 | 0.02 |
| (1,3230) | 1:A:57:ASP:HB2 | 1:A:58:LYS:HG3 | 2 | 0.02 | 0.03 |
| (1,3230) | 1:A:57:ASP:HB3 | 1:A:58:LYS:HG3 | 2 | 0.02 | 0.03 |
| (1,3193) | 1:B:54:LYS:HA | 1:B:54:LYS:HE2 | 2 | 0.06 | 0.08 |
| (1,3193) | 1:B:54:LYS:HA | 1:B:54:LYS:HE3 | 2 | 0.06 | 0.08 |
| (1,3191) | 1:B:54:LYS:H | 1:B:54:LYS:HD2 | 2 | 0.1 | 0.14 |
| (1,3191) | 1:B:54:LYS:H | 1:B:54:LYS:HD3 | 2 | 0.1 | 0.14 |
| (1,3188) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD21 | 2 | 0.07 | 0.1 |
| (1,3188) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD21 | 2 | 0.07 | 0.1 |
| (1,3185) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD22 | 2 | 0.07 | 0.07 |
| (1,3185) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD22 | 2 | 0.07 | 0.07 |
| (1,3) | 1:A:2:THR:HG21 | 1:A:4:PHE:H | 2 | 0.08 | 0.08 |
| (1,3) | 1:A:2:THR:HG22 | 1:A:4:PHE:H | 2 | 0.08 | 0.08 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,3) | 1:A:2:THR:HG23 | 1:A:4:PHE:H | 2 | 0.08 | 0.08 |
| (1,2990) | 1:A:20:ASN:HD22 | 1:B:51:ILE:HG21 | 2 | 0.08 | 0.1 |
| (1,2990) | 1:A:20:ASN:HD22 | 1:B:51:ILE:HG22 | 2 | 0.08 | 0.1 |
| (1,2990) | 1:A:20:ASN:HD22 | 1:B:51:ILE:HG23 | 2 | 0.08 | 0.1 |
| (1,2715) | 1:A:9:ARG:HE | 1:A:46:THR:HG21 | 2 | 0.14 | 0.16 |
| (1,2715) | 1:A:9:ARG:HE | 1:A:46:THR:HG22 | 2 | 0.14 | 0.16 |
| (1,2715) | 1:A:9:ARG:HE | 1:A:46:THR:HG23 | 2 | 0.14 | 0.16 |
| (1,2666) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HD11 | 2 | 0.03 | 0.05 |
| (1,2666) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HD12 | 2 | 0.03 | 0.05 |
| (1,2666) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HD13 | 2 | 0.03 | 0.05 |
| (1,2658) | 1:B:14:ASP:H | 1:B:44:ILE:HG21 | 2 | 0.04 | 0.06 |
| (1,2658) | 1:B:14:ASP:H | 1:B:44:ILE:HG22 | 2 | 0.04 | 0.06 |
| (1,2658) | 1:B:14:ASP:H | 1:B:44:ILE:HG23 | 2 | 0.04 | 0.06 |
| (1,2606) | 1:B:14:ASP:HB2 | 1:B:43:GLY:HA3 | 2 | 0.09 | 0.1 |
| (1,2605) | 1:A:14:ASP:HB2 | 1:A:43:GLY:HA3 | 2 | 0.05 | 0.09 |
| (1,2486) | 1:B:38:LEU:HD11 | 1:B:47:CYS:HG | 2 | 0.03 | 0.03 |
| (1,2486) | 1:B:38:LEU:HD12 | 1:B:47:CYS:HG | 2 | 0.03 | 0.03 |
| (1,2486) | 1:B:38:LEU:HD13 | 1:B:47:CYS:HG | 2 | 0.03 | 0.03 |
| (1,2420) | 1:B:37:VAL:HB | 1:B:48:ASN:HB2 | 2 | 0.01 | 0.01 |
| (1,2370) | 1:A:36:ILE:HG21 | 1:B:39:ASN:HB2 | 2 | 0.1 | 0.11 |
| (1,2370) | 1:A:36:ILE:HG21 | 1:B:39:ASN:HB3 | 2 | 0.1 | 0.11 |
| (1,2370) | 1:A:36:ILE:HG22 | 1:B:39:ASN:HB2 | 2 | 0.1 | 0.11 |
| (1,2370) | 1:A:36:ILE:HG22 | 1:B:39:ASN:HB3 | 2 | 0.1 | 0.11 |
| (1,2370) | 1:A:36:ILE:HG23 | 1:B:39:ASN:HB2 | 2 | 0.1 | 0.11 |
| (1,2370) | 1:A:36:ILE:HG23 | 1:B:39:ASN:HB3 | 2 | 0.1 | 0.11 |
| (1,2333) | 1:A:33:ILE:HD11 | 1:A:34:ARG:H | 2 | 0.03 | 0.03 |
| (1,2333) | 1:A:33:ILE:HD12 | 1:A:34:ARG:H | 2 | 0.03 | 0.03 |
| (1,2333) | 1:A:33:ILE:HD13 | 1:A:34:ARG:H | 2 | 0.03 | 0.03 |
| (1,2331) | 1:A:33:ILE:H | 1:A:33:ILE:HD11 | 2 | 0.01 | 0.01 |
| (1,2331) | 1:A:33:ILE:H | 1:A:33:ILE:HD12 | 2 | 0.01 | 0.01 |
| (1,2331) | 1:A:33:ILE:H | 1:A:33:ILE:HD13 | 2 | 0.01 | 0.01 |
| (1,2328) | 1:A:33:ILE:HD11 | 1:B:20:ASN:HD22 | 2 | 0.01 | 0.02 |
| (1,2328) | 1:A:33:ILE:HD12 | 1:B:20:ASN:HD22 | 2 | 0.01 | 0.02 |
| (1,2328) | 1:A:33:ILE:HD13 | 1:B:20:ASN:HD22 | 2 | 0.01 | 0.02 |
| (1,2327) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HD11 | 2 | 0.01 | 0.02 |
| (1,2327) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HD12 | 2 | 0.01 | 0.02 |
| (1,2327) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HD13 | 2 | 0.01 | 0.02 |
| (1,2323) | 1:A:20:ASN:HA | 1:B:33:ILE:HD11 | 2 | 0.01 | 0.01 |
| (1,2323) | 1:A:20:ASN:HA | 1:B:33:ILE:HD12 | 2 | 0.01 | 0.01 |
| (1,2323) | 1:A:20:ASN:HA | 1:B:33:ILE:HD13 | 2 | 0.01 | 0.01 |
| (1,2262) | 1:B:25:VAL:HA | 1:B:28:LYS:HE2 | 2 | 0.04 | 0.04 |
| (1,2262) | 1:B:25:VAL:HA | 1:B:28:LYS:HE3 | 2 | 0.04 | 0.04 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,2260) | 1:B:68:LYS:HA | 1:B:68:LYS:HD2 | 2 | 0.1 | 0.14 |
| (1,2250) | 1:B:27:SER:HG | 1:B:28:LYS:HG2 | 2 | 0.11 | 0.12 |
| (1,2249) | 1:A:27:SER:HG | 1:A:28:LYS:HG2 | 2 | 0.07 | 0.07 |
| (1,2180) | 1:B:22:ILE:HA | 1:B:25:VAL:HG21 | 2 | 0.04 | 0.05 |
| (1,2180) | 1:B:22:ILE:HA | 1:B:25:VAL:HG22 | 2 | 0.04 | 0.05 |
| (1,2180) | 1:B:22:ILE:HA | 1:B:25:VAL:HG23 | 2 | 0.04 | 0.05 |
| (1,2135) | 1:A:67:ARG:HE | 1:A:75:VAL:HG11 | 2 | 0.06 | 0.09 |
| (1,2135) | 1:A:67:ARG:HE | 1:A:75:VAL:HG12 | 2 | 0.06 | 0.09 |
| (1,2135) | 1:A:67:ARG:HE | 1:A:75:VAL:HG13 | 2 | 0.06 | 0.09 |
| (1,2024) | 1:A:22:ILE:HB | 1:A:47:CYS:HG | 2 | 0.01 | 0.01 |
| (1,2008) | 1:A:21:GLN:HG3 | 1:A:25:VAL:H | 2 | 0.02 | 0.03 |
| (1,20) | 1:B:4:PHE:H | 1:B:52:PHE:HE1 | 2 | 2.15 | 2.3 |
| (1,1990) | 1:A:21:GLN:HG2 | 1:A:25:VAL:HG21 | 2 | 0.01 | 0.01 |
| (1,1990) | 1:A:21:GLN:HG2 | 1:A:25:VAL:HG22 | 2 | 0.01 | 0.01 |
| (1,1990) | 1:A:21:GLN:HG2 | 1:A:25:VAL:HG23 | 2 | 0.01 | 0.01 |
| (1,1907) | 1:A:18:MET:HA | 1:A:21:GLN:HG2 | 2 | 0.03 | 0.03 |
| (1,1877) | 1:B:41:LYS:HE2 | 1:B:44:ILE:HD11 | 2 | 0.04 | 0.05 |
| (1,1877) | 1:B:41:LYS:HE2 | 1:B:44:ILE:HD12 | 2 | 0.04 | 0.05 |
| (1,1877) | 1:B:41:LYS:HE2 | 1:B:44:ILE:HD13 | 2 | 0.04 | 0.05 |
| (1,1877) | 1:B:41:LYS:HE3 | 1:B:44:ILE:HD11 | 2 | 0.04 | 0.05 |
| (1,1877) | 1:B:41:LYS:HE3 | 1:B:44:ILE:HD12 | 2 | 0.04 | 0.05 |
| (1,1877) | 1:B:41:LYS:HE3 | 1:B:44:ILE:HD13 | 2 | 0.04 | 0.05 |
| (1,1876) | 1:A:41:LYS:HE2 | 1:A:44:ILE:HD11 | 2 | 0.06 | 0.07 |
| (1,1876) | 1:A:41:LYS:HE2 | 1:A:44:ILE:HD12 | 2 | 0.06 | 0.07 |
| (1,1876) | 1:A:41:LYS:HE2 | 1:A:44:ILE:HD13 | 2 | 0.06 | 0.07 |
| (1,1876) | 1:A:41:LYS:HE3 | 1:A:44:ILE:HD11 | 2 | 0.06 | 0.07 |
| (1,1876) | 1:A:41:LYS:HE3 | 1:A:44:ILE:HD12 | 2 | 0.06 | 0.07 |
| (1,1876) | 1:A:41:LYS:HE3 | 1:A:44:ILE:HD13 | 2 | 0.06 | 0.07 |
| (1,1874) | 1:A:11:VAL:HG21 | 1:A:41:LYS:HE2 | 2 | 0.08 | 0.12 |
| (1,1874) | 1:A:11:VAL:HG21 | 1:A:41:LYS:HE3 | 2 | 0.08 | 0.12 |
| (1,1874) | 1:A:11:VAL:HG22 | 1:A:41:LYS:HE2 | 2 | 0.08 | 0.12 |
| (1,1874) | 1:A:11:VAL:HG22 | 1:A:41:LYS:HE3 | 2 | 0.08 | 0.12 |
| (1,1874) | 1:A:11:VAL:HG23 | 1:A:41:LYS:HE2 | 2 | 0.08 | 0.12 |
| (1,1874) | 1:A:11:VAL:HG23 | 1:A:41:LYS:HE3 | 2 | 0.08 | 0.12 |
| (1,1873) | 1:B:15:LYS:HD2 | 1:B:71:GLY:HA3 | 2 | 0.1 | 0.17 |
| (1,1873) | 1:B:15:LYS:HD3 | 1:B:71:GLY:HA3 | 2 | 0.1 | 0.17 |
| (1,1863) | 1:B:13:GLU:HB2 | 1:B:15:LYS:HG2 | 2 | 0.03 | 0.04 |
| (1,1863) | 1:B:13:GLU:HB2 | 1:B:15:LYS:HG3 | 2 | 0.03 | 0.04 |
| (1,1856) | 1:B:13:GLU:HG2 | 1:B:15:LYS:HB3 | 2 | 0.02 | 0.02 |
| (1,1856) | 1:B:13:GLU:HG3 | 1:B:15:LYS:HB3 | 2 | 0.02 | 0.02 |
| (1,1855) | 1:A:13:GLU:HG2 | 1:A:15:LYS:HB3 | 2 | 0.02 | 0.02 |
| (1,1855) | 1:A:13:GLU:HG3 | 1:A:15:LYS:HB3 | 2 | 0.02 | 0.02 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,1847) | 1:B:14:ASP:HB3 | 1:B:43:GLY:HA3 | 2 | 0.02 | 0.03 |
| (1,182) | 1:B:15:LYS:H | 1:B:18:MET:HG2 | 2 | 0.13 | 0.24 |
| (1,1806) | 1:A:13:GLU:HB2 | 1:A:15:LYS:HD2 | 2 | 0.05 | 0.08 |
| (1,1806) | 1:A:13:GLU:HB2 | 1:A:15:LYS:HD3 | 2 | 0.05 | 0.08 |
| (1,1763) | 1:B:11:VAL:HG11 | 1:B:73:PHE:HB2 | 2 | 0.01 | 0.01 |
| (1,1763) | 1:B:11:VAL:HG12 | 1:B:73:PHE:HB2 | 2 | 0.01 | 0.01 |
| (1,1763) | 1:B:11:VAL:HG13 | 1:B:73:PHE:HB2 | 2 | 0.01 | 0.01 |
| (1,1744) | 1:A:11:VAL:HG21 | 1:A:46:THR:HB | 2 | 0.03 | 0.03 |
| (1,1744) | 1:A:11:VAL:HG22 | 1:A:46:THR:HB | 2 | 0.03 | 0.03 |
| (1,1744) | 1:A:11:VAL:HG23 | 1:A:46:THR:HB | 2 | 0.03 | 0.03 |
| (1,172) | 1:B:15:LYS:H | 1:B:18:MET:HE1 | 2 | 0.04 | 0.07 |
| (1,172) | 1:B:15:LYS:H | 1:B:18:MET:HE2 | 2 | 0.04 | 0.07 |
| (1,172) | 1:B:15:LYS:H | 1:B:18:MET:HE3 | 2 | 0.04 | 0.07 |
| (1,1626) | 1:B:9:ARG:HG3 | 1:B:10:ILE:H | 2 | 0.04 | 0.04 |
| (1,1611) | 1:A:24:GLY:H | 1:A:26:ILE:HD11 | 2 | 0.01 | 0.02 |
| (1,1611) | 1:A:24:GLY:H | 1:A:26:ILE:HD12 | 2 | 0.01 | 0.02 |
| (1,1611) | 1:A:24:GLY:H | 1:A:26:ILE:HD13 | 2 | 0.01 | 0.02 |
| (1,1605) | 1:A:8:ILE:HD11 | 1:A:77:ARG:HA | 2 | 0.03 | 0.03 |
| (1,1605) | 1:A:8:ILE:HD12 | 1:A:77:ARG:HA | 2 | 0.03 | 0.03 |
| (1,1605) | 1:A:8:ILE:HD13 | 1:A:77:ARG:HA | 2 | 0.03 | 0.03 |
| (1,1570) | 1:B:8:ILE:HG21 | 1:B:63:MET:HG3 | 2 | 0.03 | 0.03 |
| (1,1570) | 1:B:8:ILE:HG22 | 1:B:63:MET:HG3 | 2 | 0.03 | 0.03 |
| (1,1570) | 1:B:8:ILE:HG23 | 1:B:63:MET:HG3 | 2 | 0.03 | 0.03 |
| (1,1419) | 1:A:40:ALA:H | 1:A:41:LYS:HD2 | 2 | 0.1 | 0.14 |
| (1,1419) | 1:A:40:ALA:H | 1:A:41:LYS:HD3 | 2 | 0.1 | 0.14 |
| (1,1356) | 1:B:77:ARG:HG2 | 1:B:78:LEU:H | 2 | 0.09 | 0.11 |
| (1,1348) | 1:B:77:ARG:H | 1:B:77:ARG:HD2 | 2 | 0.01 | 0.02 |
| (1,1348) | 1:B:77:ARG:H | 1:B:77:ARG:HD3 | 2 | 0.01 | 0.02 |
| (1,1339) | 1:A:76:GLU:HB2 | 1:A:77:ARG:H | 2 | 0.02 | 0.03 |
| (1,1338) | 1:B:77:ARG:H | 1:B:77:ARG:HB2 | 2 | 0.07 | 0.08 |
| (1,1300) | 1:B:74:THR:HG21 | 1:B:75:VAL:H | 2 | 0.01 | 0.02 |
| (1,1300) | 1:B:74:THR:HG22 | 1:B:75:VAL:H | 2 | 0.01 | 0.02 |
| (1,1300) | 1:B:74:THR:HG23 | 1:B:75:VAL:H | 2 | 0.01 | 0.02 |
| (1,1257) | 1:A:70:GLN:HA | 1:A:72:VAL:H | 2 | 0.02 | 0.02 |
| (1,1253) | 1:A:69:VAL:HG21 | 1:A:72:VAL:H | 2 | 0.03 | 0.04 |
| (1,1253) | 1:A:69:VAL:HG22 | 1:A:72:VAL:H | 2 | 0.03 | 0.04 |
| (1,1253) | 1:A:69:VAL:HG23 | 1:A:72:VAL:H | 2 | 0.03 | 0.04 |
| (1,1184) | 1:B:68:LYS:H | 1:B:75:VAL:HG21 | 2 | 0.03 | 0.04 |
| (1,1184) | 1:B:68:LYS:H | 1:B:75:VAL:HG22 | 2 | 0.03 | 0.04 |
| (1,1184) | 1:B:68:LYS:H | 1:B:75:VAL:HG23 | 2 | 0.03 | 0.04 |
| (1,1175) | 1:A:67:ARG:HE | 1:A:75:VAL:HB | 2 | 0.02 | 0.03 |
| (1,1120) | 1:B:65:LYS:H | 1:B:68:LYS:HE2 | 2 | 0.07 | 0.1 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,1120) | 1:B:65:LYS:H | 1:B:68:LYS:HE3 | 2 | 0.07 | 0.1 |
| (1,1090) | 1:A:64:ASP:H | 1:A:75:VAL:HG11 | 2 | 0.01 | 0.01 |
| (1,1090) | 1:A:64:ASP:H | 1:A:75:VAL:HG12 | 2 | 0.01 | 0.01 |
| (1,1090) | 1:A:64:ASP:H | 1:A:75:VAL:HG13 | 2 | 0.01 | 0.01 |
| (1,974) | 1:A:53:VAL:HG21 | 1:A:58:LYS:H | 1 | 0.02 | 0.02 |
| (1,974) | 1:A:53:VAL:HG22 | 1:A:58:LYS:H | 1 | 0.02 | 0.02 |
| (1,974) | 1:A:53:VAL:HG23 | 1:A:58:LYS:H | 1 | 0.02 | 0.02 |
| (1,956) | 1:A:54:LYS:HE2 | 1:A:55:ASN:HD22 | 1 | 0.04 | 0.04 |
| (1,956) | 1:A:54:LYS:HE3 | 1:A:55:ASN:HD22 | 1 | 0.04 | 0.04 |
| (1,946) | 1:A:55:ASN:H | 1:A:56:THR:HG21 | 1 | 0.08 | 0.08 |
| (1,946) | 1:A:55:ASN:H | 1:A:56:THR:HG22 | 1 | 0.08 | 0.08 |
| (1,946) | 1:A:55:ASN:H | 1:A:56:THR:HG23 | 1 | 0.08 | 0.08 |
| (1,86) | 1:A:9:ARG:HE | 1:A:10:ILE:H | 1 | 0.02 | 0.02 |
| (1,787) | 1:B:44:ILE:HB | 1:B:45:PHE:H | 1 | 0.02 | 0.02 |
| (1,761) | 1:B:44:ILE:H | 1:B:44:ILE:HG21 | 1 | 0.01 | 0.01 |
| (1,761) | 1:B:44:ILE:H | 1:B:44:ILE:HG22 | 1 | 0.01 | 0.01 |
| (1,761) | 1:B:44:ILE:H | 1:B:44:ILE:HG23 | 1 | 0.01 | 0.01 |
| (1,752) | 1:A:41:LYS:HG2 | 1:A:43:GLY:H | 1 | 0.07 | 0.07 |
| (1,752) | 1:A:41:LYS:HG3 | 1:A:43:GLY:H | 1 | 0.07 | 0.07 |
| (1,751) | 1:B:40:ALA:HB1 | 1:B:43:GLY:H | 1 | 0.08 | 0.08 |
| (1,751) | 1:B:40:ALA:HB2 | 1:B:43:GLY:H | 1 | 0.08 | 0.08 |
| (1,751) | 1:B:40:ALA:HB3 | 1:B:43:GLY:H | 1 | 0.08 | 0.08 |
| (1,743) | 1:B:41:LYS:HB2 | 1:B:42:ASP:H | 1 | 0.12 | 0.12 |
| (1,743) | 1:B:41:LYS:HB3 | 1:B:42:ASP:H | 1 | 0.12 | 0.12 |
| (1,741) | 1:B:41:LYS:HG2 | 1:B:42:ASP:H | 1 | 0.03 | 0.03 |
| (1,741) | 1:B:41:LYS:HG3 | 1:B:42:ASP:H | 1 | 0.03 | 0.03 |
| (1,739) | 1:B:41:LYS:H | 1:B:43:GLY:H | 1 | 0.01 | 0.01 |
| (1,73) | 1:A:9:ARG:H | 1:A:76:GLU:HB2 | 1 | 0.04 | 0.04 |
| (1,713) | 1:B:41:LYS:H | 1:B:41:LYS:HG2 | 1 | 0.09 | 0.09 |
| (1,713) | 1:B:41:LYS:H | 1:B:41:LYS:HG3 | 1 | 0.09 | 0.09 |
| (1,712) | 1:A:41:LYS:H | 1:A:41:LYS:HG2 | 1 | 0.07 | 0.07 |
| (1,712) | 1:A:41:LYS:H | 1:A:41:LYS:HG3 | 1 | 0.07 | 0.07 |
| (1,711) | 1:B:41:LYS:H | 1:B:44:ILE:HG21 | 1 | 0.01 | 0.01 |
| (1,711) | 1:B:41:LYS:H | 1:B:44:ILE:HG22 | 1 | 0.01 | 0.01 |
| (1,711) | 1:B:41:LYS:H | 1:B:44:ILE:HG23 | 1 | 0.01 | 0.01 |
| (1,593) | 1:A:32:ASN:HD22 | 1:B:17:GLY:H | 1 | 0.01 | 0.01 |
| (1,586) | 1:A:32:ASN:HD22 | 1:B:16:ASN:HA | 1 | 0.03 | 0.03 |
| (1,564) | 1:A:31:THR:H | 1:B:20:ASN:HD21 | 1 | 0.05 | 0.05 |
| (1,5231) | 1:B:66:LEU:HB2 | 1:B:75:VAL:HG11 | 1 | 0.01 | 0.01 |
| (1,5231) | 1:B:66:LEU:HB2 | 1:B:75:VAL:HG12 | 1 | 0.01 | 0.01 |
| (1,5231) | 1:B:66:LEU:HB2 | 1:B:75:VAL:HG13 | 1 | 0.01 | 0.01 |
| (1,5226) | 1:B:65:LYS:HA | 1:B:68:LYS:HD2 | 1 | 0.12 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,5201) | 1:B:59:LEU:HD21 | 1:B:77:ARG:HG2 | 1 | 0.12 | 0.12 |
| (1,5201) | 1:B:59:LEU:HD22 | 1:B:77:ARG:HG2 | 1 | 0.12 | 0.12 |
| (1,5201) | 1:B:59:LEU:HD23 | 1:B:77:ARG:HG2 | 1 | 0.12 | 0.12 |
| (1,5197) | 1:B:59:LEU:HB2 | 1:B:60:THR:HG21 | 1 | 0.27 | 0.27 |
| (1,5197) | 1:B:59:LEU:HB2 | 1:B:60:THR:HG22 | 1 | 0.27 | 0.27 |
| (1,5197) | 1:B:59:LEU:HB2 | 1:B:60:THR:HG23 | 1 | 0.27 | 0.27 |
| (1,5144) | 1:B:42:ASP:HB2 | 1:B:44:ILE:H | 1 | 0.07 | 0.07 |
| (1,5143) | 1:B:41:LYS:HG2 | 1:B:42:ASP:HB2 | 1 | 0.07 | 0.07 |
| (1,5143) | 1:B:41:LYS:HG3 | 1:B:42:ASP:HB2 | 1 | 0.07 | 0.07 |
| (1,5127) | 1:B:37:VAL:HG21 | 1:B:48:ASN:HB2 | 1 | 0.66 | 0.66 |
| (1,5127) | 1:B:37:VAL:HG22 | 1:B:48:ASN:HB2 | 1 | 0.66 | 0.66 |
| (1,5127) | 1:B:37:VAL:HG23 | 1:B:48:ASN:HB2 | 1 | 0.66 | 0.66 |
| (1,5105) | 1:B:34:ARG:HB2 | 1:B:35:THR:H | 1 | 0.07 | 0.07 |
| (1,5100) | 1:B:33:ILE:H | 1:B:33:ILE:HG12 | 1 | 0.23 | 0.23 |
| (1,5081) | 1:B:29:PHE:HB2 | 1:B:51:ILE:HD11 | 1 | 0.23 | 0.23 |
| (1,5081) | 1:B:29:PHE:HB2 | 1:B:51:ILE:HD12 | 1 | 0.23 | 0.23 |
| (1,5081) | 1:B:29:PHE:HB2 | 1:B:51:ILE:HD13 | 1 | 0.23 | 0.23 |
| (1,5075) | 1:B:28:LYS:HG2 | 1:B:28:LYS:HE2 | 1 | 0.1 | 0.1 |
| (1,5075) | 1:B:28:LYS:HG2 | 1:B:28:LYS:HE3 | 1 | 0.1 | 0.1 |
| (1,5058) | 1:B:26:ILE:HG12 | 1:B:29:PHE:HZ | 1 | 0.24 | 0.24 |
| (1,5002) | 1:B:15:LYS:HB2 | 1:B:18:MET:HG2 | 1 | 0.01 | 0.01 |
| (1,4980) | 1:B:9:ARG:H | 1:B:9:ARG:HG2 | 1 | 0.06 | 0.06 |
| (1,4977) | 1:B:8:ILE:HG12 | 1:B:77:ARG:HB2 | 1 | 0.01 | 0.01 |
| (1,4972) | 1:B:8:ILE:HG12 | 1:B:49:LEU:HB3 | 1 | 0.01 | 0.01 |
| (1,497) | 1:A:23:THR:HG21 | 1:A:28:LYS:H | 1 | 0.02 | 0.02 |
| (1,497) | 1:A:23:THR:HG22 | 1:A:28:LYS:H | 1 | 0.02 | 0.02 |
| (1,497) | 1:A:23:THR:HG23 | 1:A:28:LYS:H | 1 | 0.02 | 0.02 |
| (1,4919) | 1:A:66:LEU:HB2 | 1:A:75:VAL:HG11 | 1 | 0.01 | 0.01 |
| (1,4919) | 1:A:66:LEU:HB2 | 1:A:75:VAL:HG12 | 1 | 0.01 | 0.01 |
| (1,4919) | 1:A:66:LEU:HB2 | 1:A:75:VAL:HG13 | 1 | 0.01 | 0.01 |
| (1,4909) | 1:A:63:MET:HE1 | 1:A:77:ARG:HB2 | 1 | 0.01 | 0.01 |
| (1,4909) | 1:A:63:MET:HE2 | 1:A:77:ARG:HB2 | 1 | 0.01 | 0.01 |
| (1,4909) | 1:A:63:MET:HE3 | 1:A:77:ARG:HB2 | 1 | 0.01 | 0.01 |
| (1,4885) | 1:A:58:LYS:H | 1:A:58:LYS:HB2 | 1 | 0.33 | 0.33 |
| (1,4883) | 1:A:57:ASP:H | 1:A:58:LYS:HB2 | 1 | 0.56 | 0.56 |
| (1,4874) | 1:A:55:ASN:H | 1:A:58:LYS:HB2 | 1 | 0.96 | 0.96 |
| (1,4841) | 1:A:42:ASP:HB2 | 1:A:44:ILE:H | 1 | 0.02 | 0.02 |
| (1,4811) | 1:A:35:THR:HG21 | 1:B:39:ASN:HD21 | 1 | 0.18 | 0.18 |
| (1,4811) | 1:A:35:THR:HG22 | 1:B:39:ASN:HD21 | 1 | 0.18 | 0.18 |
| (1,4811) | 1:A:35:THR:HG23 | 1:B:39:ASN:HD21 | 1 | 0.18 | 0.18 |
| (1,4800) | 1:A:34:ARG:HB2 | 1:A:35:THR:H | 1 | 0.03 | 0.03 |
| (1,4797) | 1:A:33:ILE:HD11 | 1:B:20:ASN:HB2 | 1 | 0.1 | 0.1 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,4797) | 1:A:33:ILE:HD12 | 1:B:20:ASN:HB2 | 1 | 0.1 | 0.1 |
| (1,4797) | 1:A:33:ILE:HD13 | 1:B:20:ASN:HB2 | 1 | 0.1 | 0.1 |
| (1,4783) | 1:A:29:PHE:HB2 | 1:A:51:ILE:HD11 | 1 | 0.03 | 0.03 |
| (1,4783) | 1:A:29:PHE:HB2 | 1:A:51:ILE:HD12 | 1 | 0.03 | 0.03 |
| (1,4783) | 1:A:29:PHE:HB2 | 1:A:51:ILE:HD13 | 1 | 0.03 | 0.03 |
| (1,4775) | 1:A:28:LYS:HB2 | 1:A:28:LYS:HE2 | 1 | 0.09 | 0.09 |
| (1,4775) | 1:A:28:LYS:HB2 | 1:A:28:LYS:HE3 | 1 | 0.09 | 0.09 |
| (1,477) | 1:A:25:VAL:HB | 1:A:27:SER:H | 1 | 0.01 | 0.01 |
| (1,4764) | 1:A:27:SER:HB2 | 1:B:20:ASN:HA | 1 | 1.18 | 1.18 |
| (1,4722) | 1:A:20:ASN:HA | 1:B:27:SER:HB2 | 1 | 0.77 | 0.77 |
| (1,4713) | 1:A:18:MET:HG2 | 1:A:19:THR:H | 1 | 0.02 | 0.02 |
| (1,4698) | 1:A:17:GLY:H | 1:B:32:ASN:HD21 | 1 | 0.75 | 0.75 |
| (1,4674) | 1:A:14:ASP:HB2 | 1:A:44:ILE:HG21 | 1 | 0.23 | 0.23 |
| (1,4674) | 1:A:14:ASP:HB2 | 1:A:44:ILE:HG22 | 1 | 0.23 | 0.23 |
| (1,4674) | 1:A:14:ASP:HB2 | 1:A:44:ILE:HG23 | 1 | 0.23 | 0.23 |
| (1,4670) | 1:A:14:ASP:HB2 | 1:A:40:ALA:HB1 | 1 | 0.06 | 0.06 |
| (1,4670) | 1:A:14:ASP:HB2 | 1:A:40:ALA:HB2 | 1 | 0.06 | 0.06 |
| (1,4670) | 1:A:14:ASP:HB2 | 1:A:40:ALA:HB3 | 1 | 0.06 | 0.06 |
| (1,4666) | 1:A:14:ASP:H | 1:A:14:ASP:HB2 | 1 | 0.02 | 0.02 |
| (1,4658) | 1:A:9:ARG:HG2 | 1:A:11:VAL:HG21 | 1 | 0.52 | 0.52 |
| (1,4658) | 1:A:9:ARG:HG2 | 1:A:11:VAL:HG22 | 1 | 0.52 | 0.52 |
| (1,4658) | 1:A:9:ARG:HG2 | 1:A:11:VAL:HG23 | 1 | 0.52 | 0.52 |
| (1,4612) | 1:B:50:MET:HE1 | 1:B:83:HIS:HD2 | 1 | 0.1 | 0.1 |
| (1,4612) | 1:B:50:MET:HE2 | 1:B:83:HIS:HD2 | 1 | 0.1 | 0.1 |
| (1,4612) | 1:B:50:MET:HE3 | 1:B:83:HIS:HD2 | 1 | 0.1 | 0.1 |
| (1,4606) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HD2 | 1 | 0.01 | 0.01 |
| (1,4606) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HD2 | 1 | 0.01 | 0.01 |
| (1,4606) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HD2 | 1 | 0.01 | 0.01 |
| (1,4591) | 1:A:13:GLU:H | 1:A:73:PHE:HZ | 1 | 0.02 | 0.02 |
| (1,4540) | 1:B:6:ALA:H | 1:B:52:PHE:HD1 | 1 | 0.01 | 0.01 |
| (1,4540) | 1:B:6:ALA:H | 1:B:52:PHE:HD2 | 1 | 0.01 | 0.01 |
| (1,4539) | 1:A:6:ALA:H | 1:A:52:PHE:HD1 | 1 | 0.01 | 0.01 |
| (1,4539) | 1:A:6:ALA:H | 1:A:52:PHE:HD2 | 1 | 0.01 | 0.01 |
| (1,4513) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HD1 | 1 | 0.03 | 0.03 |
| (1,4513) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HD2 | 1 | 0.03 | 0.03 |
| (1,4513) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HD1 | 1 | 0.03 | 0.03 |
| (1,4513) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HD2 | 1 | 0.03 | 0.03 |
| (1,4513) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HD1 | 1 | 0.03 | 0.03 |
| (1,4513) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HD2 | 1 | 0.03 | 0.03 |
| (1,4456) | 1:B:14:ASP:HA | 1:B:45:PHE:HD1 | 1 | 0.02 | 0.02 |
| (1,4456) | 1:B:14:ASP:HA | 1:B:45:PHE:HD2 | 1 | 0.02 | 0.02 |
| (1,4451) | 1:B:18:MET:HE1 | 1:B:45:PHE:HD1 | 1 | 0.02 | 0.02 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,4451) | 1:B:18:MET:HE1 | 1:B:45:PHE:HD2 | 1 | 0.02 | 0.02 |
| (1,4451) | 1:B:18:MET:HE2 | 1:B:45:PHE:HD1 | 1 | 0.02 | 0.02 |
| (1,4451) | 1:B:18:MET:HE2 | 1:B:45:PHE:HD2 | 1 | 0.02 | 0.02 |
| (1,4451) | 1:B:18:MET:HE3 | 1:B:45:PHE:HD1 | 1 | 0.02 | 0.02 |
| (1,4451) | 1:B:18:MET:HE3 | 1:B:45:PHE:HD2 | 1 | 0.02 | 0.02 |
| (1,4447) | 1:B:40:ALA:HB1 | 1:B:45:PHE:HD1 | 1 | 0.01 | 0.01 |
| (1,4447) | 1:B:40:ALA:HB1 | 1:B:45:PHE:HD2 | 1 | 0.01 | 0.01 |
| (1,4447) | 1:B:40:ALA:HB2 | 1:B:45:PHE:HD1 | 1 | 0.01 | 0.01 |
| (1,4447) | 1:B:40:ALA:HB2 | 1:B:45:PHE:HD2 | 1 | 0.01 | 0.01 |
| (1,4447) | 1:B:40:ALA:HB3 | 1:B:45:PHE:HD1 | 1 | 0.01 | 0.01 |
| (1,4447) | 1:B:40:ALA:HB3 | 1:B:45:PHE:HD2 | 1 | 0.01 | 0.01 |
| (1,4418) | 1:A:29:PHE:H | 1:A:29:PHE:HD1 | 1 | 0.01 | 0.01 |
| (1,4418) | 1:A:29:PHE:H | 1:A:29:PHE:HD2 | 1 | 0.01 | 0.01 |
| (1,4388) | 1:A:4:PHE:HZ | 1:A:56:THR:HA | 1 | 0.01 | 0.01 |
| (1,4385) | 1:B:4:PHE:HZ | 1:B:59:LEU:HD21 | 1 | 0.01 | 0.01 |
| (1,4385) | 1:B:4:PHE:HZ | 1:B:59:LEU:HD22 | 1 | 0.01 | 0.01 |
| (1,4385) | 1:B:4:PHE:HZ | 1:B:59:LEU:HD23 | 1 | 0.01 | 0.01 |
| (1,4367) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HA | 1 | 0.08 | 0.08 |
| (1,4345) | 1:B:4:PHE:HD1 | 1:B:54:LYS:HA | 1 | 0.01 | 0.01 |
| (1,4345) | 1:B:4:PHE:HD2 | 1:B:54:LYS:HA | 1 | 0.01 | 0.01 |
| (1,4342) | 1:A:4:PHE:HD1 | 1:A:5:LEU:HB3 | 1 | 0.01 | 0.01 |
| (1,4342) | 1:A:4:PHE:HD2 | 1:A:5:LEU:HB3 | 1 | 0.01 | 0.01 |
| (1,4321) | 1:B:77:ARG:HG2 | 1:B:79:SER:HA | 1 | 0.02 | 0.02 |
| (1,4315) | 1:B:79:SER:HA | 1:B:81:LEU:HD21 | 1 | 0.02 | 0.02 |
| (1,4315) | 1:B:79:SER:HA | 1:B:81:LEU:HD22 | 1 | 0.02 | 0.02 |
| (1,4315) | 1:B:79:SER:HA | 1:B:81:LEU:HD23 | 1 | 0.02 | 0.02 |
| (1,4299) | 1:B:74:THR:HA | 1:B:75:VAL:HG21 | 1 | 0.01 | 0.01 |
| (1,4299) | 1:B:74:THR:HA | 1:B:75:VAL:HG22 | 1 | 0.01 | 0.01 |
| (1,4299) | 1:B:74:THR:HA | 1:B:75:VAL:HG23 | 1 | 0.01 | 0.01 |
| (1,4293) | 1:B:73:PHE:HA | 1:B:75:VAL:HG21 | 1 | 0.05 | 0.05 |
| (1,4293) | 1:B:73:PHE:HA | 1:B:75:VAL:HG22 | 1 | 0.05 | 0.05 |
| (1,4293) | 1:B:73:PHE:HA | 1:B:75:VAL:HG23 | 1 | 0.05 | 0.05 |
| (1,4279) | 1:B:60:THR:HB | 1:B:61:THR:H | 1 | 0.11 | 0.11 |
| (1,4257) | 1:B:41:LYS:HA | 1:B:42:ASP:H | 1 | 0.38 | 0.38 |
| (1,4190) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HB3 | 1 | 0.04 | 0.04 |
| (1,4190) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HB3 | 1 | 0.04 | 0.04 |
| (1,4190) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HB3 | 1 | 0.04 | 0.04 |
| (1,4171) | 1:B:72:VAL:HG21 | 1:B:73:PHE:HB3 | 1 | 0.01 | 0.01 |
| (1,4171) | 1:B:72:VAL:HG22 | 1:B:73:PHE:HB3 | 1 | 0.01 | 0.01 |
| (1,4171) | 1:B:72:VAL:HG23 | 1:B:73:PHE:HB3 | 1 | 0.01 | 0.01 |
| (1,4152) | 1:A:41:LYS:HE2 | 1:A:44:ILE:HB | 1 | 0.05 | 0.05 |
| (1,4152) | 1:A:41:LYS:HE3 | 1:A:44:ILE:HB | 1 | 0.05 | 0.05 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,4124) | 1:A:23:THR:H | 1:B:33:ILE:HD11 | 1 | 0.01 | 0.01 |
| (1,4124) | 1:A:23:THR:H | 1:B:33:ILE:HD12 | 1 | 0.01 | 0.01 |
| (1,4124) | 1:A:23:THR:H | 1:B:33:ILE:HD13 | 1 | 0.01 | 0.01 |
| (1,4084) | 1:A:82:GLU:HG3 | 1:A:83:HIS:HA | 1 | 0.04 | 0.04 |
| (1,4083) | 1:B:82:GLU:HA | 1:B:82:GLU:HG3 | 1 | 0.12 | 0.12 |
| (1,4081) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HA | 1 | 0.05 | 0.05 |
| (1,4080) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HA | 1 | 0.02 | 0.02 |
| (1,4071) | 1:B:79:SER:H | 1:B:81:LEU:HD21 | 1 | 0.01 | 0.01 |
| (1,4071) | 1:B:79:SER:H | 1:B:81:LEU:HD22 | 1 | 0.01 | 0.01 |
| (1,4071) | 1:B:79:SER:H | 1:B:81:LEU:HD23 | 1 | 0.01 | 0.01 |
| (1,4061) | 1:B:7:GLY:HA2 | 1:B:81:LEU:HD21 | 1 | 0.03 | 0.03 |
| (1,4061) | 1:B:7:GLY:HA2 | 1:B:81:LEU:HD22 | 1 | 0.03 | 0.03 |
| (1,4061) | 1:B:7:GLY:HA2 | 1:B:81:LEU:HD23 | 1 | 0.03 | 0.03 |
| (1,4054) | 1:A:6:ALA:H | 1:A:81:LEU:HD11 | 1 | 0.05 | 0.05 |
| (1,4054) | 1:A:6:ALA:H | 1:A:81:LEU:HD12 | 1 | 0.05 | 0.05 |
| (1,4054) | 1:A:6:ALA:H | 1:A:81:LEU:HD13 | 1 | 0.05 | 0.05 |
| (1,4039) | 1:B:50:MET:HG3 | 1:B:81:LEU:HD11 | 1 | 0.02 | 0.02 |
| (1,4039) | 1:B:50:MET:HG3 | 1:B:81:LEU:HD12 | 1 | 0.02 | 0.02 |
| (1,4039) | 1:B:50:MET:HG3 | 1:B:81:LEU:HD13 | 1 | 0.02 | 0.02 |
| (1,4037) | 1:B:50:MET:HG2 | 1:B:81:LEU:HD11 | 1 | 0.03 | 0.03 |
| (1,4037) | 1:B:50:MET:HG2 | 1:B:81:LEU:HD12 | 1 | 0.03 | 0.03 |
| (1,4037) | 1:B:50:MET:HG2 | 1:B:81:LEU:HD13 | 1 | 0.03 | 0.03 |
| (1,4036) | 1:A:50:MET:HG2 | 1:A:81:LEU:HD11 | 1 | 0.01 | 0.01 |
| (1,4036) | 1:A:50:MET:HG2 | 1:A:81:LEU:HD12 | 1 | 0.01 | 0.01 |
| (1,4036) | 1:A:50:MET:HG2 | 1:A:81:LEU:HD13 | 1 | 0.01 | 0.01 |
| (1,4022) | 1:A:80:ASN:HB3 | 1:A:81:LEU:HD21 | 1 | 0.03 | 0.03 |
| (1,4022) | 1:A:80:ASN:HB3 | 1:A:81:LEU:HD22 | 1 | 0.03 | 0.03 |
| (1,4022) | 1:A:80:ASN:HB3 | 1:A:81:LEU:HD23 | 1 | 0.03 | 0.03 |
| (1,4018) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD21 | 1 | 0.04 | 0.04 |
| (1,4018) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD22 | 1 | 0.04 | 0.04 |
| (1,4018) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD23 | 1 | 0.04 | 0.04 |
| (1,4015) | 1:B:78:LEU:HB3 | 1:B:79:SER:HB2 | 1 | 0.05 | 0.05 |
| (1,4015) | 1:B:78:LEU:HB3 | 1:B:79:SER:HB3 | 1 | 0.05 | 0.05 |
| (1,4013) | 1:B:9:ARG:H | 1:B:78:LEU:HD21 | 1 | 0.01 | 0.01 |
| (1,4013) | 1:B:9:ARG:H | 1:B:78:LEU:HD22 | 1 | 0.01 | 0.01 |
| (1,4013) | 1:B:9:ARG:H | 1:B:78:LEU:HD23 | 1 | 0.01 | 0.01 |
| (1,3987) | 1:B:48:ASN:HD21 | 1:B:78:LEU:HD11 | 1 | 0.03 | 0.03 |
| (1,3987) | 1:B:48:ASN:HD21 | 1:B:78:LEU:HD12 | 1 | 0.03 | 0.03 |
| (1,3987) | 1:B:48:ASN:HD21 | 1:B:78:LEU:HD13 | 1 | 0.03 | 0.03 |
| (1,3975) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HD11 | 1 | 0.02 | 0.02 |
| (1,3975) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HD12 | 1 | 0.02 | 0.02 |
| (1,3975) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HD13 | 1 | 0.02 | 0.02 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,3966) | 1:A:50:MET:HE1 | 1:A:78:LEU:HD11 | 1 | 0.03 | 0.03 |
| (1,3966) | 1:A:50:MET:HE1 | 1:A:78:LEU:HD12 | 1 | 0.03 | 0.03 |
| (1,3966) | 1:A:50:MET:HE1 | 1:A:78:LEU:HD13 | 1 | 0.03 | 0.03 |
| (1,3966) | 1:A:50:MET:HE2 | 1:A:78:LEU:HD11 | 1 | 0.03 | 0.03 |
| (1,3966) | 1:A:50:MET:HE2 | 1:A:78:LEU:HD12 | 1 | 0.03 | 0.03 |
| (1,3966) | 1:A:50:MET:HE2 | 1:A:78:LEU:HD13 | 1 | 0.03 | 0.03 |
| (1,3966) | 1:A:50:MET:HE3 | 1:A:78:LEU:HD11 | 1 | 0.03 | 0.03 |
| (1,3966) | 1:A:50:MET:HE3 | 1:A:78:LEU:HD12 | 1 | 0.03 | 0.03 |
| (1,3966) | 1:A:50:MET:HE3 | 1:A:78:LEU:HD13 | 1 | 0.03 | 0.03 |
| (1,3918) | 1:A:59:LEU:HD21 | 1:A:77:ARG:HD2 | 1 | 0.02 | 0.02 |
| (1,3918) | 1:A:59:LEU:HD21 | 1:A:77:ARG:HD3 | 1 | 0.02 | 0.02 |
| (1,3918) | 1:A:59:LEU:HD22 | 1:A:77:ARG:HD2 | 1 | 0.02 | 0.02 |
| (1,3918) | 1:A:59:LEU:HD22 | 1:A:77:ARG:HD3 | 1 | 0.02 | 0.02 |
| (1,3918) | 1:A:59:LEU:HD23 | 1:A:77:ARG:HD2 | 1 | 0.02 | 0.02 |
| (1,3918) | 1:A:59:LEU:HD23 | 1:A:77:ARG:HD3 | 1 | 0.02 | 0.02 |
| (1,3900) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 1 | 0.01 | 0.01 |
| (1,3900) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 1 | 0.01 | 0.01 |
| (1,3900) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 1 | 0.01 | 0.01 |
| (1,3894) | 1:A:9:ARG:HB2 | 1:A:76:GLU:HG2 | 1 | 0.01 | 0.01 |
| (1,3894) | 1:A:9:ARG:HB2 | 1:A:76:GLU:HG3 | 1 | 0.01 | 0.01 |
| (1,3894) | 1:A:9:ARG:HB3 | 1:A:76:GLU:HG2 | 1 | 0.01 | 0.01 |
| (1,3894) | 1:A:9:ARG:HB3 | 1:A:76:GLU:HG3 | 1 | 0.01 | 0.01 |
| (1,3857) | 1:A:73:PHE:HA | 1:A:74:THR:HG21 | 1 | 0.04 | 0.04 |
| (1,3857) | 1:A:73:PHE:HA | 1:A:74:THR:HG22 | 1 | 0.04 | 0.04 |
| (1,3857) | 1:A:73:PHE:HA | 1:A:74:THR:HG23 | 1 | 0.04 | 0.04 |
| (1,3845) | 1:A:10:ILE:HA | 1:A:74:THR:HB | 1 | 0.01 | 0.01 |
| (1,3814) | 1:B:66:LEU:HA | 1:B:72:VAL:HG21 | 1 | 0.01 | 0.01 |
| (1,3814) | 1:B:66:LEU:HA | 1:B:72:VAL:HG22 | 1 | 0.01 | 0.01 |
| (1,3814) | 1:B:66:LEU:HA | 1:B:72:VAL:HG23 | 1 | 0.01 | 0.01 |
| (1,3813) | 1:A:66:LEU:HA | 1:A:72:VAL:HG21 | 1 | 0.02 | 0.02 |
| (1,3813) | 1:A:66:LEU:HA | 1:A:72:VAL:HG22 | 1 | 0.02 | 0.02 |
| (1,3813) | 1:A:66:LEU:HA | 1:A:72:VAL:HG23 | 1 | 0.02 | 0.02 |
| (1,3776) | 1:B:70:GLN:HG2 | 1:B:72:VAL:H | 1 | 0.04 | 0.04 |
| (1,3776) | 1:B:70:GLN:HG3 | 1:B:72:VAL:H | 1 | 0.04 | 0.04 |
| (1,3775) | 1:A:70:GLN:HG2 | 1:A:72:VAL:H | 1 | 0.05 | 0.05 |
| (1,3775) | 1:A:70:GLN:HG3 | 1:A:72:VAL:H | 1 | 0.05 | 0.05 |
| (1,3767) | 1:A:69:VAL:HA | 1:A:70:GLN:HG2 | 1 | 0.13 | 0.13 |
| (1,3767) | 1:A:69:VAL:HA | 1:A:70:GLN:HG3 | 1 | 0.13 | 0.13 |
| (1,3747) | 1:A:69:VAL:HG11 | 1:A:70:GLN:HB2 | 1 | 0.02 | 0.02 |
| (1,3747) | 1:A:69:VAL:HG11 | 1:A:70:GLN:HB3 | 1 | 0.02 | 0.02 |
| (1,3747) | 1:A:69:VAL:HG12 | 1:A:70:GLN:HB2 | 1 | 0.02 | 0.02 |
| (1,3747) | 1:A:69:VAL:HG12 | 1:A:70:GLN:HB3 | 1 | 0.02 | 0.02 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,3747) | 1:A:69:VAL:HG13 | 1:A:70:GLN:HB2 | 1 | 0.02 | 0.02 |
| (1,3747) | 1:A:69:VAL:HG13 | 1:A:70:GLN:HB3 | 1 | 0.02 | 0.02 |
| (1,3724) | 1:B:66:LEU:HA | 1:B:69:VAL:HG21 | 1 | 0.01 | 0.01 |
| (1,3724) | 1:B:66:LEU:HA | 1:B:69:VAL:HG22 | 1 | 0.01 | 0.01 |
| (1,3724) | 1:B:66:LEU:HA | 1:B:69:VAL:HG23 | 1 | 0.01 | 0.01 |
| (1,3723) | 1:A:66:LEU:HA | 1:A:69:VAL:HG21 | 1 | 0.01 | 0.01 |
| (1,3723) | 1:A:66:LEU:HA | 1:A:69:VAL:HG22 | 1 | 0.01 | 0.01 |
| (1,3723) | 1:A:66:LEU:HA | 1:A:69:VAL:HG23 | 1 | 0.01 | 0.01 |
| (1,3706) | 1:B:68:LYS:HB3 | 1:B:69:VAL:HA | 1 | 0.02 | 0.02 |
| (1,3703) | 1:A:67:ARG:H | 1:A:68:LYS:HE2 | 1 | 0.03 | 0.03 |
| (1,3703) | 1:A:67:ARG:H | 1:A:68:LYS:HE3 | 1 | 0.03 | 0.03 |
| (1,3692) | 1:B:68:LYS:HA | 1:B:68:LYS:HE2 | 1 | 0.02 | 0.02 |
| (1,3692) | 1:B:68:LYS:HA | 1:B:68:LYS:HE3 | 1 | 0.02 | 0.02 |
| (1,3691) | 1:A:68:LYS:HA | 1:A:68:LYS:HE2 | 1 | 0.06 | 0.06 |
| (1,3691) | 1:A:68:LYS:HA | 1:A:68:LYS:HE3 | 1 | 0.06 | 0.06 |
| (1,3690) | 1:A:64:ASP:H | 1:A:65:LYS:HG2 | 1 | 0.02 | 0.02 |
| (1,369) | 1:B:21:GLN:HE22 | 1:B:69:VAL:HA | 1 | 0.04 | 0.04 |
| (1,3668) | 1:A:68:LYS:HA | 1:A:68:LYS:HD3 | 1 | 0.01 | 0.01 |
| (1,3666) | 1:A:68:LYS:HA | 1:A:68:LYS:HG3 | 1 | 0.03 | 0.03 |
| (1,3652) | 1:A:67:ARG:HD2 | 1:A:75:VAL:HG11 | 1 | 0.02 | 0.02 |
| (1,3652) | 1:A:67:ARG:HD2 | 1:A:75:VAL:HG12 | 1 | 0.02 | 0.02 |
| (1,3652) | 1:A:67:ARG:HD2 | 1:A:75:VAL:HG13 | 1 | 0.02 | 0.02 |
| (1,3652) | 1:A:67:ARG:HD3 | 1:A:75:VAL:HG11 | 1 | 0.02 | 0.02 |
| (1,3652) | 1:A:67:ARG:HD3 | 1:A:75:VAL:HG12 | 1 | 0.02 | 0.02 |
| (1,3652) | 1:A:67:ARG:HD3 | 1:A:75:VAL:HG13 | 1 | 0.02 | 0.02 |
| (1,3648) | 1:A:64:ASP:HA | 1:A:67:ARG:HG3 | 1 | 0.02 | 0.02 |
| (1,364) | 1:A:18:MET:HE1 | 1:A:21:GLN:HE22 | 1 | 0.02 | 0.02 |
| (1,364) | 1:A:18:MET:HE2 | 1:A:21:GLN:HE22 | 1 | 0.02 | 0.02 |
| (1,364) | 1:A:18:MET:HE3 | 1:A:21:GLN:HE22 | 1 | 0.02 | 0.02 |
| (1,362) | 1:A:21:GLN:HE22 | 1:A:69:VAL:HG21 | 1 | 0.04 | 0.04 |
| (1,362) | 1:A:21:GLN:HE22 | 1:A:69:VAL:HG22 | 1 | 0.04 | 0.04 |
| (1,362) | 1:A:21:GLN:HE22 | 1:A:69:VAL:HG23 | 1 | 0.04 | 0.04 |
| (1,3617) | 1:B:65:LYS:HA | 1:B:65:LYS:HE2 | 1 | 0.14 | 0.14 |
| (1,3617) | 1:B:65:LYS:HA | 1:B:65:LYS:HE3 | 1 | 0.14 | 0.14 |
| (1,3602) | 1:A:29:PHE:HZ | 1:A:65:LYS:HG2 | 1 | 0.01 | 0.01 |
| (1,358) | 1:A:21:GLN:HE22 | 1:A:69:VAL:HG11 | 1 | 0.03 | 0.03 |
| (1,358) | 1:A:21:GLN:HE22 | 1:A:69:VAL:HG12 | 1 | 0.03 | 0.03 |
| (1,358) | 1:A:21:GLN:HE22 | 1:A:69:VAL:HG13 | 1 | 0.03 | 0.03 |
| (1,3535) | 1:B:64:ASP:HB2 | 1:B:67:ARG:HB2 | 1 | 0.05 | 0.05 |
| (1,3535) | 1:B:64:ASP:HB2 | 1:B:67:ARG:HB3 | 1 | 0.05 | 0.05 |
| (1,3531) | 1:A:61:THR:HG21 | 1:A:64:ASP:HB2 | 1 | 0.04 | 0.04 |
| (1,3531) | 1:A:61:THR:HG22 | 1:A:64:ASP:HB2 | 1 | 0.04 | 0.04 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,3531) | 1:A:61:THR:HG23 | 1:A:64:ASP:HB2 | 1 | 0.04 | 0.04 |
| (1,3504) | 1:B:60:THR:HG21 | 1:B:63:MET:HE1 | 1 | 0.23 | 0.23 |
| (1,3504) | 1:B:60:THR:HG21 | 1:B:63:MET:HE2 | 1 | 0.23 | 0.23 |
| (1,3504) | 1:B:60:THR:HG21 | 1:B:63:MET:HE3 | 1 | 0.23 | 0.23 |
| (1,3504) | 1:B:60:THR:HG22 | 1:B:63:MET:HE1 | 1 | 0.23 | 0.23 |
| (1,3504) | 1:B:60:THR:HG22 | 1:B:63:MET:HE2 | 1 | 0.23 | 0.23 |
| (1,3504) | 1:B:60:THR:HG22 | 1:B:63:MET:HE3 | 1 | 0.23 | 0.23 |
| (1,3504) | 1:B:60:THR:HG23 | 1:B:63:MET:HE1 | 1 | 0.23 | 0.23 |
| (1,3504) | 1:B:60:THR:HG23 | 1:B:63:MET:HE2 | 1 | 0.23 | 0.23 |
| (1,3504) | 1:B:60:THR:HG23 | 1:B:63:MET:HE3 | 1 | 0.23 | 0.23 |
| (1,3494) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:HD21 | 1 | 0.26 | 0.26 |
| (1,3494) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:HD22 | 1 | 0.26 | 0.26 |
| (1,3494) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:HD23 | 1 | 0.26 | 0.26 |
| (1,3459) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:HD11 | 1 | 0.38 | 0.38 |
| (1,3459) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:HD12 | 1 | 0.38 | 0.38 |
| (1,3459) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:HD13 | 1 | 0.38 | 0.38 |
| (1,3448) | 1:B:62:LEU:HD11 | 1:B:63:MET:HA | 1 | 0.02 | 0.02 |
| (1,3448) | 1:B:62:LEU:HD12 | 1:B:63:MET:HA | 1 | 0.02 | 0.02 |
| (1,3448) | 1:B:62:LEU:HD13 | 1:B:63:MET:HA | 1 | 0.02 | 0.02 |
| (1,3439) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD11 | 1 | 0.02 | 0.02 |
| (1,3439) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD12 | 1 | 0.02 | 0.02 |
| (1,3439) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD13 | 1 | 0.02 | 0.02 |
| (1,3433) | 1:A:58:LYS:HG3 | 1:A:62:LEU:HD11 | 1 | 0.02 | 0.02 |
| (1,3433) | 1:A:58:LYS:HG3 | 1:A:62:LEU:HD12 | 1 | 0.02 | 0.02 |
| (1,3433) | 1:A:58:LYS:HG3 | 1:A:62:LEU:HD13 | 1 | 0.02 | 0.02 |
| (1,3364) | 1:A:61:THR:HA | 1:A:64:ASP:HB2 | 1 | 0.02 | 0.02 |
| (1,3357) | 1:B:60:THR:HA | 1:B:60:THR:HG21 | 1 | 0.05 | 0.05 |
| (1,3357) | 1:B:60:THR:HA | 1:B:60:THR:HG22 | 1 | 0.05 | 0.05 |
| (1,3357) | 1:B:60:THR:HA | 1:B:60:THR:HG23 | 1 | 0.05 | 0.05 |
| (1,3354) | 1:A:60:THR:HG21 | 1:A:63:MET:HG3 | 1 | 0.02 | 0.02 |
| (1,3354) | 1:A:60:THR:HG22 | 1:A:63:MET:HG3 | 1 | 0.02 | 0.02 |
| (1,3354) | 1:A:60:THR:HG23 | 1:A:63:MET:HG3 | 1 | 0.02 | 0.02 |
| (1,3282) | 1:A:58:LYS:HD2 | 1:A:62:LEU:H | 1 | 0.1 | 0.1 |
| (1,3282) | 1:A:58:LYS:HD3 | 1:A:62:LEU:H | 1 | 0.1 | 0.1 |
| (1,3272) | 1:A:58:LYS:HD2 | 1:A:62:LEU:HB2 | 1 | 0.03 | 0.03 |
| (1,3272) | 1:A:58:LYS:HD3 | 1:A:62:LEU:HB2 | 1 | 0.03 | 0.03 |
| (1,3248) | 1:A:31:THR:HG21 | 1:A:58:LYS:HG3 | 1 | 0.03 | 0.03 |
| (1,3248) | 1:A:31:THR:HG22 | 1:A:58:LYS:HG3 | 1 | 0.03 | 0.03 |
| (1,3248) | 1:A:31:THR:HG23 | 1:A:58:LYS:HG3 | 1 | 0.03 | 0.03 |
| (1,3240) | 1:A:55:ASN:H | 1:A:58:LYS:HB2 | 1 | 0.11 | 0.11 |
| (1,3197) | 1:B:54:LYS:H | 1:B:54:LYS:HE2 | 1 | 0.16 | 0.16 |
| (1,3197) | 1:B:54:LYS:H | 1:B:54:LYS:HE3 | 1 | 0.16 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,3196) | 1:A:54:LYS:H | 1:A:54:LYS:HE2 | 1 | 0.03 | 0.03 |
| (1,3196) | 1:A:54:LYS:H | 1:A:54:LYS:HE3 | 1 | 0.03 | 0.03 |
| (1,3132) | 1:A:5:LEU:HA | 1:A:53:VAL:HG21 | 1 | 0.02 | 0.02 |
| (1,3132) | 1:A:5:LEU:HA | 1:A:53:VAL:HG22 | 1 | 0.02 | 0.02 |
| (1,3132) | 1:A:5:LEU:HA | 1:A:53:VAL:HG23 | 1 | 0.02 | 0.02 |
| (1,3128) | 1:A:53:VAL:HG21 | 1:A:58:LYS:HA | 1 | 0.04 | 0.04 |
| (1,3128) | 1:A:53:VAL:HG22 | 1:A:58:LYS:HA | 1 | 0.04 | 0.04 |
| (1,3128) | 1:A:53:VAL:HG23 | 1:A:58:LYS:HA | 1 | 0.04 | 0.04 |
| (1,3125) | 1:B:53:VAL:HG21 | 1:B:59:LEU:HA | 1 | 0.01 | 0.01 |
| (1,3125) | 1:B:53:VAL:HG22 | 1:B:59:LEU:HA | 1 | 0.01 | 0.01 |
| (1,3125) | 1:B:53:VAL:HG23 | 1:B:59:LEU:HA | 1 | 0.01 | 0.01 |
| (1,311) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HG12 | 1 | 0.03 | 0.03 |
| (1,310) | 1:A:33:ILE:HG12 | 1:B:20:ASN:HD22 | 1 | 0.02 | 0.02 |
| (1,3099) | 1:B:52:PHE:H | 1:B:53:VAL:HG11 | 1 | 0.01 | 0.01 |
| (1,3099) | 1:B:52:PHE:H | 1:B:53:VAL:HG12 | 1 | 0.01 | 0.01 |
| (1,3099) | 1:B:52:PHE:H | 1:B:53:VAL:HG13 | 1 | 0.01 | 0.01 |
| (1,3098) | 1:A:52:PHE:H | 1:A:53:VAL:HG11 | 1 | 0.01 | 0.01 |
| (1,3098) | 1:A:52:PHE:H | 1:A:53:VAL:HG12 | 1 | 0.01 | 0.01 |
| (1,3098) | 1:A:52:PHE:H | 1:A:53:VAL:HG13 | 1 | 0.01 | 0.01 |
| (1,3097) | 1:B:53:VAL:HG11 | 1:B:55:ASN:H | 1 | 0.03 | 0.03 |
| (1,3097) | 1:B:53:VAL:HG12 | 1:B:55:ASN:H | 1 | 0.03 | 0.03 |
| (1,3097) | 1:B:53:VAL:HG13 | 1:B:55:ASN:H | 1 | 0.03 | 0.03 |
| (1,3096) | 1:A:53:VAL:HG11 | 1:A:55:ASN:H | 1 | 0.01 | 0.01 |
| (1,3096) | 1:A:53:VAL:HG12 | 1:A:55:ASN:H | 1 | 0.01 | 0.01 |
| (1,3096) | 1:A:53:VAL:HG13 | 1:A:55:ASN:H | 1 | 0.01 | 0.01 |
| (1,308) | 1:A:33:ILE:HG13 | 1:B:20:ASN:HD22 | 1 | 0.14 | 0.14 |
| (1,3063) | 1:B:53:VAL:HG11 | 1:B:62:LEU:HD21 | 1 | 0.03 | 0.03 |
| (1,3063) | 1:B:53:VAL:HG11 | 1:B:62:LEU:HD22 | 1 | 0.03 | 0.03 |
| (1,3063) | 1:B:53:VAL:HG11 | 1:B:62:LEU:HD23 | 1 | 0.03 | 0.03 |
| (1,3063) | 1:B:53:VAL:HG12 | 1:B:62:LEU:HD21 | 1 | 0.03 | 0.03 |
| (1,3063) | 1:B:53:VAL:HG12 | 1:B:62:LEU:HD22 | 1 | 0.03 | 0.03 |
| (1,3063) | 1:B:53:VAL:HG12 | 1:B:62:LEU:HD23 | 1 | 0.03 | 0.03 |
| (1,3063) | 1:B:53:VAL:HG13 | 1:B:62:LEU:HD21 | 1 | 0.03 | 0.03 |
| (1,3063) | 1:B:53:VAL:HG13 | 1:B:62:LEU:HD22 | 1 | 0.03 | 0.03 |
| (1,3063) | 1:B:53:VAL:HG13 | 1:B:62:LEU:HD23 | 1 | 0.03 | 0.03 |
| (1,303) | 1:A:33:ILE:HG13 | 1:B:20:ASN:HD21 | 1 | 0.08 | 0.08 |
| (1,2960) | 1:A:15:LYS:HG2 | 1:A:16:ASN:H | 1 | 0.08 | 0.08 |
| (1,2960) | 1:A:15:LYS:HG3 | 1:A:16:ASN:H | 1 | 0.08 | 0.08 |
| (1,2920) | 1:A:6:ALA:HA | 1:A:50:MET:HE1 | 1 | 0.02 | 0.02 |
| (1,2920) | 1:A:6:ALA:HA | 1:A:50:MET:HE2 | 1 | 0.02 | 0.02 |
| (1,2920) | 1:A:6:ALA:HA | 1:A:50:MET:HE3 | 1 | 0.02 | 0.02 |
| (1,2917) | 1:B:50:MET:HE1 | 1:B:81:LEU:HA | 1 | 0.02 | 0.02 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,2917) | 1:B:50:MET:HE2 | 1:B:81:LEU:HA | 1 | 0.02 | 0.02 |
| (1,2917) | 1:B:50:MET:HE3 | 1:B:81:LEU:HA | 1 | 0.02 | 0.02 |
| (1,2916) | 1:A:50:MET:HE1 | 1:A:81:LEU:HA | 1 | 0.01 | 0.01 |
| (1,2916) | 1:A:50:MET:HE2 | 1:A:81:LEU:HA | 1 | 0.01 | 0.01 |
| (1,2916) | 1:A:50:MET:HE3 | 1:A:81:LEU:HA | 1 | 0.01 | 0.01 |
| (1,2899) | 1:B:50:MET:HE1 | 1:B:81:LEU:HD21 | 1 | 0.02 | 0.02 |
| (1,2899) | 1:B:50:MET:HE1 | 1:B:81:LEU:HD22 | 1 | 0.02 | 0.02 |
| (1,2899) | 1:B:50:MET:HE1 | 1:B:81:LEU:HD23 | 1 | 0.02 | 0.02 |
| (1,2899) | 1:B:50:MET:HE2 | 1:B:81:LEU:HD21 | 1 | 0.02 | 0.02 |
| (1,2899) | 1:B:50:MET:HE2 | 1:B:81:LEU:HD22 | 1 | 0.02 | 0.02 |
| (1,2899) | 1:B:50:MET:HE2 | 1:B:81:LEU:HD23 | 1 | 0.02 | 0.02 |
| (1,2899) | 1:B:50:MET:HE3 | 1:B:81:LEU:HD21 | 1 | 0.02 | 0.02 |
| (1,2899) | 1:B:50:MET:HE3 | 1:B:81:LEU:HD22 | 1 | 0.02 | 0.02 |
| (1,2899) | 1:B:50:MET:HE3 | 1:B:81:LEU:HD23 | 1 | 0.02 | 0.02 |
| (1,2859) | 1:B:50:MET:HG3 | 1:B:78:LEU:HD11 | 1 | 0.01 | 0.01 |
| (1,2859) | 1:B:50:MET:HG3 | 1:B:78:LEU:HD12 | 1 | 0.01 | 0.01 |
| (1,2859) | 1:B:50:MET:HG3 | 1:B:78:LEU:HD13 | 1 | 0.01 | 0.01 |
| (1,2766) | 1:B:9:ARG:HG2 | 1:B:48:ASN:HA | 1 | 0.09 | 0.09 |
| (1,2765) | 1:A:9:ARG:HG2 | 1:A:48:ASN:HA | 1 | 0.14 | 0.14 |
| (1,2760) | 1:B:10:ILE:HD11 | 1:B:48:ASN:HA | 1 | 0.01 | 0.01 |
| (1,2760) | 1:B:10:ILE:HD12 | 1:B:48:ASN:HA | 1 | 0.01 | 0.01 |
| (1,2760) | 1:B:10:ILE:HD13 | 1:B:48:ASN:HA | 1 | 0.01 | 0.01 |
| (1,2724) | 1:B:10:ILE:H | 1:B:46:THR:HG21 | 1 | 0.02 | 0.02 |
| (1,2724) | 1:B:10:ILE:H | 1:B:46:THR:HG22 | 1 | 0.02 | 0.02 |
| (1,2724) | 1:B:10:ILE:H | 1:B:46:THR:HG23 | 1 | 0.02 | 0.02 |
| (1,2723) | 1:A:10:ILE:H | 1:A:46:THR:HG21 | 1 | 0.02 | 0.02 |
| (1,2723) | 1:A:10:ILE:H | 1:A:46:THR:HG22 | 1 | 0.02 | 0.02 |
| (1,2723) | 1:A:10:ILE:H | 1:A:46:THR:HG23 | 1 | 0.02 | 0.02 |
| (1,2701) | 1:A:41:LYS:HE2 | 1:A:46:THR:HG21 | 1 | 0.02 | 0.02 |
| (1,2701) | 1:A:41:LYS:HE2 | 1:A:46:THR:HG22 | 1 | 0.02 | 0.02 |
| (1,2701) | 1:A:41:LYS:HE2 | 1:A:46:THR:HG23 | 1 | 0.02 | 0.02 |
| (1,2701) | 1:A:41:LYS:HE3 | 1:A:46:THR:HG21 | 1 | 0.02 | 0.02 |
| (1,2701) | 1:A:41:LYS:HE3 | 1:A:46:THR:HG22 | 1 | 0.02 | 0.02 |
| (1,2701) | 1:A:41:LYS:HE3 | 1:A:46:THR:HG23 | 1 | 0.02 | 0.02 |
| (1,2677) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HZ | 1 | 0.03 | 0.03 |
| (1,2677) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HZ | 1 | 0.03 | 0.03 |
| (1,2677) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HZ | 1 | 0.03 | 0.03 |
| (1,2673) | 1:A:44:ILE:HA | 1:A:44:ILE:HD11 | 1 | 0.01 | 0.01 |
| (1,2673) | 1:A:44:ILE:HA | 1:A:44:ILE:HD12 | 1 | 0.01 | 0.01 |
| (1,2673) | 1:A:44:ILE:HA | 1:A:44:ILE:HD13 | 1 | 0.01 | 0.01 |
| (1,2657) | 1:A:14:ASP:H | 1:A:44:ILE:HG21 | 1 | 0.03 | 0.03 |
| (1,2657) | 1:A:14:ASP:H | 1:A:44:ILE:HG22 | 1 | 0.03 | 0.03 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,2657) | 1:A:14:ASP:H | 1:A:44:ILE:HG23 | 1 | 0.03 | 0.03 |
| (1,2623) | 1:A:44:ILE:HG12 | 1:A:45:PHE:H | 1 | 0.04 | 0.04 |
| (1,2613) | 1:A:12:GLY:H | 1:A:44:ILE:HB | 1 | 0.01 | 0.01 |
| (1,2588) | 1:B:15:LYS:H | 1:B:40:ALA:HB1 | 1 | 0.08 | 0.08 |
| (1,2588) | 1:B:15:LYS:H | 1:B:40:ALA:HB2 | 1 | 0.08 | 0.08 |
| (1,2588) | 1:B:15:LYS:H | 1:B:40:ALA:HB3 | 1 | 0.08 | 0.08 |
| (1,2504) | 1:B:38:LEU:HD11 | 1:B:45:PHE:HZ | 1 | 0.02 | 0.02 |
| (1,2504) | 1:B:38:LEU:HD12 | 1:B:45:PHE:HZ | 1 | 0.02 | 0.02 |
| (1,2504) | 1:B:38:LEU:HD13 | 1:B:45:PHE:HZ | 1 | 0.02 | 0.02 |
| (1,2485) | 1:A:38:LEU:HD11 | 1:A:47:CYS:HG | 1 | 0.01 | 0.01 |
| (1,2485) | 1:A:38:LEU:HD12 | 1:A:47:CYS:HG | 1 | 0.01 | 0.01 |
| (1,2485) | 1:A:38:LEU:HD13 | 1:A:47:CYS:HG | 1 | 0.01 | 0.01 |
| (1,2471) | 1:A:37:VAL:HG21 | 1:A:48:ASN:H | 1 | 0.02 | 0.02 |
| (1,2471) | 1:A:37:VAL:HG22 | 1:A:48:ASN:H | 1 | 0.02 | 0.02 |
| (1,2471) | 1:A:37:VAL:HG23 | 1:A:48:ASN:H | 1 | 0.02 | 0.02 |
| (1,247) | 1:B:19:THR:H | 1:B:40:ALA:HB1 | 1 | 0.02 | 0.02 |
| (1,247) | 1:B:19:THR:H | 1:B:40:ALA:HB2 | 1 | 0.02 | 0.02 |
| (1,247) | 1:B:19:THR:H | 1:B:40:ALA:HB3 | 1 | 0.02 | 0.02 |
| (1,2451) | 1:A:37:VAL:HG21 | 1:A:48:ASN:HB3 | 1 | 0.01 | 0.01 |
| (1,2451) | 1:A:37:VAL:HG22 | 1:A:48:ASN:HB3 | 1 | 0.01 | 0.01 |
| (1,2451) | 1:A:37:VAL:HG23 | 1:A:48:ASN:HB3 | 1 | 0.01 | 0.01 |
| (1,2432) | 1:B:37:VAL:HG11 | 1:B:48:ASN:HB3 | 1 | 0.03 | 0.03 |
| (1,2432) | 1:B:37:VAL:HG12 | 1:B:48:ASN:HB3 | 1 | 0.03 | 0.03 |
| (1,2432) | 1:B:37:VAL:HG13 | 1:B:48:ASN:HB3 | 1 | 0.03 | 0.03 |
| (1,2431) | 1:A:37:VAL:HG11 | 1:A:48:ASN:HB3 | 1 | 0.04 | 0.04 |
| (1,2431) | 1:A:37:VAL:HG12 | 1:A:48:ASN:HB3 | 1 | 0.04 | 0.04 |
| (1,2431) | 1:A:37:VAL:HG13 | 1:A:48:ASN:HB3 | 1 | 0.04 | 0.04 |
| (1,2416) | 1:B:36:ILE:HD11 | 1:B:38:LEU:H | 1 | 0.07 | 0.07 |
| (1,2416) | 1:B:36:ILE:HD12 | 1:B:38:LEU:H | 1 | 0.07 | 0.07 |
| (1,2416) | 1:B:36:ILE:HD13 | 1:B:38:LEU:H | 1 | 0.07 | 0.07 |
| (1,2415) | 1:A:36:ILE:HD11 | 1:A:38:LEU:H | 1 | 0.02 | 0.02 |
| (1,2415) | 1:A:36:ILE:HD12 | 1:A:38:LEU:H | 1 | 0.02 | 0.02 |
| (1,2415) | 1:A:36:ILE:HD13 | 1:A:38:LEU:H | 1 | 0.02 | 0.02 |
| (1,2412) | 1:B:23:THR:H | 1:B:36:ILE:HD11 | 1 | 0.01 | 0.01 |
| (1,2412) | 1:B:23:THR:H | 1:B:36:ILE:HD12 | 1 | 0.01 | 0.01 |
| (1,2412) | 1:B:23:THR:H | 1:B:36:ILE:HD13 | 1 | 0.01 | 0.01 |
| (1,2402) | 1:B:23:THR:HG1 | 1:B:36:ILE:HD11 | 1 | 0.06 | 0.06 |
| (1,2402) | 1:B:23:THR:HG1 | 1:B:36:ILE:HD12 | 1 | 0.06 | 0.06 |
| (1,2402) | 1:B:23:THR:HG1 | 1:B:36:ILE:HD13 | 1 | 0.06 | 0.06 |
| (1,2374) | 1:B:35:THR:HB | 1:B:36:ILE:HG21 | 1 | 0.02 | 0.02 |
| (1,2374) | 1:B:35:THR:HB | 1:B:36:ILE:HG22 | 1 | 0.02 | 0.02 |
| (1,2374) | 1:B:35:THR:HB | 1:B:36:ILE:HG23 | 1 | 0.02 | 0.02 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|-----|--------|--------|--------|----------|---------|
| (1,2373) | 1:A:35:THR:HB | 1:A:36:ILE:HG21 | 1 | 0.01 | 0.01 |
| (1,2373) | 1:A:35:THR:HB | 1:A:36:ILE:HG22 | 1 | 0.01 | 0.01 |
| (1,2373) | 1:A:35:THR:HB | 1:A:36:ILE:HG23 | 1 | 0.01 | 0.01 |
| (1,2329) | 1:A:20:ASN:HD21 | 1:B:33:ILE:HD11 | 1 | 0.03 | 0.03 |
| (1,2329) | 1:A:20:ASN:HD21 | 1:B:33:ILE:HD12 | 1 | 0.03 | 0.03 |
| (1,2329) | 1:A:20:ASN:HD21 | 1:B:33:ILE:HD13 | 1 | 0.03 | 0.03 |
| (1,2287) | 1:A:31:THR:HG21 | 1:A:52:PHE:H | 1 | 0.01 | 0.01 |
| (1,2287) | 1:A:31:THR:HG22 | 1:A:52:PHE:H | 1 | 0.01 | 0.01 |
| (1,2287) | 1:A:31:THR:HG23 | 1:A:52:PHE:H | 1 | 0.01 | 0.01 |
| (1,2274) | 1:B:31:THR:HG21 | 1:B:51:ILE:HD11 | 1 | 0.03 | 0.03 |
| (1,2274) | 1:B:31:THR:HG21 | 1:B:51:ILE:HD12 | 1 | 0.03 | 0.03 |
| (1,2274) | 1:B:31:THR:HG21 | 1:B:51:ILE:HD13 | 1 | 0.03 | 0.03 |
| (1,2274) | 1:B:31:THR:HG22 | 1:B:51:ILE:HD11 | 1 | 0.03 | 0.03 |
| (1,2274) | 1:B:31:THR:HG22 | 1:B:51:ILE:HD12 | 1 | 0.03 | 0.03 |
| (1,2274) | 1:B:31:THR:HG22 | 1:B:51:ILE:HD13 | 1 | 0.03 | 0.03 |
| (1,2274) | 1:B:31:THR:HG23 | 1:B:51:ILE:HD11 | 1 | 0.03 | 0.03 |
| (1,2274) | 1:B:31:THR:HG23 | 1:B:51:ILE:HD12 | 1 | 0.03 | 0.03 |
| (1,2274) | 1:B:31:THR:HG23 | 1:B:51:ILE:HD13 | 1 | 0.03 | 0.03 |
| (1,2264) | 1:B:28:LYS:HA | 1:B:28:LYS:HE2 | 1 | 0.16 | 0.16 |
| (1,2264) | 1:B:28:LYS:HA | 1:B:28:LYS:HE3 | 1 | 0.16 | 0.16 |
| (1,2263) | 1:A:28:LYS:HA | 1:A:28:LYS:HE2 | 1 | 0.01 | 0.01 |
| (1,2263) | 1:A:28:LYS:HA | 1:A:28:LYS:HE3 | 1 | 0.01 | 0.01 |
| (1,226) | 1:A:18:MET:H | 1:A:18:MET:HG3 | 1 | 0.01 | 0.01 |
| (1,2253) | 1:A:27:SER:HG | 1:A:28:LYS:HG3 | 1 | 0.16 | 0.16 |
| (1,2248) | 1:B:28:LYS:HA | 1:B:28:LYS:HG2 | 1 | 0.23 | 0.23 |
| (1,2237) | 1:A:23:THR:HG21 | 1:A:27:SER:HB3 | 1 | 0.01 | 0.01 |
| (1,2237) | 1:A:23:THR:HG22 | 1:A:27:SER:HB3 | 1 | 0.01 | 0.01 |
| (1,2237) | 1:A:23:THR:HG23 | 1:A:27:SER:HB3 | 1 | 0.01 | 0.01 |
| (1,2233) | 1:A:23:THR:HG21 | 1:A:27:SER:HB2 | 1 | 0.04 | 0.04 |
| (1,2233) | 1:A:23:THR:HG22 | 1:A:27:SER:HB2 | 1 | 0.04 | 0.04 |
| (1,2233) | 1:A:23:THR:HG23 | 1:A:27:SER:HB2 | 1 | 0.04 | 0.04 |
| (1,2229) | 1:A:20:ASN:HD22 | 1:B:27:SER:HA | 1 | 0.02 | 0.02 |
| (1,2186) | 1:B:25:VAL:HG21 | 1:B:29:PHE:HD1 | 1 | 0.02 | 0.02 |
| (1,2186) | 1:B:25:VAL:HG21 | 1:B:29:PHE:HD2 | 1 | 0.02 | 0.02 |
| (1,2186) | 1:B:25:VAL:HG22 | 1:B:29:PHE:HD1 | 1 | 0.02 | 0.02 |
| (1,2186) | 1:B:25:VAL:HG22 | 1:B:29:PHE:HD2 | 1 | 0.02 | 0.02 |
| (1,2186) | 1:B:25:VAL:HG23 | 1:B:29:PHE:HD1 | 1 | 0.02 | 0.02 |
| (1,2186) | 1:B:25:VAL:HG23 | 1:B:29:PHE:HD2 | 1 | 0.02 | 0.02 |
| (1,2185) | 1:A:25:VAL:HG21 | 1:A:29:PHE:HD1 | 1 | 0.03 | 0.03 |
| (1,2185) | 1:A:25:VAL:HG21 | 1:A:29:PHE:HD2 | 1 | 0.03 | 0.03 |
| (1,2185) | 1:A:25:VAL:HG22 | 1:A:29:PHE:HD1 | 1 | 0.03 | 0.03 |
| (1,2185) | 1:A:25:VAL:HG22 | 1:A:29:PHE:HD2 | 1 | 0.03 | 0.03 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,2185) | 1:A:25:VAL:HG23 | 1:A:29:PHE:HD1 | 1 | 0.03 | 0.03 |
| (1,2185) | 1:A:25:VAL:HG23 | 1:A:29:PHE:HD2 | 1 | 0.03 | 0.03 |
| (1,2175) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HE2 | 1 | 0.09 | 0.09 |
| (1,2175) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HE3 | 1 | 0.09 | 0.09 |
| (1,2175) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HE2 | 1 | 0.09 | 0.09 |
| (1,2175) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HE3 | 1 | 0.09 | 0.09 |
| (1,2175) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HE2 | 1 | 0.09 | 0.09 |
| (1,2175) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HE3 | 1 | 0.09 | 0.09 |
| (1,2168) | 1:B:25:VAL:HG11 | 1:B:69:VAL:H | 1 | 0.01 | 0.01 |
| (1,2168) | 1:B:25:VAL:HG12 | 1:B:69:VAL:H | 1 | 0.01 | 0.01 |
| (1,2168) | 1:B:25:VAL:HG13 | 1:B:69:VAL:H | 1 | 0.01 | 0.01 |
| (1,2151) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HD3 | 1 | 0.02 | 0.02 |
| (1,2151) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HD3 | 1 | 0.02 | 0.02 |
| (1,2151) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HD3 | 1 | 0.02 | 0.02 |
| (1,2136) | 1:B:67:ARG:HE | 1:B:75:VAL:HG11 | 1 | 0.09 | 0.09 |
| (1,2136) | 1:B:67:ARG:HE | 1:B:75:VAL:HG12 | 1 | 0.09 | 0.09 |
| (1,2136) | 1:B:67:ARG:HE | 1:B:75:VAL:HG13 | 1 | 0.09 | 0.09 |
| (1,2103) | 1:A:22:ILE:HA | 1:A:22:ILE:HD11 | 1 | 0.01 | 0.01 |
| (1,2103) | 1:A:22:ILE:HA | 1:A:22:ILE:HD12 | 1 | 0.01 | 0.01 |
| (1,2103) | 1:A:22:ILE:HA | 1:A:22:ILE:HD13 | 1 | 0.01 | 0.01 |
| (1,2091) | 1:A:22:ILE:HD11 | 1:A:69:VAL:HG21 | 1 | 0.03 | 0.03 |
| (1,2091) | 1:A:22:ILE:HD11 | 1:A:69:VAL:HG22 | 1 | 0.03 | 0.03 |
| (1,2091) | 1:A:22:ILE:HD11 | 1:A:69:VAL:HG23 | 1 | 0.03 | 0.03 |
| (1,2091) | 1:A:22:ILE:HD12 | 1:A:69:VAL:HG21 | 1 | 0.03 | 0.03 |
| (1,2091) | 1:A:22:ILE:HD12 | 1:A:69:VAL:HG22 | 1 | 0.03 | 0.03 |
| (1,2091) | 1:A:22:ILE:HD12 | 1:A:69:VAL:HG23 | 1 | 0.03 | 0.03 |
| (1,2091) | 1:A:22:ILE:HD13 | 1:A:69:VAL:HG21 | 1 | 0.03 | 0.03 |
| (1,2091) | 1:A:22:ILE:HD13 | 1:A:69:VAL:HG22 | 1 | 0.03 | 0.03 |
| (1,2091) | 1:A:22:ILE:HD13 | 1:A:69:VAL:HG23 | 1 | 0.03 | 0.03 |
| (1,2021) | 1:B:19:THR:HG21 | 1:B:22:ILE:HB | 1 | 0.02 | 0.02 |
| (1,2021) | 1:B:19:THR:HG22 | 1:B:22:ILE:HB | 1 | 0.02 | 0.02 |
| (1,2021) | 1:B:19:THR:HG23 | 1:B:22:ILE:HB | 1 | 0.02 | 0.02 |
| (1,2020) | 1:A:19:THR:HG21 | 1:A:22:ILE:HB | 1 | 0.03 | 0.03 |
| (1,2020) | 1:A:19:THR:HG22 | 1:A:22:ILE:HB | 1 | 0.03 | 0.03 |
| (1,2020) | 1:A:19:THR:HG23 | 1:A:22:ILE:HB | 1 | 0.03 | 0.03 |
| (1,1991) | 1:B:21:GLN:HG2 | 1:B:25:VAL:HG21 | 1 | 0.04 | 0.04 |
| (1,1991) | 1:B:21:GLN:HG2 | 1:B:25:VAL:HG22 | 1 | 0.04 | 0.04 |
| (1,1991) | 1:B:21:GLN:HG2 | 1:B:25:VAL:HG23 | 1 | 0.04 | 0.04 |
| (1,1989) | 1:B:21:GLN:HG2 | 1:B:69:VAL:HG11 | 1 | 0.05 | 0.05 |
| (1,1989) | 1:B:21:GLN:HG2 | 1:B:69:VAL:HG12 | 1 | 0.05 | 0.05 |
| (1,1989) | 1:B:21:GLN:HG2 | 1:B:69:VAL:HG13 | 1 | 0.05 | 0.05 |
| (1,1977) | 1:B:21:GLN:HB3 | 1:B:69:VAL:HG11 | 1 | 0.03 | 0.03 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,1977) | 1:B:21:GLN:HB3 | 1:B:69:VAL:HG12 | 1 | 0.03 | 0.03 |
| (1,1977) | 1:B:21:GLN:HB3 | 1:B:69:VAL:HG13 | 1 | 0.03 | 0.03 |
| (1,1943) | 1:B:18:MET:HE1 | 1:B:70:GLN:H | 1 | 0.01 | 0.01 |
| (1,1943) | 1:B:18:MET:HE2 | 1:B:70:GLN:H | 1 | 0.01 | 0.01 |
| (1,1943) | 1:B:18:MET:HE3 | 1:B:70:GLN:H | 1 | 0.01 | 0.01 |
| (1,1914) | 1:B:17:GLY:H | 1:B:18:MET:HG3 | 1 | 0.01 | 0.01 |
| (1,1899) | 1:A:16:ASN:HA | 1:A:17:GLY:HA3 | 1 | 0.02 | 0.02 |
| (1,1891) | 1:B:15:LYS:HA | 1:B:15:LYS:HE2 | 1 | 0.01 | 0.01 |
| (1,1891) | 1:B:15:LYS:HA | 1:B:15:LYS:HE3 | 1 | 0.01 | 0.01 |
| (1,1882) | 1:A:15:LYS:HG2 | 1:A:15:LYS:HE2 | 1 | 0.02 | 0.02 |
| (1,1882) | 1:A:15:LYS:HG2 | 1:A:15:LYS:HE3 | 1 | 0.02 | 0.02 |
| (1,1882) | 1:A:15:LYS:HG3 | 1:A:15:LYS:HE2 | 1 | 0.02 | 0.02 |
| (1,1882) | 1:A:15:LYS:HG3 | 1:A:15:LYS:HE3 | 1 | 0.02 | 0.02 |
| (1,1862) | 1:A:13:GLU:HB2 | 1:A:15:LYS:HG2 | 1 | 0.07 | 0.07 |
| (1,1862) | 1:A:13:GLU:HB2 | 1:A:15:LYS:HG3 | 1 | 0.07 | 0.07 |
| (1,1859) | 1:B:14:ASP:HA | 1:B:15:LYS:HB3 | 1 | 0.11 | 0.11 |
| (1,1857) | 1:B:15:LYS:HB3 | 1:B:16:ASN:HB2 | 1 | 0.03 | 0.03 |
| (1,1839) | 1:B:13:GLU:HG2 | 1:B:44:ILE:HA | 1 | 0.03 | 0.03 |
| (1,1839) | 1:B:13:GLU:HG3 | 1:B:44:ILE:HA | 1 | 0.03 | 0.03 |
| (1,1838) | 1:A:13:GLU:HG2 | 1:A:44:ILE:HA | 1 | 0.01 | 0.01 |
| (1,1838) | 1:A:13:GLU:HG3 | 1:A:44:ILE:HA | 1 | 0.01 | 0.01 |
| (1,1797) | 1:B:13:GLU:HB3 | 1:B:15:LYS:HG2 | 1 | 0.04 | 0.04 |
| (1,1797) | 1:B:13:GLU:HB3 | 1:B:15:LYS:HG3 | 1 | 0.04 | 0.04 |
| (1,178) | 1:B:15:LYS:H | 1:B:18:MET:HB2 | 1 | 0.01 | 0.01 |
| (1,177) | 1:A:15:LYS:H | 1:A:18:MET:HB3 | 1 | 0.01 | 0.01 |
| (1,1761) | 1:B:11:VAL:HG11 | 1:B:41:LYS:HE2 | 1 | 0.02 | 0.02 |
| (1,1761) | 1:B:11:VAL:HG11 | 1:B:41:LYS:HE3 | 1 | 0.02 | 0.02 |
| (1,1761) | 1:B:11:VAL:HG12 | 1:B:41:LYS:HE2 | 1 | 0.02 | 0.02 |
| (1,1761) | 1:B:11:VAL:HG12 | 1:B:41:LYS:HE3 | 1 | 0.02 | 0.02 |
| (1,1761) | 1:B:11:VAL:HG13 | 1:B:41:LYS:HE2 | 1 | 0.02 | 0.02 |
| (1,1761) | 1:B:11:VAL:HG13 | 1:B:41:LYS:HE3 | 1 | 0.02 | 0.02 |
| (1,1745) | 1:B:11:VAL:HG21 | 1:B:46:THR:HB | 1 | 0.05 | 0.05 |
| (1,1745) | 1:B:11:VAL:HG22 | 1:B:46:THR:HB | 1 | 0.05 | 0.05 |
| (1,1745) | 1:B:11:VAL:HG23 | 1:B:46:THR:HB | 1 | 0.05 | 0.05 |
| (1,1731) | 1:B:10:ILE:HD11 | 1:B:49:LEU:H | 1 | 0.01 | 0.01 |
| (1,1731) | 1:B:10:ILE:HD12 | 1:B:49:LEU:H | 1 | 0.01 | 0.01 |
| (1,1731) | 1:B:10:ILE:HD13 | 1:B:49:LEU:H | 1 | 0.01 | 0.01 |
| (1,1730) | 1:A:10:ILE:HD11 | 1:A:49:LEU:H | 1 | 0.01 | 0.01 |
| (1,1730) | 1:A:10:ILE:HD12 | 1:A:49:LEU:H | 1 | 0.01 | 0.01 |
| (1,1730) | 1:A:10:ILE:HD13 | 1:A:49:LEU:H | 1 | 0.01 | 0.01 |
| (1,1721) | 1:B:10:ILE:HD11 | 1:B:11:VAL:H | 1 | 0.01 | 0.01 |
| (1,1721) | 1:B:10:ILE:HD12 | 1:B:11:VAL:H | 1 | 0.01 | 0.01 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,1721) | 1:B:10:ILE:HD13 | 1:B:11:VAL:H | 1 | 0.01 | 0.01 |
| (1,1720) | 1:A:10:ILE:HD11 | 1:A:11:VAL:H | 1 | 0.03 | 0.03 |
| (1,1720) | 1:A:10:ILE:HD12 | 1:A:11:VAL:H | 1 | 0.03 | 0.03 |
| (1,1720) | 1:A:10:ILE:HD13 | 1:A:11:VAL:H | 1 | 0.03 | 0.03 |
| (1,1685) | 1:B:9:ARG:HA | 1:B:10:ILE:HG21 | 1 | 0.02 | 0.02 |
| (1,1685) | 1:B:9:ARG:HA | 1:B:10:ILE:HG22 | 1 | 0.02 | 0.02 |
| (1,1685) | 1:B:9:ARG:HA | 1:B:10:ILE:HG23 | 1 | 0.02 | 0.02 |
| (1,165) | 1:B:13:GLU:H | 1:B:73:PHE:H | 1 | 0.05 | 0.05 |
| (1,164) | 1:A:13:GLU:H | 1:A:73:PHE:H | 1 | 0.01 | 0.01 |
| (1,1633) | 1:B:9:ARG:HD2 | 1:B:76:GLU:HG2 | 1 | 0.05 | 0.05 |
| (1,1633) | 1:B:9:ARG:HD2 | 1:B:76:GLU:HG3 | 1 | 0.05 | 0.05 |
| (1,1633) | 1:B:9:ARG:HD3 | 1:B:76:GLU:HG2 | 1 | 0.05 | 0.05 |
| (1,1633) | 1:B:9:ARG:HD3 | 1:B:76:GLU:HG3 | 1 | 0.05 | 0.05 |
| (1,1629) | 1:A:9:ARG:HD2 | 1:A:76:GLU:HB2 | 1 | 0.04 | 0.04 |
| (1,1629) | 1:A:9:ARG:HD3 | 1:A:76:GLU:HB2 | 1 | 0.04 | 0.04 |
| (1,1604) | 1:B:23:THR:HA | 1:B:26:ILE:HD11 | 1 | 0.01 | 0.01 |
| (1,1604) | 1:B:23:THR:HA | 1:B:26:ILE:HD12 | 1 | 0.01 | 0.01 |
| (1,1604) | 1:B:23:THR:HA | 1:B:26:ILE:HD13 | 1 | 0.01 | 0.01 |
| (1,1569) | 1:A:8:ILE:HG21 | 1:A:63:MET:HG3 | 1 | 0.02 | 0.02 |
| (1,1569) | 1:A:8:ILE:HG22 | 1:A:63:MET:HG3 | 1 | 0.02 | 0.02 |
| (1,1569) | 1:A:8:ILE:HG23 | 1:A:63:MET:HG3 | 1 | 0.02 | 0.02 |
| (1,155) | 1:B:13:GLU:H | 1:B:44:ILE:HA | 1 | 0.01 | 0.01 |
| (1,1525) | 1:A:5:LEU:HD21 | 1:A:51:ILE:HA | 1 | 0.01 | 0.01 |
| (1,1525) | 1:A:5:LEU:HD22 | 1:A:51:ILE:HA | 1 | 0.01 | 0.01 |
| (1,1525) | 1:A:5:LEU:HD23 | 1:A:51:ILE:HA | 1 | 0.01 | 0.01 |
| (1,148) | 1:A:13:GLU:H | 1:A:13:GLU:HG2 | 1 | 0.01 | 0.01 |
| (1,148) | 1:A:13:GLU:H | 1:A:13:GLU:HG3 | 1 | 0.01 | 0.01 |
| (1,1430) | 1:B:45:PHE:H | 1:B:45:PHE:HE1 | 1 | 0.05 | 0.05 |
| (1,1400) | 1:B:81:LEU:HA | 1:B:82:GLU:H | 1 | 0.05 | 0.05 |
| (1,1398) | 1:B:82:GLU:H | 1:B:82:GLU:HG2 | 1 | 0.03 | 0.03 |
| (1,1394) | 1:B:81:LEU:HB3 | 1:B:82:GLU:H | 1 | 0.01 | 0.01 |
| (1,1381) | 1:A:81:LEU:H | 1:A:81:LEU:HD11 | 1 | 0.02 | 0.02 |
| (1,1381) | 1:A:81:LEU:H | 1:A:81:LEU:HD12 | 1 | 0.02 | 0.02 |
| (1,1381) | 1:A:81:LEU:H | 1:A:81:LEU:HD13 | 1 | 0.02 | 0.02 |
| (1,1347) | 1:A:77:ARG:H | 1:A:77:ARG:HD2 | 1 | 0.04 | 0.04 |
| (1,1347) | 1:A:77:ARG:H | 1:A:77:ARG:HD3 | 1 | 0.04 | 0.04 |
| (1,13) | 1:A:4:PHE:H | 1:A:54:LYS:HA | 1 | 0.05 | 0.05 |
| (1,1299) | 1:A:74:THR:HG21 | 1:A:75:VAL:H | 1 | 0.01 | 0.01 |
| (1,1299) | 1:A:74:THR:HG22 | 1:A:75:VAL:H | 1 | 0.01 | 0.01 |
| (1,1299) | 1:A:74:THR:HG23 | 1:A:75:VAL:H | 1 | 0.01 | 0.01 |
| (1,1277) | 1:A:74:THR:H | 1:A:75:VAL:HG21 | 1 | 0.03 | 0.03 |
| (1,1277) | 1:A:74:THR:H | 1:A:75:VAL:HG22 | 1 | 0.03 | 0.03 |

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| Key | Atom-1 | Atom-2 | Models | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| (1,1277) | 1:A:74:THR:H | 1:A:75:VAL:HG23 | 1 | 0.03 | 0.03 |
| (1,1254) | 1:B:69:VAL:HG21 | 1:B:72:VAL:H | 1 | 0.03 | 0.03 |
| (1,1254) | 1:B:69:VAL:HG22 | 1:B:72:VAL:H | 1 | 0.03 | 0.03 |
| (1,1254) | 1:B:69:VAL:HG23 | 1:B:72:VAL:H | 1 | 0.03 | 0.03 |
| (1,1182) | 1:B:67:ARG:HE | 1:B:75:VAL:H | 1 | 0.1 | 0.1 |
| (1,1165) | 1:A:67:ARG:H | 1:A:67:ARG:HE | 1 | 0.01 | 0.01 |
| (1,1160) | 1:B:67:ARG:H | 1:B:67:ARG:HD2 | 1 | 0.08 | 0.08 |
| (1,1160) | 1:B:67:ARG:H | 1:B:67:ARG:HD3 | 1 | 0.08 | 0.08 |
| (1,1149) | 1:A:67:ARG:H | 1:A:69:VAL:HG21 | 1 | 0.02 | 0.02 |
| (1,1149) | 1:A:67:ARG:H | 1:A:69:VAL:HG22 | 1 | 0.02 | 0.02 |
| (1,1149) | 1:A:67:ARG:H | 1:A:69:VAL:HG23 | 1 | 0.02 | 0.02 |
| (1,1115) | 1:A:64:ASP:HB2 | 1:A:65:LYS:H | 1 | 0.04 | 0.04 |

## 8.8 All distance violations

### 8.8.1 Histogram : Distribution of distance violations

The following histogram shows the distribution of violations in the ensemble.
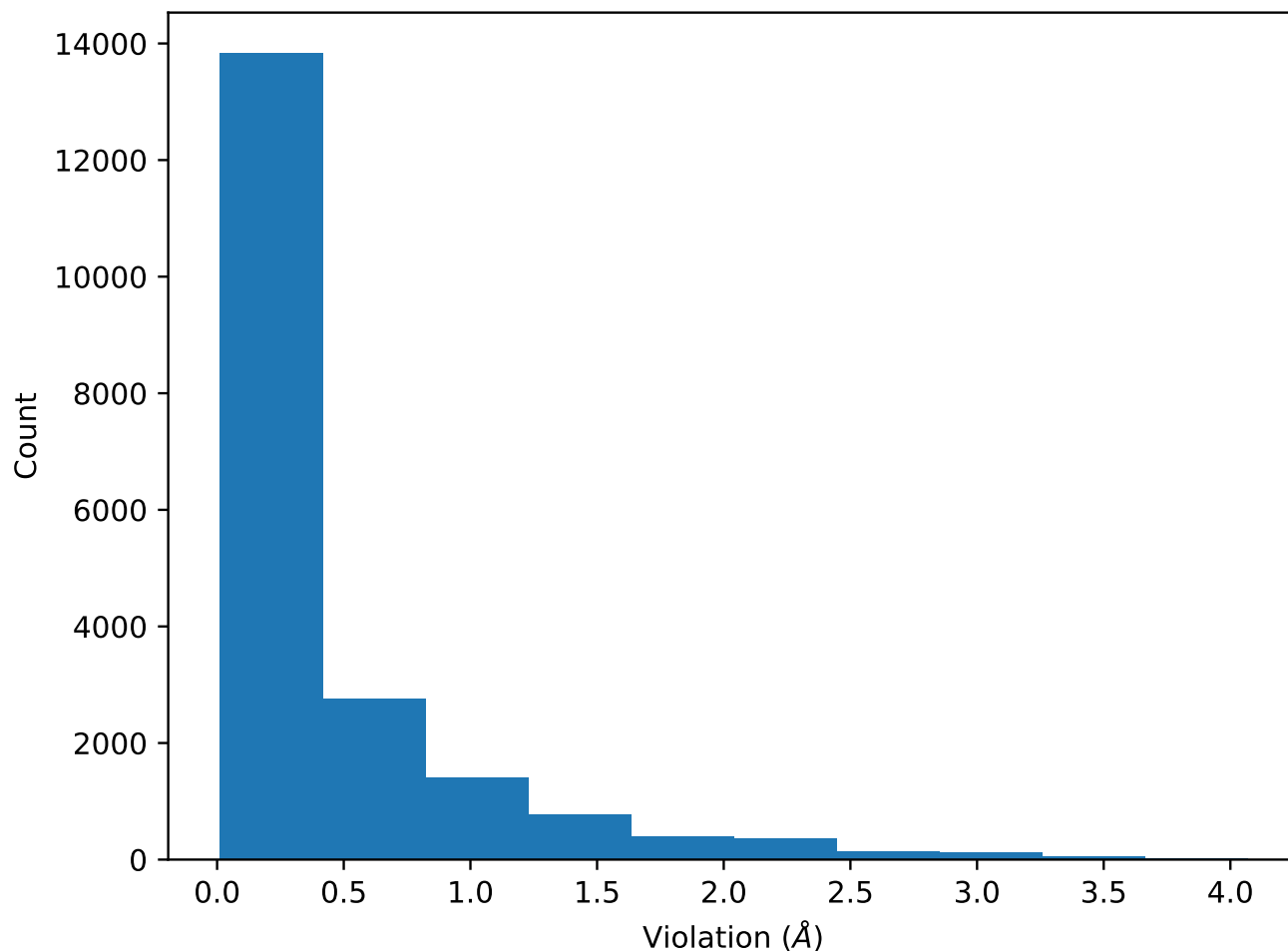


### 8.8.2 Table : All distance violations

The following table lists the violations in the ensemble sorted by violation value

| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 8 | 4.07 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 19 | 4.06 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 5 | 4.05 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 2 | 3.98 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 7 | 3.97 |
| (1,4370) | 1:A:4:PHE:HE1 | 1:A:55:ASN:HA | 15 | 3.95 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 10 | 3.9 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 9 | 3.89 |
| (1,4370) | 1:A:4:PHE:HE1 | 1:A:55:ASN:HA | 1 | 3.88 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 13 | 3.87 |
| (1,4371) | 1:B:4:PHE:HE1 | 1:B:55:ASN:HA | 12 | 3.87 |
| (1,4370) | 1:A:4:PHE:HE1 | 1:A:55:ASN:HA | 3 | 3.85 |
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 6 | 3.78 |
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 11 | 3.78 |
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 10 | 3.75 |
| (1,4370) | 1:A:4:PHE:HE1 | 1:A:55:ASN:HA | 10 | 3.75 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 12 | 3.73 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 17 | 3.73 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 15 | 3.72 |
| (1,4371) | 1:B:4:PHE:HE1 | 1:B:55:ASN:HA | 2 | 3.72 |
| (1,4370) | 1:A:4:PHE:HE1 | 1:A:55:ASN:HA | 9 | 3.71 |
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 7 | 3.7 |
| (1,4379) | 1:B:4:PHE:HE1 | 1:B:7:GLY:H | 7 | 3.7 |
| (1,4379) | 1:B:4:PHE:HE1 | 1:B:7:GLY:H | 9 | 3.7 |
| (1,4370) | 1:A:4:PHE:HE1 | 1:A:55:ASN:HA | 6 | 3.7 |
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 8 | 3.69 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 18 | 3.68 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 20 | 3.66 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 1 | 3.65 |
| (1,4370) | 1:A:4:PHE:HE1 | 1:A:55:ASN:HA | 2 | 3.65 |
| (1,4379) | 1:B:4:PHE:HE1 | 1:B:7:GLY:H | 8 | 3.64 |
| (1,4371) | 1:B:4:PHE:HE1 | 1:B:55:ASN:HA | 10 | 3.64 |
| (1,4378) | 1:A:4:PHE:HE1 | 1:A:7:GLY:H | 7 | 3.63 |
| (1,4379) | 1:B:4:PHE:HE1 | 1:B:7:GLY:H | 18 | 3.62 |
| (1,4378) | 1:A:4:PHE:HE1 | 1:A:7:GLY:H | 13 | 3.6 |
| (1,4371) | 1:B:4:PHE:HE1 | 1:B:55:ASN:HA | 3 | 3.6 |
| (1,4378) | 1:A:4:PHE:HE1 | 1:A:7:GLY:H | 14 | 3.59 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 16 | 3.56 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 3 | 3.55 |
| (1,4378) | 1:A:4:PHE:HE1 | 1:A:7:GLY:H | 12 | 3.54 |
| (1,4370) | 1:A:4:PHE:HE1 | 1:A:55:ASN:HA | 8 | 3.54 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 13 | 3.53 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 2 | 3.52 |
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 5 | 3.52 |
| (1,4379) | 1:B:4:PHE:HE1 | 1:B:7:GLY:H | 5 | 3.51 |
| (1,4370) | 1:A:4:PHE:HE1 | 1:A:55:ASN:HA | 17 | 3.51 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 19 | 3.48 |
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 3 | 3.48 |
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 13 | 3.45 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4371) | 1:B:4:PHE:HE1 | 1:B:55:ASN:HA | 14 | 3.44 |
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 17 | 3.42 |
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 16 | 3.4 |
| (1,4490) | 1:B:18:MET:HB2 | 1:B:45:PHE:HE1 | 5 | 3.4 |
| (1,1663) | 1:B:10:ILE:HG13 | 1:B:45:PHE:HE1 | 9 | 3.4 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 3 | 3.39 |
| (1,4371) | 1:B:4:PHE:HE1 | 1:B:55:ASN:HA | 17 | 3.38 |
| (1,4371) | 1:B:4:PHE:HE1 | 1:B:55:ASN:HA | 20 | 3.38 |
| (1,4490) | 1:B:18:MET:HB2 | 1:B:45:PHE:HE1 | 8 | 3.35 |
| (1,1819) | 1:B:13:GLU:HB2 | 1:B:73:PHE:HE1 | 8 | 3.35 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 15 | 3.34 |
| (1,1818) | 1:A:13:GLU:HB2 | 1:A:73:PHE:HE1 | 20 | 3.33 |
| (1,1663) | 1:B:10:ILE:HG13 | 1:B:45:PHE:HE1 | 6 | 3.33 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 11 | 3.32 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 11 | 3.32 |
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 2 | 3.31 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 12 | 3.31 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 12 | 3.31 |
| (1,1818) | 1:A:13:GLU:HB2 | 1:A:73:PHE:HE1 | 9 | 3.31 |
| (1,1818) | 1:A:13:GLU:HB2 | 1:A:73:PHE:HE1 | 17 | 3.31 |
| (1,1662) | 1:A:10:ILE:HG13 | 1:A:45:PHE:HE1 | 1 | 3.31 |
| (1,1662) | 1:A:10:ILE:HG13 | 1:A:45:PHE:HE1 | 12 | 3.31 |
| (1,1663) | 1:B:10:ILE:HG13 | 1:B:45:PHE:HE1 | 16 | 3.29 |
| (1,1662) | 1:A:10:ILE:HG13 | 1:A:45:PHE:HE1 | 19 | 3.29 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 10 | 3.28 |
| (1,1818) | 1:A:13:GLU:HB2 | 1:A:73:PHE:HE1 | 7 | 3.28 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 12 | 3.27 |
| (1,1662) | 1:A:10:ILE:HG13 | 1:A:45:PHE:HE1 | 4 | 3.27 |
| (1,1819) | 1:B:13:GLU:HB2 | 1:B:73:PHE:HE1 | 5 | 3.25 |
| (1,4577) | 1:A:13:GLU:HG2 | 1:A:73:PHE:HE1 | 18 | 3.23 |
| (1,4577) | 1:A:13:GLU:HG3 | 1:A:73:PHE:HE1 | 18 | 3.23 |
| (1,4370) | 1:A:4:PHE:HE1 | 1:A:55:ASN:HA | 5 | 3.23 |
| (1,1819) | 1:B:13:GLU:HB2 | 1:B:73:PHE:HE1 | 16 | 3.23 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 17 | 3.22 |
| (1,4578) | 1:B:13:GLU:HG2 | 1:B:73:PHE:HE1 | 1 | 3.22 |
| (1,4578) | 1:B:13:GLU:HG3 | 1:B:73:PHE:HE1 | 1 | 3.22 |
| (1,4578) | 1:B:13:GLU:HG2 | 1:B:73:PHE:HE1 | 10 | 3.21 |
| (1,4578) | 1:B:13:GLU:HG3 | 1:B:73:PHE:HE1 | 10 | 3.21 |
| (1,4490) | 1:B:18:MET:HB2 | 1:B:45:PHE:HE1 | 7 | 3.21 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 4 | 3.2 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 11 | 3.2 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 2 | 3.2 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4577) | 1:A:13:GLU:HG2 | 1:A:73:PHE:HE1 | 2 | 3.19 |
| (1,4577) | 1:A:13:GLU:HG3 | 1:A:73:PHE:HE1 | 2 | 3.19 |
| (1,1819) | 1:B:13:GLU:HB2 | 1:B:73:PHE:HE1 | 18 | 3.19 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 7 | 3.18 |
| (1,4577) | 1:A:13:GLU:HG2 | 1:A:73:PHE:HE1 | 3 | 3.18 |
| (1,4577) | 1:A:13:GLU:HG3 | 1:A:73:PHE:HE1 | 3 | 3.18 |
| (1,4552) | 1:B:4:PHE:HA | 1:B:52:PHE:HE1 | 12 | 3.18 |
| (1,4371) | 1:B:4:PHE:HE1 | 1:B:55:ASN:HA | 13 | 3.18 |
| (1,1819) | 1:B:13:GLU:HB2 | 1:B:73:PHE:HE1 | 3 | 3.18 |
| (1,1818) | 1:A:13:GLU:HB2 | 1:A:73:PHE:HE1 | 6 | 3.18 |
| (1,1818) | 1:A:13:GLU:HB2 | 1:A:73:PHE:HE1 | 8 | 3.18 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 19 | 3.17 |
| (1,4578) | 1:B:13:GLU:HG2 | 1:B:73:PHE:HE1 | 2 | 3.17 |
| (1,4578) | 1:B:13:GLU:HG3 | 1:B:73:PHE:HE1 | 2 | 3.17 |
| (1,4578) | 1:B:13:GLU:HG2 | 1:B:73:PHE:HE1 | 12 | 3.17 |
| (1,4578) | 1:B:13:GLU:HG3 | 1:B:73:PHE:HE1 | 12 | 3.17 |
| (1,4370) | 1:A:4:PHE:HE1 | 1:A:55:ASN:HA | 4 | 3.17 |
| (1,1818) | 1:A:13:GLU:HB2 | 1:A:73:PHE:HE1 | 16 | 3.17 |
| (1,1818) | 1:A:13:GLU:HB2 | 1:A:73:PHE:HE1 | 18 | 3.17 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 5 | 3.16 |
| (1,1818) | 1:A:13:GLU:HB2 | 1:A:73:PHE:HE1 | 12 | 3.16 |
| (1,1818) | 1:A:13:GLU:HB2 | 1:A:73:PHE:HE1 | 19 | 3.16 |
| (1,1663) | 1:B:10:ILE:HG13 | 1:B:45:PHE:HE1 | 17 | 3.16 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 5 | 3.15 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 14 | 3.15 |
| (1,4577) | 1:A:13:GLU:HG2 | 1:A:73:PHE:HE1 | 8 | 3.15 |
| (1,4577) | 1:A:13:GLU:HG3 | 1:A:73:PHE:HE1 | 8 | 3.15 |
| (1,4577) | 1:A:13:GLU:HG2 | 1:A:73:PHE:HE1 | 16 | 3.15 |
| (1,4577) | 1:A:13:GLU:HG3 | 1:A:73:PHE:HE1 | 16 | 3.15 |
| (1,1818) | 1:A:13:GLU:HB2 | 1:A:73:PHE:HE1 | 2 | 3.15 |
| (1,1818) | 1:A:13:GLU:HB2 | 1:A:73:PHE:HE1 | 14 | 3.15 |
| (1,4370) | 1:A:4:PHE:HE1 | 1:A:55:ASN:HA | 11 | 3.14 |
| (1,1819) | 1:B:13:GLU:HB2 | 1:B:73:PHE:HE1 | 9 | 3.14 |
| (1,1819) | 1:B:13:GLU:HB2 | 1:B:73:PHE:HE1 | 10 | 3.14 |
| (1,1819) | 1:B:13:GLU:HB2 | 1:B:73:PHE:HE1 | 12 | 3.14 |
| (1,4578) | 1:B:13:GLU:HG2 | 1:B:73:PHE:HE1 | 18 | 3.12 |
| (1,4578) | 1:B:13:GLU:HG3 | 1:B:73:PHE:HE1 | 18 | 3.12 |
| (1,4577) | 1:A:13:GLU:HG2 | 1:A:73:PHE:HE1 | 6 | 3.11 |
| (1,4577) | 1:A:13:GLU:HG3 | 1:A:73:PHE:HE1 | 6 | 3.11 |
| (1,1662) | 1:A:10:ILE:HG13 | 1:A:45:PHE:HE1 | 18 | 3.11 |
| (1,1818) | 1:A:13:GLU:HB2 | 1:A:73:PHE:HE1 | 3 | 3.1 |
| (1,4577) | 1:A:13:GLU:HG2 | 1:A:73:PHE:HE1 | 17 | 3.09 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4577) | 1:A:13:GLU:HG3 | 1:A:73:PHE:HE1 | 17 | 3.09 |
| (1,4577) | 1:A:13:GLU:HG2 | 1:A:73:PHE:HE1 | 19 | 3.09 |
| (1,4577) | 1:A:13:GLU:HG3 | 1:A:73:PHE:HE1 | 19 | 3.09 |
| (1,4371) | 1:B:4:PHE:HE1 | 1:B:55:ASN:HA | 1 | 3.09 |
| (1,4577) | 1:A:13:GLU:HG2 | 1:A:73:PHE:HE1 | 14 | 3.08 |
| (1,4577) | 1:A:13:GLU:HG3 | 1:A:73:PHE:HE1 | 14 | 3.08 |
| (1,4578) | 1:B:13:GLU:HG2 | 1:B:73:PHE:HE1 | 7 | 3.07 |
| (1,4578) | 1:B:13:GLU:HG3 | 1:B:73:PHE:HE1 | 7 | 3.07 |
| (1,4577) | 1:A:13:GLU:HG2 | 1:A:73:PHE:HE1 | 9 | 3.07 |
| (1,4577) | 1:A:13:GLU:HG3 | 1:A:73:PHE:HE1 | 9 | 3.07 |
| (1,4371) | 1:B:4:PHE:HE1 | 1:B:55:ASN:HA | 15 | 3.07 |
| (1,1662) | 1:A:10:ILE:HG13 | 1:A:45:PHE:HE1 | 15 | 3.07 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 13 | 3.06 |
| (1,4578) | 1:B:13:GLU:HG2 | 1:B:73:PHE:HE1 | 3 | 3.06 |
| (1,4578) | 1:B:13:GLU:HG3 | 1:B:73:PHE:HE1 | 3 | 3.06 |
| (1,4577) | 1:A:13:GLU:HG2 | 1:A:73:PHE:HE1 | 12 | 3.06 |
| (1,4577) | 1:A:13:GLU:HG3 | 1:A:73:PHE:HE1 | 12 | 3.06 |
| (1,4578) | 1:B:13:GLU:HG2 | 1:B:73:PHE:HE1 | 8 | 3.05 |
| (1,4578) | 1:B:13:GLU:HG3 | 1:B:73:PHE:HE1 | 8 | 3.05 |
| (1,4486) | 1:B:10:ILE:HB | 1:B:45:PHE:HE1 | 9 | 3.05 |
| (1,1819) | 1:B:13:GLU:HB2 | 1:B:73:PHE:HE1 | 1 | 3.05 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 18 | 3.04 |
| (1,1819) | 1:B:13:GLU:HB2 | 1:B:73:PHE:HE1 | 7 | 3.04 |
| (1,1409) | 1:A:15:LYS:H | 1:A:45:PHE:HE1 | 17 | 3.04 |
| (1,4370) | 1:A:4:PHE:HE1 | 1:A:55:ASN:HA | 18 | 3.03 |
| (1,1819) | 1:B:13:GLU:HB2 | 1:B:73:PHE:HE1 | 2 | 3.03 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 1 | 3.02 |
| (1,4552) | 1:B:4:PHE:HA | 1:B:52:PHE:HE1 | 11 | 3.02 |
| (1,4486) | 1:B:10:ILE:HB | 1:B:45:PHE:HE1 | 6 | 3.02 |
| (1,4485) | 1:A:10:ILE:HB | 1:A:45:PHE:HE1 | 1 | 3.02 |
| (1,4371) | 1:B:4:PHE:HE1 | 1:B:55:ASN:HA | 19 | 3.0 |
| (1,1663) | 1:B:10:ILE:HG13 | 1:B:45:PHE:HE1 | 4 | 3.0 |
| (1,4490) | 1:B:18:MET:HB2 | 1:B:45:PHE:HE1 | 10 | 2.99 |
| (1,4577) | 1:A:13:GLU:HG2 | 1:A:73:PHE:HE1 | 20 | 2.98 |
| (1,4577) | 1:A:13:GLU:HG3 | 1:A:73:PHE:HE1 | 20 | 2.98 |
| (1,4486) | 1:B:10:ILE:HB | 1:B:45:PHE:HE1 | 16 | 2.98 |
| (1,1409) | 1:A:15:LYS:H | 1:A:45:PHE:HE1 | 6 | 2.98 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 16 | 2.97 |
| (1,4578) | 1:B:13:GLU:HG2 | 1:B:73:PHE:HE1 | 16 | 2.97 |
| (1,4578) | 1:B:13:GLU:HG3 | 1:B:73:PHE:HE1 | 16 | 2.97 |
| (1,4485) | 1:A:10:ILE:HB | 1:A:45:PHE:HE1 | 19 | 2.97 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 8 | 2.96 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4578) | 1:B:13:GLU:HG2 | 1:B:73:PHE:HE1 | 5 | 2.96 |
| (1,4578) | 1:B:13:GLU:HG3 | 1:B:73:PHE:HE1 | 5 | 2.96 |
| (1,4487) | 1:A:18:MET:HB2 | 1:A:45:PHE:HE1 | 9 | 2.96 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 14 | 2.95 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 8 | 2.95 |
| (1,4370) | 1:A:4:PHE:HE1 | 1:A:55:ASN:HA | 16 | 2.95 |
| (1,4485) | 1:A:10:ILE:HB | 1:A:45:PHE:HE1 | 12 | 2.94 |
| (1,4371) | 1:B:4:PHE:HE1 | 1:B:55:ASN:HA | 4 | 2.93 |
| (1,4487) | 1:A:18:MET:HB2 | 1:A:45:PHE:HE1 | 6 | 2.92 |
| (1,4371) | 1:B:4:PHE:HE1 | 1:B:55:ASN:HA | 16 | 2.92 |
| (1,4578) | 1:B:13:GLU:HG2 | 1:B:73:PHE:HE1 | 9 | 2.91 |
| (1,4578) | 1:B:13:GLU:HG3 | 1:B:73:PHE:HE1 | 9 | 2.91 |
| (1,4490) | 1:B:18:MET:HB2 | 1:B:45:PHE:HE1 | 13 | 2.91 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 2 | 2.9 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 11 | 2.9 |
| (1,4490) | 1:B:18:MET:HB2 | 1:B:45:PHE:HE1 | 2 | 2.9 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 12 | 2.89 |
| (1,4577) | 1:A:13:GLU:HG2 | 1:A:73:PHE:HE1 | 7 | 2.87 |
| (1,4577) | 1:A:13:GLU:HG3 | 1:A:73:PHE:HE1 | 7 | 2.87 |
| (1,4485) | 1:A:10:ILE:HB | 1:A:45:PHE:HE1 | 4 | 2.87 |
| (1,4486) | 1:B:10:ILE:HB | 1:B:45:PHE:HE1 | 17 | 2.86 |
| (1,4370) | 1:A:4:PHE:HE1 | 1:A:55:ASN:HA | 20 | 2.86 |
| (1,4498) | 1:B:13:GLU:H | 1:B:45:PHE:HE1 | 2 | 2.85 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 9 | 2.83 |
| (1,4487) | 1:A:18:MET:HB2 | 1:A:45:PHE:HE1 | 7 | 2.82 |
| (1,4485) | 1:A:10:ILE:HB | 1:A:45:PHE:HE1 | 18 | 2.8 |
| (1,1409) | 1:A:15:LYS:H | 1:A:45:PHE:HE1 | 2 | 2.8 |
| (1,4497) | 1:A:13:GLU:H | 1:A:45:PHE:HE1 | 20 | 2.79 |
| (1,4487) | 1:A:18:MET:HB2 | 1:A:45:PHE:HE1 | 8 | 2.79 |
| (1,4487) | 1:A:18:MET:HB2 | 1:A:45:PHE:HE1 | 11 | 2.79 |
| (1,1409) | 1:A:15:LYS:H | 1:A:45:PHE:HE1 | 16 | 2.79 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 13 | 2.78 |
| (1,4371) | 1:B:4:PHE:HE1 | 1:B:55:ASN:HA | 11 | 2.78 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 20 | 2.77 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 20 | 2.77 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 20 | 2.77 |
| (1,4490) | 1:B:18:MET:HB2 | 1:B:45:PHE:HE1 | 3 | 2.77 |
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 20 | 2.76 |
| (1,4490) | 1:B:18:MET:HB2 | 1:B:45:PHE:HE1 | 12 | 2.75 |
| (1,4498) | 1:B:13:GLU:H | 1:B:45:PHE:HE1 | 7 | 2.73 |
| (1,4497) | 1:A:13:GLU:H | 1:A:45:PHE:HE1 | 2 | 2.72 |
| (1,4490) | 1:B:18:MET:HB2 | 1:B:45:PHE:HE1 | 18 | 2.72 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4487) | 1:A:18:MET:HB2 | 1:A:45:PHE:HE1 | 17 | 2.72 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD21 | 18 | 2.72 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD22 | 18 | 2.72 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD23 | 18 | 2.72 |
| (1,4370) | 1:A:4:PHE:HE1 | 1:A:55:ASN:HA | 19 | 2.71 |
| (1,4490) | 1:B:18:MET:HB2 | 1:B:45:PHE:HE1 | 19 | 2.7 |
| (1,4486) | 1:B:10:ILE:HB | 1:B:45:PHE:HE1 | 4 | 2.7 |
| (1,4485) | 1:A:10:ILE:HB | 1:A:45:PHE:HE1 | 15 | 2.7 |
| (1,4371) | 1:B:4:PHE:HE1 | 1:B:55:ASN:HA | 6 | 2.7 |
| (1,4490) | 1:B:18:MET:HB2 | 1:B:45:PHE:HE1 | 20 | 2.69 |
| (1,4487) | 1:A:18:MET:HB2 | 1:A:45:PHE:HE1 | 10 | 2.68 |
| (1,1410) | 1:B:15:LYS:H | 1:B:45:PHE:HE1 | 2 | 2.66 |
| (1,1410) | 1:B:15:LYS:H | 1:B:45:PHE:HE1 | 5 | 2.66 |
| (1,1409) | 1:A:15:LYS:H | 1:A:45:PHE:HE1 | 13 | 2.66 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 6 | 2.65 |
| (1,1410) | 1:B:15:LYS:H | 1:B:45:PHE:HE1 | 8 | 2.63 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 14 | 2.62 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 8 | 2.61 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 8 | 2.61 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 8 | 2.61 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 16 | 2.61 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 16 | 2.61 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 16 | 2.61 |
| (1,4487) | 1:A:18:MET:HB2 | 1:A:45:PHE:HE1 | 2 | 2.61 |
| (1,1715) | 1:B:10:ILE:HD11 | 1:B:45:PHE:HE1 | 9 | 2.6 |
| (1,1715) | 1:B:10:ILE:HD12 | 1:B:45:PHE:HE1 | 9 | 2.6 |
| (1,1715) | 1:B:10:ILE:HD13 | 1:B:45:PHE:HE1 | 9 | 2.6 |
| (1,4491) | 1:A:45:PHE:HE1 | 1:A:47:CYS:HB2 | 14 | 2.59 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD21 | 7 | 2.59 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD22 | 7 | 2.59 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD23 | 7 | 2.59 |
| (1,1662) | 1:A:10:ILE:HG13 | 1:A:45:PHE:HE1 | 14 | 2.59 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 2 | 2.58 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 2 | 2.58 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 2 | 2.58 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 6 | 2.56 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 6 | 2.56 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 6 | 2.56 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 8 | 2.56 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 8 | 2.56 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 8 | 2.56 |
| (1,4490) | 1:B:18:MET:HB2 | 1:B:45:PHE:HE1 | 1 | 2.55 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4487) | 1:A:18:MET:HB2 | 1:A:45:PHE:HE1 | 3 | 2.55 |
| (1,1714) | 1:A:10:ILE:HD11 | 1:A:45:PHE:HE1 | 12 | 2.55 |
| (1,1714) | 1:A:10:ILE:HD12 | 1:A:45:PHE:HE1 | 12 | 2.55 |
| (1,1714) | 1:A:10:ILE:HD13 | 1:A:45:PHE:HE1 | 12 | 2.55 |
| (1,1410) | 1:B:15:LYS:H | 1:B:45:PHE:HE1 | 7 | 2.55 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD21 | 5 | 2.53 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD22 | 5 | 2.53 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD23 | 5 | 2.53 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 3 | 2.52 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 3 | 2.52 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 3 | 2.52 |
| (1,4497) | 1:A:13:GLU:H | 1:A:45:PHE:HE1 | 17 | 2.52 |
| (1,4490) | 1:B:18:MET:HB2 | 1:B:45:PHE:HE1 | 14 | 2.52 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 12 | 2.51 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 12 | 2.51 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 12 | 2.51 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 1 | 2.5 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 1 | 2.5 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 1 | 2.5 |
| (1,1715) | 1:B:10:ILE:HD11 | 1:B:45:PHE:HE1 | 16 | 2.5 |
| (1,1715) | 1:B:10:ILE:HD12 | 1:B:45:PHE:HE1 | 16 | 2.5 |
| (1,1715) | 1:B:10:ILE:HD13 | 1:B:45:PHE:HE1 | 16 | 2.5 |
| (1,1714) | 1:A:10:ILE:HD11 | 1:A:45:PHE:HE1 | 19 | 2.5 |
| (1,1714) | 1:A:10:ILE:HD12 | 1:A:45:PHE:HE1 | 19 | 2.5 |
| (1,1714) | 1:A:10:ILE:HD13 | 1:A:45:PHE:HE1 | 19 | 2.5 |
| (1,1410) | 1:B:15:LYS:H | 1:B:45:PHE:HE1 | 20 | 2.5 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 16 | 2.49 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 9 | 2.49 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 9 | 2.49 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 9 | 2.49 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 14 | 2.49 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 14 | 2.49 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 14 | 2.49 |
| (1,4498) | 1:B:13:GLU:H | 1:B:45:PHE:HE1 | 14 | 2.49 |
| (1,1409) | 1:A:15:LYS:H | 1:A:45:PHE:HE1 | 11 | 2.49 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 5 | 2.48 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 5 | 2.48 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 5 | 2.48 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 10 | 2.48 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 10 | 2.48 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 10 | 2.48 |
| (1,4498) | 1:B:13:GLU:H | 1:B:45:PHE:HE1 | 3 | 2.48 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1715) | 1:B:10:ILE:HD11 | 1:B:45:PHE:HE1 | 6 | 2.48 |
| (1,1715) | 1:B:10:ILE:HD12 | 1:B:45:PHE:HE1 | 6 | 2.48 |
| (1,1715) | 1:B:10:ILE:HD13 | 1:B:45:PHE:HE1 | 6 | 2.48 |
| (1,1410) | 1:B:15:LYS:H | 1:B:45:PHE:HE1 | 10 | 2.48 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 7 | 2.47 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 7 | 2.47 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 7 | 2.47 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 11 | 2.47 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 11 | 2.47 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 11 | 2.47 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 12 | 2.47 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 12 | 2.47 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 12 | 2.47 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 15 | 2.47 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 15 | 2.47 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 15 | 2.47 |
| (1,4498) | 1:B:13:GLU:H | 1:B:45:PHE:HE1 | 12 | 2.47 |
| (1,4497) | 1:A:13:GLU:H | 1:A:45:PHE:HE1 | 16 | 2.47 |
| (1,1714) | 1:A:10:ILE:HD11 | 1:A:45:PHE:HE1 | 1 | 2.47 |
| (1,1714) | 1:A:10:ILE:HD12 | 1:A:45:PHE:HE1 | 1 | 2.47 |
| (1,1714) | 1:A:10:ILE:HD13 | 1:A:45:PHE:HE1 | 1 | 2.47 |
| (1,4498) | 1:B:13:GLU:H | 1:B:45:PHE:HE1 | 11 | 2.46 |
| (1,4498) | 1:B:13:GLU:H | 1:B:45:PHE:HE1 | 15 | 2.46 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD21 | 8 | 2.46 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD22 | 8 | 2.46 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD23 | 8 | 2.46 |
| (1,3929) | 1:B:4:PHE:HE1 | 1:B:77:ARG:HD2 | 18 | 2.46 |
| (1,3929) | 1:B:4:PHE:HE1 | 1:B:77:ARG:HD3 | 18 | 2.46 |
| (1,4490) | 1:B:18:MET:HB2 | 1:B:45:PHE:HE1 | 15 | 2.45 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD21 | 12 | 2.45 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD22 | 12 | 2.45 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD23 | 12 | 2.45 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 3 | 2.44 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 3 | 2.44 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 3 | 2.44 |
| (1,4487) | 1:A:18:MET:HB2 | 1:A:45:PHE:HE1 | 13 | 2.44 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD21 | 13 | 2.44 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD22 | 13 | 2.44 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD23 | 13 | 2.44 |
| (1,1714) | 1:A:10:ILE:HD11 | 1:A:45:PHE:HE1 | 4 | 2.44 |
| (1,1714) | 1:A:10:ILE:HD12 | 1:A:45:PHE:HE1 | 4 | 2.44 |
| (1,1714) | 1:A:10:ILE:HD13 | 1:A:45:PHE:HE1 | 4 | 2.44 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 2 | 2.43 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 2 | 2.43 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 2 | 2.43 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 5 | 2.43 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 5 | 2.43 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 5 | 2.43 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 16 | 2.43 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 16 | 2.43 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 16 | 2.43 |
| (1,4497) | 1:A:13:GLU:H | 1:A:45:PHE:HE1 | 7 | 2.43 |
| (1,4485) | 1:A:10:ILE:HB | 1:A:45:PHE:HE1 | 14 | 2.43 |
| (1,1409) | 1:A:15:LYS:H | 1:A:45:PHE:HE1 | 7 | 2.43 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 19 | 2.42 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 4 | 2.42 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 4 | 2.42 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 4 | 2.42 |
| (1,4576) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HE1 | 8 | 2.42 |
| (1,4575) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HE1 | 7 | 2.42 |
| (1,4491) | 1:A:45:PHE:HE1 | 1:A:47:CYS:HB2 | 1 | 2.42 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 20 | 2.42 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 20 | 2.42 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 20 | 2.42 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 7 | 2.41 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 7 | 2.41 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 7 | 2.41 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 9 | 2.41 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 9 | 2.41 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 9 | 2.41 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 19 | 2.41 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 19 | 2.41 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 19 | 2.41 |
| (1,4576) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HE1 | 16 | 2.41 |
| (1,4497) | 1:A:13:GLU:H | 1:A:45:PHE:HE1 | 8 | 2.41 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD21 | 14 | 2.41 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD22 | 14 | 2.41 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD23 | 14 | 2.41 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 17 | 2.4 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 17 | 2.4 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 17 | 2.4 |
| (1,3928) | 1:A:4:PHE:HE1 | 1:A:77:ARG:HD2 | 7 | 2.4 |
| (1,3928) | 1:A:4:PHE:HE1 | 1:A:77:ARG:HD3 | 7 | 2.4 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 15 | 2.39 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 15 | 2.39 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 15 | 2.39 |
| (1,1840) | 1:A:13:GLU:HG2 | 1:A:45:PHE:HE1 | 20 | 2.39 |
| (1,1840) | 1:A:13:GLU:HG3 | 1:A:45:PHE:HE1 | 20 | 2.39 |
| (1,1410) | 1:B:15:LYS:H | 1:B:45:PHE:HE1 | 12 | 2.39 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 19 | 2.38 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 19 | 2.38 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 19 | 2.38 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 20 | 2.38 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 20 | 2.38 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 20 | 2.38 |
| (1,4576) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HE1 | 10 | 2.38 |
| (1,4576) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HE1 | 12 | 2.38 |
| (1,4575) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HE1 | 9 | 2.38 |
| (1,4497) | 1:A:13:GLU:H | 1:A:45:PHE:HE1 | 5 | 2.38 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 13 | 2.37 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 13 | 2.37 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 13 | 2.37 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 14 | 2.37 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 14 | 2.37 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 14 | 2.37 |
| (1,4575) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HE1 | 8 | 2.37 |
| (1,1715) | 1:B:10:ILE:HD11 | 1:B:45:PHE:HE1 | 17 | 2.37 |
| (1,1715) | 1:B:10:ILE:HD12 | 1:B:45:PHE:HE1 | 17 | 2.37 |
| (1,1715) | 1:B:10:ILE:HD13 | 1:B:45:PHE:HE1 | 17 | 2.37 |
| (1,1714) | 1:A:10:ILE:HD11 | 1:A:45:PHE:HE1 | 15 | 2.37 |
| (1,1714) | 1:A:10:ILE:HD12 | 1:A:45:PHE:HE1 | 15 | 2.37 |
| (1,1714) | 1:A:10:ILE:HD13 | 1:A:45:PHE:HE1 | 15 | 2.37 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 17 | 2.36 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 17 | 2.36 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 17 | 2.36 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 18 | 2.36 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 18 | 2.36 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 18 | 2.36 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 10 | 2.36 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 10 | 2.36 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 10 | 2.36 |
| (1,4576) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HE1 | 5 | 2.36 |
| (1,4575) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HE1 | 3 | 2.36 |
| (1,4498) | 1:B:13:GLU:H | 1:B:45:PHE:HE1 | 20 | 2.36 |
| (1,1410) | 1:B:15:LYS:H | 1:B:45:PHE:HE1 | 3 | 2.36 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 13 | 2.35 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 13 | 2.35 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 13 | 2.35 |
| (1,4575) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HE1 | 12 | 2.35 |
| (1,4575) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HE1 | 14 | 2.35 |
| (1,4497) | 1:A:13:GLU:H | 1:A:45:PHE:HE1 | 9 | 2.35 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 6 | 2.35 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 6 | 2.35 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 6 | 2.35 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 11 | 2.34 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 11 | 2.34 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 11 | 2.34 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 18 | 2.34 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 18 | 2.34 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 18 | 2.34 |
| (1,4576) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HE1 | 9 | 2.34 |
| (1,4575) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HE1 | 20 | 2.34 |
| (1,4497) | 1:A:13:GLU:H | 1:A:45:PHE:HE1 | 6 | 2.34 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 16 | 2.34 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 16 | 2.34 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 16 | 2.34 |
| (1,4576) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HE1 | 1 | 2.33 |
| (1,4575) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HE1 | 2 | 2.33 |
| (1,4575) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HE1 | 17 | 2.33 |
| (1,4498) | 1:B:13:GLU:H | 1:B:45:PHE:HE1 | 13 | 2.33 |
| (1,1409) | 1:A:15:LYS:H | 1:A:45:PHE:HE1 | 9 | 2.33 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 6 | 2.31 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 6 | 2.31 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 6 | 2.31 |
| (1,4576) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HE1 | 3 | 2.31 |
| (1,4576) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HE1 | 18 | 2.31 |
| (1,4575) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HE1 | 19 | 2.31 |
| (1,4498) | 1:B:13:GLU:H | 1:B:45:PHE:HE1 | 5 | 2.31 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD21 | 7 | 2.31 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD22 | 7 | 2.31 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD23 | 7 | 2.31 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 8 | 2.31 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 8 | 2.31 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 8 | 2.31 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 3 | 2.31 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 3 | 2.31 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 3 | 2.31 |
| (1,1714) | 1:A:10:ILE:HD11 | 1:A:45:PHE:HE1 | 18 | 2.31 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1714) | 1:A:10:ILE:HD12 | 1:A:45:PHE:HE1 | 18 | 2.31 |
| (1,1714) | 1:A:10:ILE:HD13 | 1:A:45:PHE:HE1 | 18 | 2.31 |
| (1,4576) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HE1 | 2 | 2.3 |
| (1,4575) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HE1 | 18 | 2.3 |
| (1,4498) | 1:B:13:GLU:H | 1:B:45:PHE:HE1 | 8 | 2.3 |
| (1,4497) | 1:A:13:GLU:H | 1:A:45:PHE:HE1 | 13 | 2.3 |
| (1,4490) | 1:B:18:MET:HB2 | 1:B:45:PHE:HE1 | 11 | 2.3 |
| (1,20) | 1:B:4:PHE:H | 1:B:52:PHE:HE1 | 11 | 2.3 |
| (1,4497) | 1:A:13:GLU:H | 1:A:45:PHE:HE1 | 3 | 2.29 |
| (1,4491) | 1:A:45:PHE:HE1 | 1:A:47:CYS:HB2 | 4 | 2.29 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 9 | 2.29 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 9 | 2.29 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 9 | 2.29 |
| (1,1841) | 1:B:13:GLU:HG2 | 1:B:45:PHE:HE1 | 2 | 2.29 |
| (1,1841) | 1:B:13:GLU:HG3 | 1:B:45:PHE:HE1 | 2 | 2.29 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 5 | 2.28 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 5 | 2.28 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 5 | 2.28 |
| (1,4575) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HE1 | 6 | 2.28 |
| (1,4575) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HE1 | 16 | 2.28 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 12 | 2.28 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 12 | 2.28 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 12 | 2.28 |
| (1,1410) | 1:B:15:LYS:H | 1:B:45:PHE:HE1 | 15 | 2.28 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD21 | 4 | 2.27 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD22 | 4 | 2.27 |
| (1,4600) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD23 | 4 | 2.27 |
| (1,3928) | 1:A:4:PHE:HE1 | 1:A:77:ARG:HD2 | 12 | 2.27 |
| (1,3928) | 1:A:4:PHE:HE1 | 1:A:77:ARG:HD3 | 12 | 2.27 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 7 | 2.27 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 7 | 2.27 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 7 | 2.27 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 8 | 2.27 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 8 | 2.27 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 8 | 2.27 |
| (1,1841) | 1:B:13:GLU:HG2 | 1:B:45:PHE:HE1 | 7 | 2.27 |
| (1,1841) | 1:B:13:GLU:HG3 | 1:B:45:PHE:HE1 | 7 | 2.27 |
| (1,1410) | 1:B:15:LYS:H | 1:B:45:PHE:HE1 | 13 | 2.27 |
| (1,4576) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HE1 | 7 | 2.26 |
| (1,4498) | 1:B:13:GLU:H | 1:B:45:PHE:HE1 | 18 | 2.26 |
| (1,4492) | 1:B:45:PHE:HE1 | 1:B:47:CYS:HB2 | 16 | 2.26 |
| (1,4487) | 1:A:18:MET:HB2 | 1:A:45:PHE:HE1 | 5 | 2.26 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 12 | 2.26 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 12 | 2.26 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 12 | 2.26 |
| (1,1840) | 1:A:13:GLU:HG2 | 1:A:45:PHE:HE1 | 2 | 2.26 |
| (1,1840) | 1:A:13:GLU:HG3 | 1:A:45:PHE:HE1 | 2 | 2.26 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD21 | 1 | 2.25 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD22 | 1 | 2.25 |
| (1,4599) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD23 | 1 | 2.25 |
| (1,4491) | 1:A:45:PHE:HE1 | 1:A:47:CYS:HB2 | 19 | 2.25 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 1 | 2.25 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 1 | 2.25 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 1 | 2.25 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 3 | 2.25 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 3 | 2.25 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 3 | 2.25 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 11 | 2.25 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 11 | 2.25 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 11 | 2.25 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 15 | 2.25 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 15 | 2.25 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 15 | 2.25 |
| (1,1410) | 1:B:15:LYS:H | 1:B:45:PHE:HE1 | 1 | 2.25 |
| (1,1409) | 1:A:15:LYS:H | 1:A:45:PHE:HE1 | 8 | 2.25 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 3 | 2.24 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 3 | 2.24 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 3 | 2.24 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 14 | 2.24 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 14 | 2.24 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 14 | 2.24 |
| (1,4498) | 1:B:13:GLU:H | 1:B:45:PHE:HE1 | 10 | 2.23 |
| (1,4491) | 1:A:45:PHE:HE1 | 1:A:47:CYS:HB2 | 12 | 2.23 |
| (1,1409) | 1:A:15:LYS:H | 1:A:45:PHE:HE1 | 3 | 2.23 |
| (1,1409) | 1:A:15:LYS:H | 1:A:45:PHE:HE1 | 10 | 2.23 |
| (1,4498) | 1:B:13:GLU:H | 1:B:45:PHE:HE1 | 19 | 2.22 |
| (1,1715) | 1:B:10:ILE:HD11 | 1:B:45:PHE:HE1 | 4 | 2.22 |
| (1,1715) | 1:B:10:ILE:HD12 | 1:B:45:PHE:HE1 | 4 | 2.22 |
| (1,1715) | 1:B:10:ILE:HD13 | 1:B:45:PHE:HE1 | 4 | 2.22 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 18 | 2.22 |
| (1,4682) | 1:A:15:LYS:HB2 | 1:A:16:ASN:HB2 | 3 | 2.21 |
| (1,4498) | 1:B:13:GLU:H | 1:B:45:PHE:HE1 | 1 | 2.21 |
| (1,4492) | 1:B:45:PHE:HE1 | 1:B:47:CYS:HB2 | 9 | 2.21 |
| (1,1409) | 1:A:15:LYS:H | 1:A:45:PHE:HE1 | 20 | 2.21 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 8 | 2.2 |
| (1,4492) | 1:B:45:PHE:HE1 | 1:B:47:CYS:HB2 | 17 | 2.2 |
| (1,1410) | 1:B:15:LYS:H | 1:B:45:PHE:HE1 | 14 | 2.2 |
| (1,4491) | 1:A:45:PHE:HE1 | 1:A:47:CYS:HB2 | 15 | 2.19 |
| (1,4358) | 1:A:4:PHE:HE1 | 1:A:6:ALA:HB1 | 7 | 2.19 |
| (1,4358) | 1:A:4:PHE:HE1 | 1:A:6:ALA:HB2 | 7 | 2.19 |
| (1,4358) | 1:A:4:PHE:HE1 | 1:A:6:ALA:HB3 | 7 | 2.19 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 2 | 2.19 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 2 | 2.19 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 2 | 2.19 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 9 | 2.18 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 9 | 2.18 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 9 | 2.18 |
| (1,4497) | 1:A:13:GLU:H | 1:A:45:PHE:HE1 | 11 | 2.18 |
| (1,1840) | 1:A:13:GLU:HG2 | 1:A:45:PHE:HE1 | 16 | 2.18 |
| (1,1840) | 1:A:13:GLU:HG3 | 1:A:45:PHE:HE1 | 16 | 2.18 |
| (1,1840) | 1:A:13:GLU:HG2 | 1:A:45:PHE:HE1 | 17 | 2.18 |
| (1,1840) | 1:A:13:GLU:HG3 | 1:A:45:PHE:HE1 | 17 | 2.18 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 7 | 2.17 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD21 | 9 | 2.17 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD22 | 9 | 2.17 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD23 | 9 | 2.17 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 20 | 2.17 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 1 | 2.16 |
| (1,4491) | 1:A:45:PHE:HE1 | 1:A:47:CYS:HB2 | 18 | 2.16 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB1 | 7 | 2.16 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB2 | 7 | 2.16 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB3 | 7 | 2.16 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 4 | 2.16 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 4 | 2.16 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 4 | 2.16 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 3 | 2.15 |
| (1,4487) | 1:A:18:MET:HB2 | 1:A:45:PHE:HE1 | 16 | 2.15 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 10 | 2.15 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 10 | 2.15 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 10 | 2.15 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 5 | 2.14 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 18 | 2.14 |
| (1,4497) | 1:A:13:GLU:H | 1:A:45:PHE:HE1 | 10 | 2.14 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 14 | 2.14 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 14 | 2.14 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 14 | 2.14 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 2 | 2.14 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 2 | 2.14 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 2 | 2.14 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 20 | 2.13 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB1 | 5 | 2.13 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB2 | 5 | 2.13 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB3 | 5 | 2.13 |
| (1,3929) | 1:B:4:PHE:HE1 | 1:B:77:ARG:HD2 | 9 | 2.13 |
| (1,3929) | 1:B:4:PHE:HE1 | 1:B:77:ARG:HD3 | 9 | 2.13 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 15 | 2.13 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 17 | 2.12 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 17 | 2.12 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 17 | 2.12 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 19 | 2.12 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 19 | 2.12 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 19 | 2.12 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 17 | 2.11 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 17 | 2.11 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 17 | 2.11 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 5 | 2.11 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 5 | 2.11 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 5 | 2.11 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 10 | 2.11 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 10 | 2.11 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 10 | 2.11 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 13 | 2.11 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 13 | 2.11 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 13 | 2.11 |
| (1,1410) | 1:B:15:LYS:H | 1:B:45:PHE:HE1 | 19 | 2.11 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 10 | 2.11 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 17 | 2.11 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 7 | 2.1 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 7 | 2.1 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 7 | 2.1 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 10 | 2.1 |
| (1,4579) | 1:A:13:GLU:HA | 1:A:73:PHE:HE1 | 17 | 2.09 |
| (1,4471) | 1:A:22:ILE:HG21 | 1:A:45:PHE:HE1 | 19 | 2.09 |
| (1,4471) | 1:A:22:ILE:HG22 | 1:A:45:PHE:HE1 | 19 | 2.09 |
| (1,4471) | 1:A:22:ILE:HG23 | 1:A:45:PHE:HE1 | 19 | 2.09 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 3 | 2.09 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 5 | 2.09 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 15 | 2.08 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|----------------|
| (1,4682) | 1:A:15:LYS:HB2 | 1:A:16:ASN:HB2 | 10 | 2.08 |
| (1,4492) | 1:B:45:PHE:HE1 | 1:B:47:CYS:HB2 | 4 | 2.08 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB1 | 8 | 2.08 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB2 | 8 | 2.08 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB3 | 8 | 2.08 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 5 | 2.08 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 5 | 2.08 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 5 | 2.08 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 15 | 2.08 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 15 | 2.08 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 15 | 2.08 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 11 | 2.08 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 20 | 2.07 |
| (1,4554) | 1:B:5:LEU:H | 1:B:52:PHE:HE1 | 11 | 2.07 |
| (1,4492) | 1:B:45:PHE:HE1 | 1:B:47:CYS:HB2 | 6 | 2.07 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB1 | 18 | 2.07 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB2 | 18 | 2.07 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB3 | 18 | 2.07 |
| (1,4358) | 1:A:4:PHE:HE1 | 1:A:6:ALA:HB1 | 13 | 2.07 |
| (1,4358) | 1:A:4:PHE:HE1 | 1:A:6:ALA:HB2 | 13 | 2.07 |
| (1,4358) | 1:A:4:PHE:HE1 | 1:A:6:ALA:HB3 | 13 | 2.07 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 19 | 2.07 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 19 | 2.07 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 19 | 2.07 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 18 | 2.07 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 18 | 2.07 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 18 | 2.07 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 19 | 2.07 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB1 | 9 | 2.06 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB2 | 9 | 2.06 |
| (1,4359) | 1:B:4:PHE:HE1 | 1:B:6:ALA:HB3 | 9 | 2.06 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 20 | 2.06 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 20 | 2.06 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 20 | 2.06 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 17 | 2.06 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 8 | 2.05 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 8 | 2.05 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 8 | 2.05 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 2 | 2.05 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 16 | 2.05 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 16 | 2.05 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 16 | 2.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1840) | 1:A:13:GLU:HG2 | 1:A:45:PHE:HE1 | 6 | 2.05 |
| (1,1840) | 1:A:13:GLU:HG3 | 1:A:45:PHE:HE1 | 6 | 2.05 |
| (1,1840) | 1:A:13:GLU:HG2 | 1:A:45:PHE:HE1 | 13 | 2.05 |
| (1,1840) | 1:A:13:GLU:HG3 | 1:A:45:PHE:HE1 | 13 | 2.05 |
| (1,4682) | 1:A:15:LYS:HB2 | 1:A:16:ASN:HB2 | 12 | 2.04 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 4 | 2.04 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 4 | 2.04 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 4 | 2.04 |
| (1,4579) | 1:A:13:GLU:HA | 1:A:73:PHE:HE1 | 20 | 2.04 |
| (1,4554) | 1:B:5:LEU:H | 1:B:52:PHE:HE1 | 12 | 2.04 |
| (1,4358) | 1:A:4:PHE:HE1 | 1:A:6:ALA:HB1 | 14 | 2.04 |
| (1,4358) | 1:A:4:PHE:HE1 | 1:A:6:ALA:HB2 | 14 | 2.04 |
| (1,4358) | 1:A:4:PHE:HE1 | 1:A:6:ALA:HB3 | 14 | 2.04 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 9 | 2.04 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 9 | 2.04 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 9 | 2.04 |
| (1,1410) | 1:B:15:LYS:H | 1:B:45:PHE:HE1 | 18 | 2.04 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 12 | 2.03 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 12 | 2.03 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 12 | 2.03 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 13 | 2.03 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 13 | 2.03 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 13 | 2.03 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 11 | 2.0 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 11 | 2.0 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 11 | 2.0 |
| (1,4487) | 1:A:18:MET:HB2 | 1:A:45:PHE:HE1 | 20 | 2.0 |
| (1,2757) | 1:A:45:PHE:HE1 | 1:A:47:CYS:HB3 | 19 | 2.0 |
| (1,20) | 1:B:4:PHE:H | 1:B:52:PHE:HE1 | 12 | 2.0 |
| (1,1841) | 1:B:13:GLU:HG2 | 1:B:45:PHE:HE1 | 3 | 2.0 |
| (1,1841) | 1:B:13:GLU:HG3 | 1:B:45:PHE:HE1 | 3 | 2.0 |
| (1,1410) | 1:B:15:LYS:H | 1:B:45:PHE:HE1 | 11 | 2.0 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 4 | 1.99 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 4 | 1.99 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 4 | 1.99 |
| (1,4358) | 1:A:4:PHE:HE1 | 1:A:6:ALA:HB1 | 12 | 1.99 |
| (1,4358) | 1:A:4:PHE:HE1 | 1:A:6:ALA:HB2 | 12 | 1.99 |
| (1,4358) | 1:A:4:PHE:HE1 | 1:A:6:ALA:HB3 | 12 | 1.99 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 12 | 1.99 |
| (1,4579) | 1:A:13:GLU:HA | 1:A:73:PHE:HE1 | 18 | 1.98 |
| (1,4472) | 1:B:22:ILE:HG21 | 1:B:45:PHE:HE1 | 16 | 1.98 |
| (1,4472) | 1:B:22:ILE:HG22 | 1:B:45:PHE:HE1 | 16 | 1.98 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4472) | 1:B:22:ILE:HG23 | 1:B:45:PHE:HE1 | 16 | 1.98 |
| (1,4472) | 1:B:22:ILE:HG21 | 1:B:45:PHE:HE1 | 17 | 1.98 |
| (1,4472) | 1:B:22:ILE:HG22 | 1:B:45:PHE:HE1 | 17 | 1.98 |
| (1,4472) | 1:B:22:ILE:HG23 | 1:B:45:PHE:HE1 | 17 | 1.98 |
| (1,4471) | 1:A:22:ILE:HG21 | 1:A:45:PHE:HE1 | 15 | 1.98 |
| (1,4471) | 1:A:22:ILE:HG22 | 1:A:45:PHE:HE1 | 15 | 1.98 |
| (1,4471) | 1:A:22:ILE:HG23 | 1:A:45:PHE:HE1 | 15 | 1.98 |
| (1,3929) | 1:B:4:PHE:HE1 | 1:B:77:ARG:HD2 | 8 | 1.98 |
| (1,3929) | 1:B:4:PHE:HE1 | 1:B:77:ARG:HD3 | 8 | 1.98 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 4 | 1.98 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 4 | 1.98 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 4 | 1.98 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 11 | 1.98 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 11 | 1.98 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 11 | 1.98 |
| (1,2758) | 1:B:45:PHE:HE1 | 1:B:47:CYS:HB3 | 9 | 1.98 |
| (1,2757) | 1:A:45:PHE:HE1 | 1:A:47:CYS:HB3 | 15 | 1.98 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 9 | 1.97 |
| (1,1840) | 1:A:13:GLU:HG2 | 1:A:45:PHE:HE1 | 8 | 1.97 |
| (1,1840) | 1:A:13:GLU:HG3 | 1:A:45:PHE:HE1 | 8 | 1.97 |
| (1,5145) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG12 | 1 | 1.96 |
| (1,4842) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG12 | 7 | 1.96 |
| (1,4682) | 1:A:15:LYS:HB2 | 1:A:16:ASN:HB2 | 5 | 1.96 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 10 | 1.96 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 10 | 1.96 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 10 | 1.96 |
| (1,2758) | 1:B:45:PHE:HE1 | 1:B:47:CYS:HB3 | 16 | 1.96 |
| (1,2757) | 1:A:45:PHE:HE1 | 1:A:47:CYS:HB3 | 4 | 1.96 |
| (1,2757) | 1:A:45:PHE:HE1 | 1:A:47:CYS:HB3 | 12 | 1.96 |
| (1,1841) | 1:B:13:GLU:HG2 | 1:B:45:PHE:HE1 | 15 | 1.96 |
| (1,1841) | 1:B:13:GLU:HG3 | 1:B:45:PHE:HE1 | 15 | 1.96 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 20 | 1.95 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 6 | 1.94 |
| (1,4682) | 1:A:15:LYS:HB2 | 1:A:16:ASN:HB2 | 7 | 1.94 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 17 | 1.94 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 17 | 1.94 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 17 | 1.94 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 6 | 1.94 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 6 | 1.94 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 6 | 1.94 |
| (1,2757) | 1:A:45:PHE:HE1 | 1:A:47:CYS:HB3 | 1 | 1.94 |
| (1,1841) | 1:B:13:GLU:HG2 | 1:B:45:PHE:HE1 | 12 | 1.94 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1841) | 1:B:13:GLU:HG3 | 1:B:45:PHE:HE1 | 12 | 1.94 |
| (1,1409) | 1:A:15:LYS:H | 1:A:45:PHE:HE1 | 5 | 1.94 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 9 | 1.94 |
| (1,5145) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG12 | 18 | 1.93 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 6 | 1.93 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 12 | 1.93 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 12 | 1.93 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 12 | 1.93 |
| (1,4471) | 1:A:22:ILE:HG21 | 1:A:45:PHE:HE1 | 12 | 1.93 |
| (1,4471) | 1:A:22:ILE:HG22 | 1:A:45:PHE:HE1 | 12 | 1.93 |
| (1,4471) | 1:A:22:ILE:HG23 | 1:A:45:PHE:HE1 | 12 | 1.93 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD11 | 1 | 1.93 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD12 | 1 | 1.93 |
| (1,2820) | 1:A:29:PHE:HE1 | 1:A:49:LEU:HD13 | 1 | 1.93 |
| (1,1841) | 1:B:13:GLU:HG2 | 1:B:45:PHE:HE1 | 14 | 1.93 |
| (1,1841) | 1:B:13:GLU:HG3 | 1:B:45:PHE:HE1 | 14 | 1.93 |
| (1,1841) | 1:B:13:GLU:HG2 | 1:B:45:PHE:HE1 | 20 | 1.93 |
| (1,1841) | 1:B:13:GLU:HG3 | 1:B:45:PHE:HE1 | 20 | 1.93 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 10 | 1.92 |
| (1,4842) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG12 | 11 | 1.92 |
| (1,4472) | 1:B:22:ILE:HG21 | 1:B:45:PHE:HE1 | 6 | 1.92 |
| (1,4472) | 1:B:22:ILE:HG22 | 1:B:45:PHE:HE1 | 6 | 1.92 |
| (1,4472) | 1:B:22:ILE:HG23 | 1:B:45:PHE:HE1 | 6 | 1.92 |
| (1,4471) | 1:A:22:ILE:HG21 | 1:A:45:PHE:HE1 | 1 | 1.92 |
| (1,4471) | 1:A:22:ILE:HG22 | 1:A:45:PHE:HE1 | 1 | 1.92 |
| (1,4471) | 1:A:22:ILE:HG23 | 1:A:45:PHE:HE1 | 1 | 1.92 |
| (1,1841) | 1:B:13:GLU:HG2 | 1:B:45:PHE:HE1 | 11 | 1.92 |
| (1,1841) | 1:B:13:GLU:HG3 | 1:B:45:PHE:HE1 | 11 | 1.92 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 4 | 1.92 |
| (1,4579) | 1:A:13:GLU:HA | 1:A:73:PHE:HE1 | 9 | 1.91 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 2 | 1.91 |
| (1,4471) | 1:A:22:ILE:HG21 | 1:A:45:PHE:HE1 | 18 | 1.91 |
| (1,4471) | 1:A:22:ILE:HG22 | 1:A:45:PHE:HE1 | 18 | 1.91 |
| (1,4471) | 1:A:22:ILE:HG23 | 1:A:45:PHE:HE1 | 18 | 1.91 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 4 | 1.9 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 1 | 1.9 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 1 | 1.9 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 1 | 1.9 |
| (1,4581) | 1:A:13:GLU:H | 1:A:73:PHE:HE1 | 16 | 1.9 |
| (1,1840) | 1:A:13:GLU:HG2 | 1:A:45:PHE:HE1 | 9 | 1.9 |
| (1,1840) | 1:A:13:GLU:HG3 | 1:A:45:PHE:HE1 | 9 | 1.9 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 8 | 1.9 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 19 | 1.9 |
| (1,4471) | 1:A:22:ILE:HG21 | 1:A:45:PHE:HE1 | 4 | 1.89 |
| (1,4471) | 1:A:22:ILE:HG22 | 1:A:45:PHE:HE1 | 4 | 1.89 |
| (1,4471) | 1:A:22:ILE:HG23 | 1:A:45:PHE:HE1 | 4 | 1.89 |
| (1,5145) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG12 | 10 | 1.88 |
| (1,4807) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HE1 | 11 | 1.88 |
| (1,4580) | 1:B:13:GLU:HA | 1:B:73:PHE:HE1 | 8 | 1.88 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 4 | 1.88 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 15 | 1.87 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 15 | 1.87 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 15 | 1.87 |
| (1,4579) | 1:A:13:GLU:HA | 1:A:73:PHE:HE1 | 6 | 1.87 |
| (1,4579) | 1:A:13:GLU:HA | 1:A:73:PHE:HE1 | 16 | 1.87 |
| (1,4473) | 1:A:38:LEU:HD11 | 1:A:45:PHE:HE1 | 14 | 1.87 |
| (1,4473) | 1:A:38:LEU:HD12 | 1:A:45:PHE:HE1 | 14 | 1.87 |
| (1,4473) | 1:A:38:LEU:HD13 | 1:A:45:PHE:HE1 | 14 | 1.87 |
| (1,1714) | 1:A:10:ILE:HD11 | 1:A:45:PHE:HE1 | 14 | 1.87 |
| (1,1714) | 1:A:10:ILE:HD12 | 1:A:45:PHE:HE1 | 14 | 1.87 |
| (1,1714) | 1:A:10:ILE:HD13 | 1:A:45:PHE:HE1 | 14 | 1.87 |
| (1,5145) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG12 | 14 | 1.86 |
| (1,4925) | 1:A:67:ARG:HG2 | 1:A:75:VAL:H | 16 | 1.86 |
| (1,4682) | 1:A:15:LYS:HB2 | 1:A:16:ASN:HB2 | 9 | 1.86 |
| (1,5237) | 1:B:67:ARG:HG2 | 1:B:75:VAL:H | 2 | 1.85 |
| (1,5237) | 1:B:67:ARG:HG2 | 1:B:75:VAL:H | 3 | 1.85 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 18 | 1.85 |
| (1,4682) | 1:A:15:LYS:HB2 | 1:A:16:ASN:HB2 | 1 | 1.85 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 18 | 1.85 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 18 | 1.85 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 18 | 1.85 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG21 | 6 | 1.85 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG22 | 6 | 1.85 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG23 | 6 | 1.85 |
| (1,3929) | 1:B:4:PHE:HE1 | 1:B:77:ARG:HD2 | 5 | 1.85 |
| (1,3929) | 1:B:4:PHE:HE1 | 1:B:77:ARG:HD3 | 5 | 1.85 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD11 | 18 | 1.85 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD12 | 18 | 1.85 |
| (1,2821) | 1:B:29:PHE:HE1 | 1:B:49:LEU:HD13 | 18 | 1.85 |
| (1,1841) | 1:B:13:GLU:HG2 | 1:B:45:PHE:HE1 | 5 | 1.85 |
| (1,1841) | 1:B:13:GLU:HG3 | 1:B:45:PHE:HE1 | 5 | 1.85 |
| (1,1841) | 1:B:13:GLU:HG2 | 1:B:45:PHE:HE1 | 13 | 1.85 |
| (1,1841) | 1:B:13:GLU:HG3 | 1:B:45:PHE:HE1 | 13 | 1.85 |
| (1,1066) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:H | 3 | 1.85 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 7 | 1.84 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 7 | 1.84 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 7 | 1.84 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG21 | 14 | 1.84 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG22 | 14 | 1.84 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG23 | 14 | 1.84 |
| (1,4472) | 1:B:22:ILE:HG21 | 1:B:45:PHE:HE1 | 9 | 1.84 |
| (1,4472) | 1:B:22:ILE:HG22 | 1:B:45:PHE:HE1 | 9 | 1.84 |
| (1,4472) | 1:B:22:ILE:HG23 | 1:B:45:PHE:HE1 | 9 | 1.84 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 19 | 1.83 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 19 | 1.83 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 19 | 1.83 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG21 | 1 | 1.83 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG22 | 1 | 1.83 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG23 | 1 | 1.83 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 3 | 1.83 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 3 | 1.83 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 3 | 1.83 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 7 | 1.83 |
| (1,4952) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HB2 | 12 | 1.82 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 6 | 1.82 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 6 | 1.82 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 6 | 1.82 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG21 | 11 | 1.82 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG22 | 11 | 1.82 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG23 | 11 | 1.82 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG21 | 11 | 1.82 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG22 | 11 | 1.82 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG23 | 11 | 1.82 |
| (1,3929) | 1:B:4:PHE:HE1 | 1:B:77:ARG:HD2 | 7 | 1.82 |
| (1,3929) | 1:B:4:PHE:HE1 | 1:B:77:ARG:HD3 | 7 | 1.82 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 20 | 1.82 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 20 | 1.82 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 20 | 1.82 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 11 | 1.82 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 17 | 1.81 |
| (1,4842) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG12 | 1 | 1.81 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG21 | 15 | 1.81 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG22 | 15 | 1.81 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG23 | 15 | 1.81 |
| (1,1841) | 1:B:13:GLU:HG2 | 1:B:45:PHE:HE1 | 8 | 1.81 |
| (1,1841) | 1:B:13:GLU:HG3 | 1:B:45:PHE:HE1 | 8 | 1.81 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1841) | 1:B:13:GLU:HG2 | 1:B:45:PHE:HE1 | 19 | 1.81 |
| (1,1841) | 1:B:13:GLU:HG3 | 1:B:45:PHE:HE1 | 19 | 1.81 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 3 | 1.81 |
| (1,4629) | 1:A:3:ASP:HB2 | 1:A:52:PHE:HB2 | 1 | 1.8 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 9 | 1.8 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 9 | 1.8 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 9 | 1.8 |
| (1,4581) | 1:A:13:GLU:H | 1:A:73:PHE:HE1 | 6 | 1.8 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG21 | 13 | 1.8 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG22 | 13 | 1.8 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG23 | 13 | 1.8 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG21 | 5 | 1.8 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG22 | 5 | 1.8 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG23 | 5 | 1.8 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG21 | 10 | 1.8 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG22 | 10 | 1.8 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG23 | 10 | 1.8 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG21 | 15 | 1.8 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG22 | 15 | 1.8 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG23 | 15 | 1.8 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 15 | 1.8 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 15 | 1.8 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 15 | 1.8 |
| (1,1841) | 1:B:13:GLU:HG2 | 1:B:45:PHE:HE1 | 18 | 1.8 |
| (1,1841) | 1:B:13:GLU:HG3 | 1:B:45:PHE:HE1 | 18 | 1.8 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 17 | 1.79 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG21 | 19 | 1.79 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG22 | 19 | 1.79 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG23 | 19 | 1.79 |
| (1,3038) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HZ1 | 10 | 1.79 |
| (1,3038) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HZ1 | 10 | 1.79 |
| (1,3038) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HZ1 | 10 | 1.79 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 13 | 1.79 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 3 | 1.78 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 3 | 1.78 |
| (1,4682) | 1:A:15:LYS:HB2 | 1:A:16:ASN:HB2 | 11 | 1.78 |
| (1,4580) | 1:B:13:GLU:HA | 1:B:73:PHE:HE1 | 18 | 1.78 |
| (1,4579) | 1:A:13:GLU:HA | 1:A:73:PHE:HE1 | 2 | 1.78 |
| (1,4488) | 1:B:18:MET:HB3 | 1:B:45:PHE:HE1 | 5 | 1.78 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 18 | 1.78 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 18 | 1.78 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 18 | 1.78 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,2758) | 1:B:45:PHE:HE1 | 1:B:47:CYS:HB3 | 6 | 1.78 |
| (1,4582) | 1:B:13:GLU:H | 1:B:73:PHE:HE1 | 18 | 1.77 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 7 | 1.77 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 2 | 1.77 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 2 | 1.77 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 2 | 1.77 |
| (1,2757) | 1:A:45:PHE:HE1 | 1:A:47:CYS:HB3 | 18 | 1.77 |
| (1,1066) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:H | 20 | 1.77 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 11 | 1.76 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 4 | 1.76 |
| (1,4488) | 1:B:18:MET:HB3 | 1:B:45:PHE:HE1 | 8 | 1.76 |
| (1,4471) | 1:A:22:ILE:HG21 | 1:A:45:PHE:HE1 | 14 | 1.76 |
| (1,4471) | 1:A:22:ILE:HG22 | 1:A:45:PHE:HE1 | 14 | 1.76 |
| (1,4471) | 1:A:22:ILE:HG23 | 1:A:45:PHE:HE1 | 14 | 1.76 |
| (1,2758) | 1:B:45:PHE:HE1 | 1:B:47:CYS:HB3 | 17 | 1.76 |
| (1,2757) | 1:A:45:PHE:HE1 | 1:A:47:CYS:HB3 | 14 | 1.76 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 8 | 1.76 |
| (1,4925) | 1:A:67:ARG:HG2 | 1:A:75:VAL:H | 9 | 1.75 |
| (1,4842) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG12 | 5 | 1.75 |
| (1,4581) | 1:A:13:GLU:H | 1:A:73:PHE:HE1 | 18 | 1.75 |
| (1,4580) | 1:B:13:GLU:HA | 1:B:73:PHE:HE1 | 3 | 1.75 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG21 | 20 | 1.75 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG22 | 20 | 1.75 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG23 | 20 | 1.75 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 7 | 1.75 |
| (1,4472) | 1:B:22:ILE:HG21 | 1:B:45:PHE:HE1 | 4 | 1.75 |
| (1,4472) | 1:B:22:ILE:HG22 | 1:B:45:PHE:HE1 | 4 | 1.75 |
| (1,4472) | 1:B:22:ILE:HG23 | 1:B:45:PHE:HE1 | 4 | 1.75 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 14 | 1.74 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 14 | 1.74 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 14 | 1.74 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 11 | 1.74 |
| (1,3928) | 1:A:4:PHE:HE1 | 1:A:77:ARG:HD2 | 14 | 1.74 |
| (1,3928) | 1:A:4:PHE:HE1 | 1:A:77:ARG:HD3 | 14 | 1.74 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 3 | 1.74 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 3 | 1.74 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 3 | 1.74 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 18 | 1.74 |
| (1,5145) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG12 | 7 | 1.73 |
| (1,4925) | 1:A:67:ARG:HG2 | 1:A:75:VAL:H | 5 | 1.73 |
| (1,4724) | 1:A:20:ASN:HB2 | 1:A:21:GLN:HE21 | 16 | 1.73 |
| (1,4581) | 1:A:13:GLU:H | 1:A:73:PHE:HE1 | 8 | 1.73 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4580) | 1:B:13:GLU:HA | 1:B:73:PHE:HE1 | 5 | 1.73 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 13 | 1.73 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 13 | 1.73 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 13 | 1.73 |
| (1,1840) | 1:A:13:GLU:HG2 | 1:A:45:PHE:HE1 | 3 | 1.73 |
| (1,1840) | 1:A:13:GLU:HG3 | 1:A:45:PHE:HE1 | 3 | 1.73 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 3 | 1.73 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 20 | 1.72 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 20 | 1.72 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 20 | 1.72 |
| (1,4581) | 1:A:13:GLU:H | 1:A:73:PHE:HE1 | 17 | 1.72 |
| (1,4581) | 1:A:13:GLU:H | 1:A:73:PHE:HE1 | 20 | 1.72 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG21 | 1 | 1.72 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG22 | 1 | 1.72 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG23 | 1 | 1.72 |
| (1,2758) | 1:B:45:PHE:HE1 | 1:B:47:CYS:HB3 | 4 | 1.72 |
| (1,1840) | 1:A:13:GLU:HG2 | 1:A:45:PHE:HE1 | 10 | 1.72 |
| (1,1840) | 1:A:13:GLU:HG3 | 1:A:45:PHE:HE1 | 10 | 1.72 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 13 | 1.72 |
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 11 | 1.71 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 3 | 1.71 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 3 | 1.71 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 3 | 1.71 |
| (1,4581) | 1:A:13:GLU:H | 1:A:73:PHE:HE1 | 9 | 1.71 |
| (1,4579) | 1:A:13:GLU:HA | 1:A:73:PHE:HE1 | 8 | 1.71 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 3 | 1.71 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 18 | 1.71 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 20 | 1.71 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 5 | 1.71 |
| (1,4473) | 1:A:38:LEU:HD11 | 1:A:45:PHE:HE1 | 18 | 1.71 |
| (1,4473) | 1:A:38:LEU:HD12 | 1:A:45:PHE:HE1 | 18 | 1.71 |
| (1,4473) | 1:A:38:LEU:HD13 | 1:A:45:PHE:HE1 | 18 | 1.71 |
| (1,1841) | 1:B:13:GLU:HG2 | 1:B:45:PHE:HE1 | 10 | 1.71 |
| (1,1841) | 1:B:13:GLU:HG3 | 1:B:45:PHE:HE1 | 10 | 1.71 |
| (1,1840) | 1:A:13:GLU:HG2 | 1:A:45:PHE:HE1 | 5 | 1.71 |
| (1,1840) | 1:A:13:GLU:HG3 | 1:A:45:PHE:HE1 | 5 | 1.71 |
| (1,4870) | 1:A:54:LYS:HG2 | 1:A:55:ASN:HD21 | 19 | 1.7 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 2 | 1.7 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 2 | 1.7 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 2 | 1.7 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG21 | 4 | 1.7 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG22 | 4 | 1.7 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG23 | 4 | 1.7 |
| (1,4473) | 1:A:38:LEU:HD11 | 1:A:45:PHE:HE1 | 15 | 1.7 |
| (1,4473) | 1:A:38:LEU:HD12 | 1:A:45:PHE:HE1 | 15 | 1.7 |
| (1,4473) | 1:A:38:LEU:HD13 | 1:A:45:PHE:HE1 | 15 | 1.7 |
| (1,1840) | 1:A:13:GLU:HG2 | 1:A:45:PHE:HE1 | 7 | 1.7 |
| (1,1840) | 1:A:13:GLU:HG3 | 1:A:45:PHE:HE1 | 7 | 1.7 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 8 | 1.69 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 8 | 1.69 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 8 | 1.69 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 16 | 1.69 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 16 | 1.69 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 16 | 1.69 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 20 | 1.69 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 20 | 1.69 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 20 | 1.69 |
| (1,4581) | 1:A:13:GLU:H | 1:A:73:PHE:HE1 | 2 | 1.69 |
| (1,4579) | 1:A:13:GLU:HA | 1:A:73:PHE:HE1 | 19 | 1.69 |
| (1,5029) | 1:B:20:ASN:HB2 | 1:B:21:GLN:HE21 | 18 | 1.68 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 6 | 1.68 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 14 | 1.68 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 1 | 1.68 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 15 | 1.68 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 15 | 1.68 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 15 | 1.68 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 8 | 1.68 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 20 | 1.68 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 20 | 1.68 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 20 | 1.68 |
| (1,1066) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:H | 10 | 1.68 |
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 13 | 1.67 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 5 | 1.67 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 5 | 1.67 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 5 | 1.67 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 14 | 1.67 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 14 | 1.67 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 14 | 1.67 |
| (1,1841) | 1:B:13:GLU:HG2 | 1:B:45:PHE:HE1 | 1 | 1.67 |
| (1,1841) | 1:B:13:GLU:HG3 | 1:B:45:PHE:HE1 | 1 | 1.67 |
| (1,1840) | 1:A:13:GLU:HG2 | 1:A:45:PHE:HE1 | 11 | 1.67 |
| (1,1840) | 1:A:13:GLU:HG3 | 1:A:45:PHE:HE1 | 11 | 1.67 |
| (1,5039) | 1:B:24:GLY:HA2 | 1:B:26:ILE:HG12 | 10 | 1.66 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 15 | 1.66 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3038) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HZ1 | 3 | 1.66 |
| (1,3038) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HZ1 | 3 | 1.66 |
| (1,3038) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HZ1 | 3 | 1.66 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 17 | 1.66 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 17 | 1.66 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 17 | 1.66 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 11 | 1.66 |
| (1,5039) | 1:B:24:GLY:HA2 | 1:B:26:ILE:HG12 | 2 | 1.65 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 19 | 1.65 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 19 | 1.65 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 19 | 1.65 |
| (1,4582) | 1:B:13:GLU:H | 1:B:73:PHE:HE1 | 1 | 1.65 |
| (1,4580) | 1:B:13:GLU:HA | 1:B:73:PHE:HE1 | 10 | 1.65 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG21 | 4 | 1.65 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG22 | 4 | 1.65 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG23 | 4 | 1.65 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 14 | 1.65 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 4 | 1.65 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 4 | 1.65 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 4 | 1.65 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 10 | 1.65 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 10 | 1.65 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 10 | 1.65 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 13 | 1.64 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 2 | 1.64 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 2 | 1.64 |
| (1,4842) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG12 | 19 | 1.64 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 14 | 1.64 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 14 | 1.64 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 14 | 1.64 |
| (1,4489) | 1:A:18:MET:HB3 | 1:A:45:PHE:HE1 | 17 | 1.64 |
| (1,4488) | 1:B:18:MET:HB3 | 1:B:45:PHE:HE1 | 7 | 1.64 |
| (1,4474) | 1:B:38:LEU:HD11 | 1:B:45:PHE:HE1 | 16 | 1.64 |
| (1,4474) | 1:B:38:LEU:HD12 | 1:B:45:PHE:HE1 | 16 | 1.64 |
| (1,4474) | 1:B:38:LEU:HD13 | 1:B:45:PHE:HE1 | 16 | 1.64 |
| (1,4473) | 1:A:38:LEU:HD11 | 1:A:45:PHE:HE1 | 1 | 1.64 |
| (1,4473) | 1:A:38:LEU:HD12 | 1:A:45:PHE:HE1 | 1 | 1.64 |
| (1,4473) | 1:A:38:LEU:HD13 | 1:A:45:PHE:HE1 | 1 | 1.64 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 8 | 1.64 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 8 | 1.64 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 8 | 1.64 |
| (1,4842) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG12 | 12 | 1.63 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4582) | 1:B:13:GLU:H | 1:B:73:PHE:HE1 | 3 | 1.63 |
| (1,4582) | 1:B:13:GLU:H | 1:B:73:PHE:HE1 | 10 | 1.63 |
| (1,4579) | 1:A:13:GLU:HA | 1:A:73:PHE:HE1 | 7 | 1.63 |
| (1,4579) | 1:A:13:GLU:HA | 1:A:73:PHE:HE1 | 14 | 1.63 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 19 | 1.63 |
| (1,3038) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HZ1 | 13 | 1.63 |
| (1,3038) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HZ1 | 13 | 1.63 |
| (1,3038) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HZ1 | 13 | 1.63 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 4 | 1.63 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 4 | 1.63 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 4 | 1.63 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 7 | 1.63 |
| (1,840) | 1:A:45:PHE:HE1 | 1:A:47:CYS:H | 14 | 1.62 |
| (1,5039) | 1:B:24:GLY:HA2 | 1:B:26:ILE:HG12 | 19 | 1.62 |
| (1,4582) | 1:B:13:GLU:H | 1:B:73:PHE:HE1 | 8 | 1.62 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG21 | 17 | 1.62 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG22 | 17 | 1.62 |
| (1,4570) | 1:B:73:PHE:HE1 | 1:B:74:THR:HG23 | 17 | 1.62 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 16 | 1.62 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 16 | 1.62 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 16 | 1.62 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 3 | 1.62 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 3 | 1.62 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 3 | 1.62 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 13 | 1.62 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 14 | 1.62 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 16 | 1.62 |
| (1,5039) | 1:B:24:GLY:HA2 | 1:B:26:ILE:HG12 | 8 | 1.61 |
| (1,5039) | 1:B:24:GLY:HA2 | 1:B:26:ILE:HG12 | 12 | 1.61 |
| (1,4582) | 1:B:13:GLU:H | 1:B:73:PHE:HE1 | 5 | 1.61 |
| (1,4581) | 1:A:13:GLU:H | 1:A:73:PHE:HE1 | 3 | 1.61 |
| (1,4581) | 1:A:13:GLU:H | 1:A:73:PHE:HE1 | 12 | 1.61 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 7 | 1.61 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 7 | 1.61 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 7 | 1.61 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 8 | 1.61 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 8 | 1.61 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 8 | 1.61 |
| (1,840) | 1:A:45:PHE:HE1 | 1:A:47:CYS:H | 1 | 1.6 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 18 | 1.6 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 18 | 1.6 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 9 | 1.6 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 5 | 1.6 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 5 | 1.6 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 5 | 1.6 |
| (1,4581) | 1:A:13:GLU:H | 1:A:73:PHE:HE1 | 19 | 1.6 |
| (1,4580) | 1:B:13:GLU:HA | 1:B:73:PHE:HE1 | 12 | 1.6 |
| (1,4566) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HE1 | 14 | 1.6 |
| (1,4566) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HE1 | 14 | 1.6 |
| (1,4566) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HE1 | 14 | 1.6 |
| (1,4482) | 1:B:10:ILE:HG21 | 1:B:45:PHE:HE1 | 9 | 1.6 |
| (1,4482) | 1:B:10:ILE:HG22 | 1:B:45:PHE:HE1 | 9 | 1.6 |
| (1,4482) | 1:B:10:ILE:HG23 | 1:B:45:PHE:HE1 | 9 | 1.6 |
| (1,4481) | 1:A:10:ILE:HG21 | 1:A:45:PHE:HE1 | 12 | 1.6 |
| (1,4481) | 1:A:10:ILE:HG22 | 1:A:45:PHE:HE1 | 12 | 1.6 |
| (1,4481) | 1:A:10:ILE:HG23 | 1:A:45:PHE:HE1 | 12 | 1.6 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG21 | 14 | 1.6 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG22 | 14 | 1.6 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG23 | 14 | 1.6 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 11 | 1.6 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 11 | 1.6 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 11 | 1.6 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 6 | 1.6 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 6 | 1.6 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 6 | 1.6 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 5 | 1.6 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 5 | 1.6 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 5 | 1.6 |
| (1,1752) | 1:A:11:VAL:HG21 | 1:A:45:PHE:HE1 | 4 | 1.6 |
| (1,1752) | 1:A:11:VAL:HG22 | 1:A:45:PHE:HE1 | 4 | 1.6 |
| (1,1752) | 1:A:11:VAL:HG23 | 1:A:45:PHE:HE1 | 4 | 1.6 |
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 6 | 1.59 |
| (1,5039) | 1:B:24:GLY:HA2 | 1:B:26:ILE:HG12 | 6 | 1.59 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 2 | 1.59 |
| (1,4582) | 1:B:13:GLU:H | 1:B:73:PHE:HE1 | 2 | 1.59 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 6 | 1.58 |
| (1,5039) | 1:B:24:GLY:HA2 | 1:B:26:ILE:HG12 | 15 | 1.58 |
| (1,5039) | 1:B:24:GLY:HA2 | 1:B:26:ILE:HG12 | 18 | 1.58 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 10 | 1.58 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 11 | 1.58 |
| (1,4579) | 1:A:13:GLU:HA | 1:A:73:PHE:HE1 | 3 | 1.58 |
| (1,4565) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HE1 | 5 | 1.58 |
| (1,4565) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HE1 | 5 | 1.58 |
| (1,4565) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HE1 | 5 | 1.58 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 6 | 1.58 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 6 | 1.58 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 6 | 1.58 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 18 | 1.58 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 18 | 1.58 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 18 | 1.58 |
| (1,1753) | 1:B:11:VAL:HG21 | 1:B:45:PHE:HE1 | 9 | 1.58 |
| (1,1753) | 1:B:11:VAL:HG22 | 1:B:45:PHE:HE1 | 9 | 1.58 |
| (1,1753) | 1:B:11:VAL:HG23 | 1:B:45:PHE:HE1 | 9 | 1.58 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 7 | 1.58 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 14 | 1.57 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 14 | 1.57 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 8 | 1.57 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 12 | 1.57 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 19 | 1.57 |
| (1,4481) | 1:A:10:ILE:HG21 | 1:A:45:PHE:HE1 | 4 | 1.57 |
| (1,4481) | 1:A:10:ILE:HG22 | 1:A:45:PHE:HE1 | 4 | 1.57 |
| (1,4481) | 1:A:10:ILE:HG23 | 1:A:45:PHE:HE1 | 4 | 1.57 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 19 | 1.57 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 19 | 1.57 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 19 | 1.57 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 1 | 1.57 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 1 | 1.57 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 1 | 1.57 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 3 | 1.56 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 3 | 1.56 |
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 7 | 1.56 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 9 | 1.56 |
| (1,4801) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG2 | 11 | 1.56 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 5 | 1.56 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 6 | 1.56 |
| (1,4724) | 1:A:20:ASN:HB2 | 1:A:21:GLN:HE21 | 14 | 1.56 |
| (1,4686) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HB2 | 9 | 1.56 |
| (1,4686) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HB2 | 9 | 1.56 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 2 | 1.56 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 2 | 1.56 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 2 | 1.56 |
| (1,4579) | 1:A:13:GLU:HA | 1:A:73:PHE:HE1 | 12 | 1.56 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 8 | 1.56 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 16 | 1.56 |
| (1,4473) | 1:A:38:LEU:HD11 | 1:A:45:PHE:HE1 | 12 | 1.56 |
| (1,4473) | 1:A:38:LEU:HD12 | 1:A:45:PHE:HE1 | 12 | 1.56 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4473) | 1:A:38:LEU:HD13 | 1:A:45:PHE:HE1 | 12 | 1.56 |
| (1,3928) | 1:A:4:PHE:HE1 | 1:A:77:ARG:HD2 | 13 | 1.56 |
| (1,3928) | 1:A:4:PHE:HE1 | 1:A:77:ARG:HD3 | 13 | 1.56 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 6 | 1.56 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 6 | 1.56 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 6 | 1.56 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 19 | 1.56 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 19 | 1.56 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 19 | 1.56 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 2 | 1.56 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 2 | 1.56 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 2 | 1.56 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 11 | 1.56 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 11 | 1.56 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 11 | 1.56 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 13 | 1.55 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 13 | 1.55 |
| (1,5039) | 1:B:24:GLY:HA2 | 1:B:26:ILE:HG12 | 17 | 1.55 |
| (1,4767) | 1:A:27:SER:HG | 1:A:28:LYS:HD2 | 2 | 1.55 |
| (1,4767) | 1:A:27:SER:HG | 1:A:28:LYS:HD2 | 17 | 1.55 |
| (1,4629) | 1:A:3:ASP:HB2 | 1:A:52:PHE:HB2 | 17 | 1.55 |
| (1,4580) | 1:B:13:GLU:HA | 1:B:73:PHE:HE1 | 7 | 1.55 |
| (1,4580) | 1:B:13:GLU:HA | 1:B:73:PHE:HE1 | 16 | 1.55 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 14 | 1.55 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 12 | 1.55 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 11 | 1.55 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 11 | 1.55 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 11 | 1.55 |
| (1,1753) | 1:B:11:VAL:HG21 | 1:B:45:PHE:HE1 | 16 | 1.55 |
| (1,1753) | 1:B:11:VAL:HG22 | 1:B:45:PHE:HE1 | 16 | 1.55 |
| (1,1753) | 1:B:11:VAL:HG23 | 1:B:45:PHE:HE1 | 16 | 1.55 |
| (1,841) | 1:B:45:PHE:HE1 | 1:B:47:CYS:H | 16 | 1.54 |
| (1,840) | 1:A:45:PHE:HE1 | 1:A:47:CYS:H | 15 | 1.54 |
| (1,840) | 1:A:45:PHE:HE1 | 1:A:47:CYS:H | 19 | 1.54 |
| (1,5039) | 1:B:24:GLY:HA2 | 1:B:26:ILE:HG12 | 1 | 1.54 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 5 | 1.54 |
| (1,4925) | 1:A:67:ARG:HG2 | 1:A:75:VAL:H | 18 | 1.54 |
| (1,4834) | 1:A:39:ASN:HD21 | 1:A:46:THR:HB | 12 | 1.54 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 16 | 1.54 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 1 | 1.54 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 6 | 1.54 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 6 | 1.54 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 6 | 1.54 |
| (1,4582) | 1:B:13:GLU:H | 1:B:73:PHE:HE1 | 12 | 1.54 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 9 | 1.54 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 9 | 1.54 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 9 | 1.54 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 12 | 1.54 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 12 | 1.54 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 12 | 1.54 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 9 | 1.54 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 9 | 1.54 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 9 | 1.54 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 13 | 1.53 |
| (1,4806) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HD1 | 19 | 1.53 |
| (1,4806) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HD2 | 19 | 1.53 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 7 | 1.53 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 14 | 1.53 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 10 | 1.53 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 10 | 1.53 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 10 | 1.53 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 16 | 1.53 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 16 | 1.53 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 16 | 1.53 |
| (1,4580) | 1:B:13:GLU:HA | 1:B:73:PHE:HE1 | 1 | 1.53 |
| (1,4580) | 1:B:13:GLU:HA | 1:B:73:PHE:HE1 | 2 | 1.53 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 13 | 1.53 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 6 | 1.53 |
| (1,4474) | 1:B:38:LEU:HD11 | 1:B:45:PHE:HE1 | 17 | 1.53 |
| (1,4474) | 1:B:38:LEU:HD12 | 1:B:45:PHE:HE1 | 17 | 1.53 |
| (1,4474) | 1:B:38:LEU:HD13 | 1:B:45:PHE:HE1 | 17 | 1.53 |
| (1,841) | 1:B:45:PHE:HE1 | 1:B:47:CYS:H | 9 | 1.52 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 6 | 1.52 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD2 | 13 | 1.52 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD3 | 13 | 1.52 |
| (1,5106) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG2 | 18 | 1.52 |
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 14 | 1.52 |
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 14 | 1.52 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 14 | 1.52 |
| (1,5039) | 1:B:24:GLY:HA2 | 1:B:26:ILE:HG12 | 11 | 1.52 |
| (1,5039) | 1:B:24:GLY:HA2 | 1:B:26:ILE:HG12 | 14 | 1.52 |
| (1,4925) | 1:A:67:ARG:HG2 | 1:A:75:VAL:H | 13 | 1.52 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 16 | 1.52 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 20 | 1.52 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4724) | 1:A:20:ASN:HB2 | 1:A:21:GLN:HE21 | 13 | 1.52 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 11 | 1.52 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 11 | 1.52 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 11 | 1.52 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 13 | 1.52 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 13 | 1.52 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 13 | 1.52 |
| (1,4565) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HE1 | 1 | 1.52 |
| (1,4565) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HE1 | 1 | 1.52 |
| (1,4565) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HE1 | 1 | 1.52 |
| (1,4489) | 1:A:18:MET:HB3 | 1:A:45:PHE:HE1 | 2 | 1.52 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 2 | 1.52 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 2 | 1.52 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 2 | 1.52 |
| (1,1752) | 1:A:11:VAL:HG21 | 1:A:45:PHE:HE1 | 12 | 1.52 |
| (1,1752) | 1:A:11:VAL:HG22 | 1:A:45:PHE:HE1 | 12 | 1.52 |
| (1,1752) | 1:A:11:VAL:HG23 | 1:A:45:PHE:HE1 | 12 | 1.52 |
| (1,5237) | 1:B:67:ARG:HG2 | 1:B:75:VAL:H | 5 | 1.51 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 20 | 1.51 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 8 | 1.51 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 9 | 1.51 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 9 | 1.51 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 9 | 1.51 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 11 | 1.51 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 11 | 1.51 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 11 | 1.51 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 3 | 1.51 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 6 | 1.51 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 8 | 1.51 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 8 | 1.51 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 8 | 1.51 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 18 | 1.51 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 18 | 1.51 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 18 | 1.51 |
| (1,4565) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HE1 | 10 | 1.51 |
| (1,4565) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HE1 | 10 | 1.51 |
| (1,4565) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HE1 | 10 | 1.51 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 3 | 1.51 |
| (1,4488) | 1:B:18:MET:HB3 | 1:B:45:PHE:HE1 | 2 | 1.51 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 16 | 1.51 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 16 | 1.51 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 16 | 1.51 |

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 15 | 1.51 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 15 | 1.51 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 15 | 1.51 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 16 | 1.51 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 16 | 1.51 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 16 | 1.51 |
| (1,840) | 1:A:45:PHE:HE1 | 1:A:47:CYS:H | 4 | 1.5 |
| (1,840) | 1:A:45:PHE:HE1 | 1:A:47:CYS:H | 12 | 1.5 |
| (1,840) | 1:A:45:PHE:HE1 | 1:A:47:CYS:H | 18 | 1.5 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 2 | 1.5 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 2 | 1.5 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 2 | 1.5 |
| (1,4582) | 1:B:13:GLU:H | 1:B:73:PHE:HE1 | 16 | 1.5 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 5 | 1.5 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 10 | 1.49 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 2 | 1.49 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 2 | 1.49 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 3 | 1.49 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 13 | 1.49 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 18 | 1.49 |
| (1,4686) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HB2 | 10 | 1.49 |
| (1,4686) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HB2 | 10 | 1.49 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 10 | 1.49 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 10 | 1.49 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 12 | 1.49 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 12 | 1.49 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 12 | 1.49 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 1 | 1.48 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 1 | 1.48 |
| (1,5039) | 1:B:24:GLY:HA2 | 1:B:26:ILE:HG12 | 13 | 1.48 |
| (1,5007) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HB2 | 9 | 1.48 |
| (1,5007) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HB2 | 9 | 1.48 |
| (1,4879) | 1:A:55:ASN:HD21 | 1:A:58:LYS:HG3 | 5 | 1.48 |
| (1,4834) | 1:A:39:ASN:HD21 | 1:A:46:THR:HB | 13 | 1.48 |
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 10 | 1.48 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 10 | 1.48 |
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 10 | 1.48 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 19 | 1.48 |
| (1,4582) | 1:B:13:GLU:H | 1:B:73:PHE:HE1 | 7 | 1.48 |
| (1,4581) | 1:A:13:GLU:H | 1:A:73:PHE:HE1 | 7 | 1.48 |
| (1,4489) | 1:A:18:MET:HB3 | 1:A:45:PHE:HE1 | 9 | 1.48 |
| (1,4488) | 1:B:18:MET:HB3 | 1:B:45:PHE:HE1 | 10 | 1.48 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 9 | 1.48 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 9 | 1.48 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 9 | 1.48 |
| (1,1753) | 1:B:11:VAL:HG21 | 1:B:45:PHE:HE1 | 6 | 1.48 |
| (1,1753) | 1:B:11:VAL:HG22 | 1:B:45:PHE:HE1 | 6 | 1.48 |
| (1,1753) | 1:B:11:VAL:HG23 | 1:B:45:PHE:HE1 | 6 | 1.48 |
| (1,841) | 1:B:45:PHE:HE1 | 1:B:47:CYS:H | 6 | 1.47 |
| (1,841) | 1:B:45:PHE:HE1 | 1:B:47:CYS:H | 17 | 1.47 |
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 14 | 1.47 |
| (1,5039) | 1:B:24:GLY:HA2 | 1:B:26:ILE:HG12 | 3 | 1.47 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 9 | 1.47 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 9 | 1.47 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 16 | 1.47 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 16 | 1.47 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 13 | 1.47 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 17 | 1.47 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 17 | 1.47 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 17 | 1.47 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 1 | 1.47 |
| (1,4482) | 1:B:10:ILE:HG21 | 1:B:45:PHE:HE1 | 6 | 1.47 |
| (1,4482) | 1:B:10:ILE:HG22 | 1:B:45:PHE:HE1 | 6 | 1.47 |
| (1,4482) | 1:B:10:ILE:HG23 | 1:B:45:PHE:HE1 | 6 | 1.47 |
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 5 | 1.46 |
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 20 | 1.46 |
| (1,5039) | 1:B:24:GLY:HA2 | 1:B:26:ILE:HG12 | 16 | 1.46 |
| (1,4925) | 1:A:67:ARG:HG2 | 1:A:75:VAL:H | 17 | 1.46 |
| (1,4686) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HB2 | 5 | 1.46 |
| (1,4686) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HB2 | 5 | 1.46 |
| (1,4686) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HB2 | 11 | 1.46 |
| (1,4686) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HB2 | 11 | 1.46 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 13 | 1.46 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 13 | 1.46 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 13 | 1.46 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG21 | 18 | 1.46 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG22 | 18 | 1.46 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG23 | 18 | 1.46 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 12 | 1.46 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 12 | 1.46 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 12 | 1.46 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 14 | 1.46 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 14 | 1.46 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 14 | 1.46 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1934) | 1:A:18:MET:HE1 | 1:A:45:PHE:HE1 | 2 | 1.46 |
| (1,1934) | 1:A:18:MET:HE2 | 1:A:45:PHE:HE1 | 2 | 1.46 |
| (1,1934) | 1:A:18:MET:HE3 | 1:A:45:PHE:HE1 | 2 | 1.46 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 10 | 1.45 |
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 10 | 1.45 |
| (1,4965) | 1:B:7:GLY:H | 1:B:77:ARG:HG2 | 8 | 1.45 |
| (1,4879) | 1:A:55:ASN:HD21 | 1:A:58:LYS:HG3 | 12 | 1.45 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE2 | 7 | 1.45 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE3 | 7 | 1.45 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 5 | 1.45 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 13 | 1.45 |
| (1,4482) | 1:B:10:ILE:HG21 | 1:B:45:PHE:HE1 | 16 | 1.45 |
| (1,4482) | 1:B:10:ILE:HG22 | 1:B:45:PHE:HE1 | 16 | 1.45 |
| (1,4482) | 1:B:10:ILE:HG23 | 1:B:45:PHE:HE1 | 16 | 1.45 |
| (1,4481) | 1:A:10:ILE:HG21 | 1:A:45:PHE:HE1 | 19 | 1.45 |
| (1,4481) | 1:A:10:ILE:HG22 | 1:A:45:PHE:HE1 | 19 | 1.45 |
| (1,4481) | 1:A:10:ILE:HG23 | 1:A:45:PHE:HE1 | 19 | 1.45 |
| (1,4475) | 1:A:22:ILE:HD11 | 1:A:45:PHE:HE1 | 12 | 1.45 |
| (1,4475) | 1:A:22:ILE:HD12 | 1:A:45:PHE:HE1 | 12 | 1.45 |
| (1,4475) | 1:A:22:ILE:HD13 | 1:A:45:PHE:HE1 | 12 | 1.45 |
| (1,4474) | 1:B:38:LEU:HD11 | 1:B:45:PHE:HE1 | 4 | 1.45 |
| (1,4474) | 1:B:38:LEU:HD12 | 1:B:45:PHE:HE1 | 4 | 1.45 |
| (1,4474) | 1:B:38:LEU:HD13 | 1:B:45:PHE:HE1 | 4 | 1.45 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 7 | 1.45 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 7 | 1.45 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 7 | 1.45 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 2 | 1.45 |
| (1,5173) | 1:B:54:LYS:HG2 | 1:B:55:ASN:HD21 | 10 | 1.44 |
| (1,5173) | 1:B:54:LYS:HG2 | 1:B:55:ASN:HD21 | 11 | 1.44 |
| (1,5112) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HE1 | 18 | 1.44 |
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 3 | 1.44 |
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 3 | 1.44 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 3 | 1.44 |
| (1,5039) | 1:B:24:GLY:HA2 | 1:B:26:ILE:HG12 | 7 | 1.44 |
| (1,5029) | 1:B:20:ASN:HB2 | 1:B:21:GLN:HE21 | 7 | 1.44 |
| (1,4879) | 1:A:55:ASN:HD21 | 1:A:58:LYS:HG3 | 4 | 1.44 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 2 | 1.44 |
| (1,4581) | 1:A:13:GLU:H | 1:A:73:PHE:HE1 | 14 | 1.44 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 17 | 1.44 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 2 | 1.44 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 2 | 1.44 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 2 | 1.44 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 3 | 1.44 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 3 | 1.44 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 3 | 1.44 |
| (1,1753) | 1:B:11:VAL:HG21 | 1:B:45:PHE:HE1 | 17 | 1.44 |
| (1,1753) | 1:B:11:VAL:HG22 | 1:B:45:PHE:HE1 | 17 | 1.44 |
| (1,1753) | 1:B:11:VAL:HG23 | 1:B:45:PHE:HE1 | 17 | 1.44 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 14 | 1.44 |
| (1,841) | 1:B:45:PHE:HE1 | 1:B:47:CYS:H | 4 | 1.43 |
| (1,5182) | 1:B:55:ASN:HD21 | 1:B:58:LYS:HG3 | 7 | 1.43 |
| (1,5029) | 1:B:20:ASN:HB2 | 1:B:21:GLN:HE21 | 14 | 1.43 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 15 | 1.43 |
| (1,4834) | 1:A:39:ASN:HD21 | 1:A:46:THR:HB | 6 | 1.43 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 7 | 1.43 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 7 | 1.43 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 7 | 1.43 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 11 | 1.43 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG21 | 13 | 1.43 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG22 | 13 | 1.43 |
| (1,4569) | 1:A:73:PHE:HE1 | 1:A:74:THR:HG23 | 13 | 1.43 |
| (1,4488) | 1:B:18:MET:HB3 | 1:B:45:PHE:HE1 | 13 | 1.43 |
| (1,4473) | 1:A:38:LEU:HD11 | 1:A:45:PHE:HE1 | 19 | 1.43 |
| (1,4473) | 1:A:38:LEU:HD12 | 1:A:45:PHE:HE1 | 19 | 1.43 |
| (1,4473) | 1:A:38:LEU:HD13 | 1:A:45:PHE:HE1 | 19 | 1.43 |
| (1,3370) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HB | 18 | 1.43 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 8 | 1.43 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 8 | 1.43 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 8 | 1.43 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 8 | 1.43 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 8 | 1.43 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 8 | 1.43 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 10 | 1.43 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 10 | 1.43 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 10 | 1.43 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 14 | 1.43 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 14 | 1.43 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 14 | 1.43 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 5 | 1.43 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 5 | 1.43 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 5 | 1.43 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 17 | 1.42 |
| (1,5106) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG2 | 20 | 1.42 |
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 18 | 1.42 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 18 | 1.42 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 18 | 1.42 |
| (1,5029) | 1:B:20:ASN:HB2 | 1:B:21:GLN:HE21 | 11 | 1.42 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 9 | 1.42 |
| (1,4582) | 1:B:13:GLU:H | 1:B:73:PHE:HE1 | 9 | 1.42 |
| (1,4481) | 1:A:10:ILE:HG21 | 1:A:45:PHE:HE1 | 1 | 1.42 |
| (1,4481) | 1:A:10:ILE:HG22 | 1:A:45:PHE:HE1 | 1 | 1.42 |
| (1,4481) | 1:A:10:ILE:HG23 | 1:A:45:PHE:HE1 | 1 | 1.42 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 5 | 1.42 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 5 | 1.42 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 5 | 1.42 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 12 | 1.42 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 12 | 1.42 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 12 | 1.42 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 16 | 1.42 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 16 | 1.42 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 16 | 1.42 |
| (1,1752) | 1:A:11:VAL:HG21 | 1:A:45:PHE:HE1 | 1 | 1.42 |
| (1,1752) | 1:A:11:VAL:HG22 | 1:A:45:PHE:HE1 | 1 | 1.42 |
| (1,1752) | 1:A:11:VAL:HG23 | 1:A:45:PHE:HE1 | 1 | 1.42 |
| (1,1066) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:H | 17 | 1.42 |
| (1,5106) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG2 | 10 | 1.41 |
| (1,4801) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG2 | 17 | 1.41 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 6 | 1.41 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 6 | 1.41 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 6 | 1.41 |
| (1,4580) | 1:B:13:GLU:HA | 1:B:73:PHE:HE1 | 9 | 1.41 |
| (1,4565) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HE1 | 15 | 1.41 |
| (1,4565) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HE1 | 15 | 1.41 |
| (1,4565) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HE1 | 15 | 1.41 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 9 | 1.41 |
| (1,4475) | 1:A:22:ILE:HD11 | 1:A:45:PHE:HE1 | 4 | 1.41 |
| (1,4475) | 1:A:22:ILE:HD12 | 1:A:45:PHE:HE1 | 4 | 1.41 |
| (1,4475) | 1:A:22:ILE:HD13 | 1:A:45:PHE:HE1 | 4 | 1.41 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 11 | 1.41 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 11 | 1.41 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 11 | 1.41 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 9 | 1.41 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 9 | 1.41 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 9 | 1.41 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 1 | 1.41 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 1 | 1.41 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 1 | 1.41 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 8 | 1.41 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 8 | 1.41 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 8 | 1.41 |
| (1,1752) | 1:A:11:VAL:HG21 | 1:A:45:PHE:HE1 | 18 | 1.41 |
| (1,1752) | 1:A:11:VAL:HG22 | 1:A:45:PHE:HE1 | 18 | 1.41 |
| (1,1752) | 1:A:11:VAL:HG23 | 1:A:45:PHE:HE1 | 18 | 1.41 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 9 | 1.4 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 9 | 1.4 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 18 | 1.4 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 18 | 1.4 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 18 | 1.4 |
| (1,5007) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HB2 | 18 | 1.4 |
| (1,5007) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HB2 | 18 | 1.4 |
| (1,4740) | 1:A:24:GLY:HA2 | 1:A:26:ILE:HG12 | 15 | 1.4 |
| (1,4598) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HE1 | 17 | 1.4 |
| (1,4598) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HE1 | 17 | 1.4 |
| (1,4598) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HE1 | 17 | 1.4 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 15 | 1.4 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 11 | 1.4 |
| (1,4489) | 1:A:18:MET:HB3 | 1:A:45:PHE:HE1 | 6 | 1.4 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 8 | 1.4 |
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 3 | 1.39 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 19 | 1.39 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 19 | 1.39 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 19 | 1.39 |
| (1,5029) | 1:B:20:ASN:HB2 | 1:B:21:GLN:HE21 | 12 | 1.39 |
| (1,4686) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HB2 | 12 | 1.39 |
| (1,4686) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HB2 | 12 | 1.39 |
| (1,4597) | 1:A:26:ILE:HG21 | 1:A:29:PHE:HE1 | 1 | 1.39 |
| (1,4597) | 1:A:26:ILE:HG22 | 1:A:29:PHE:HE1 | 1 | 1.39 |
| (1,4597) | 1:A:26:ILE:HG23 | 1:A:29:PHE:HE1 | 1 | 1.39 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 9 | 1.39 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 9 | 1.39 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 9 | 1.39 |
| (1,4473) | 1:A:38:LEU:HD11 | 1:A:45:PHE:HE1 | 4 | 1.39 |
| (1,4473) | 1:A:38:LEU:HD12 | 1:A:45:PHE:HE1 | 4 | 1.39 |
| (1,4473) | 1:A:38:LEU:HD13 | 1:A:45:PHE:HE1 | 4 | 1.39 |
| (1,5145) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG12 | 16 | 1.38 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 19 | 1.38 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 19 | 1.38 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 1 | 1.38 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 1 | 1.38 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 1 | 1.38 |
| (1,2549) | 1:A:38:LEU:HD21 | 1:A:45:PHE:HE1 | 14 | 1.38 |
| (1,2549) | 1:A:38:LEU:HD22 | 1:A:45:PHE:HE1 | 14 | 1.38 |
| (1,2549) | 1:A:38:LEU:HD23 | 1:A:45:PHE:HE1 | 14 | 1.38 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 15 | 1.38 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 7 | 1.37 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 5 | 1.37 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 15 | 1.37 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 12 | 1.37 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 12 | 1.37 |
| (1,4953) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HD1 | 12 | 1.37 |
| (1,4953) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HD2 | 12 | 1.37 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 7 | 1.37 |
| (1,4686) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HB2 | 3 | 1.37 |
| (1,4686) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HB2 | 3 | 1.37 |
| (1,4565) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HE1 | 11 | 1.37 |
| (1,4565) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HE1 | 11 | 1.37 |
| (1,4565) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HE1 | 11 | 1.37 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 14 | 1.37 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 6 | 1.37 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 6 | 1.37 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 6 | 1.37 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 16 | 1.37 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 16 | 1.37 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 16 | 1.37 |
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 4 | 1.36 |
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 17 | 1.36 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 17 | 1.36 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 20 | 1.36 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 2 | 1.36 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 17 | 1.36 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 17 | 1.36 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 17 | 1.36 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 16 | 1.35 |
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 9 | 1.35 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 6 | 1.35 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 6 | 1.35 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 6 | 1.35 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 17 | 1.35 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 17 | 1.35 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 17 | 1.35 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 20 | 1.35 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 20 | 1.35 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 4 | 1.35 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 4 | 1.35 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 4 | 1.35 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 4 | 1.35 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 12 | 1.35 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 12 | 1.35 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 12 | 1.35 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 16 | 1.35 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 16 | 1.35 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 16 | 1.35 |
| (1,4724) | 1:A:20:ASN:HB2 | 1:A:21:GLN:HE21 | 7 | 1.35 |
| (1,4720) | 1:A:20:ASN:H | 1:B:32:ASN:HB2 | 16 | 1.35 |
| (1,4689) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HB2 | 9 | 1.35 |
| (1,4689) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HB2 | 9 | 1.35 |
| (1,4489) | 1:A:18:MET:HB3 | 1:A:45:PHE:HE1 | 11 | 1.34 |
| (1,5174) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HB2 | 6 | 1.33 |
| (1,5174) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HB2 | 6 | 1.33 |
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 12 | 1.33 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 14 | 1.33 |
| (1,5029) | 1:B:20:ASN:HB2 | 1:B:21:GLN:HE21 | 15 | 1.33 |
| (1,4481) | 1:A:10:ILE:HG21 | 1:A:45:PHE:HE1 | 15 | 1.33 |
| (1,4481) | 1:A:10:ILE:HG22 | 1:A:45:PHE:HE1 | 15 | 1.33 |
| (1,4481) | 1:A:10:ILE:HG23 | 1:A:45:PHE:HE1 | 15 | 1.33 |
| (1,4474) | 1:B:38:LEU:HD11 | 1:B:45:PHE:HE1 | 9 | 1.33 |
| (1,4474) | 1:B:38:LEU:HD12 | 1:B:45:PHE:HE1 | 9 | 1.33 |
| (1,4474) | 1:B:38:LEU:HD13 | 1:B:45:PHE:HE1 | 9 | 1.33 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 4 | 1.33 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 4 | 1.33 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 4 | 1.33 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 7 | 1.33 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 7 | 1.33 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 7 | 1.33 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 16 | 1.32 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 16 | 1.32 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 16 | 1.32 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 10 | 1.32 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 8 | 1.32 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 1 | 1.32 |
| (1,5182) | 1:B:55:ASN:HD21 | 1:B:58:LYS:HG3 | 11 | 1.31 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 10 | 1.31 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 8 | 1.31 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 15 | 1.31 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 15 | 1.31 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 15 | 1.31 |
| (1,4871) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HB2 | 11 | 1.31 |
| (1,4871) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HB2 | 11 | 1.31 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 1 | 1.31 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 1 | 1.31 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 1 | 1.31 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 17 | 1.31 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 17 | 1.31 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 17 | 1.31 |
| (1,4474) | 1:B:38:LEU:HD11 | 1:B:45:PHE:HE1 | 6 | 1.31 |
| (1,4474) | 1:B:38:LEU:HD12 | 1:B:45:PHE:HE1 | 6 | 1.31 |
| (1,4474) | 1:B:38:LEU:HD13 | 1:B:45:PHE:HE1 | 6 | 1.31 |
| (1,3038) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HZ1 | 6 | 1.31 |
| (1,3038) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HZ1 | 6 | 1.31 |
| (1,3038) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HZ1 | 6 | 1.31 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 10 | 1.31 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 10 | 1.31 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 10 | 1.31 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 19 | 1.31 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 19 | 1.31 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 19 | 1.31 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 15 | 1.3 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 2 | 1.3 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 3 | 1.3 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 13 | 1.3 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 10 | 1.3 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 10 | 1.3 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 10 | 1.3 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 14 | 1.3 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 14 | 1.3 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 14 | 1.3 |
| (1,4952) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HB2 | 4 | 1.3 |
| (1,4686) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HB2 | 1 | 1.3 |
| (1,4686) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HB2 | 1 | 1.3 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 17 | 1.3 |
| (1,1752) | 1:A:11:VAL:HG21 | 1:A:45:PHE:HE1 | 19 | 1.3 |
| (1,1752) | 1:A:11:VAL:HG22 | 1:A:45:PHE:HE1 | 19 | 1.3 |
| (1,1752) | 1:A:11:VAL:HG23 | 1:A:45:PHE:HE1 | 19 | 1.3 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 12 | 1.29 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 1 | 1.29 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 2 | 1.29 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 12 | 1.29 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 2 | 1.29 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 2 | 1.29 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 2 | 1.29 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 5 | 1.29 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 5 | 1.29 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 5 | 1.29 |
| (1,4629) | 1:A:3:ASP:HB2 | 1:A:52:PHE:HB2 | 13 | 1.29 |
| (1,4566) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HE1 | 11 | 1.29 |
| (1,4566) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HE1 | 11 | 1.29 |
| (1,4566) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HE1 | 11 | 1.29 |
| (1,4489) | 1:A:18:MET:HB3 | 1:A:45:PHE:HE1 | 7 | 1.29 |
| (1,4482) | 1:B:10:ILE:HG21 | 1:B:45:PHE:HE1 | 17 | 1.29 |
| (1,4482) | 1:B:10:ILE:HG22 | 1:B:45:PHE:HE1 | 17 | 1.29 |
| (1,4482) | 1:B:10:ILE:HG23 | 1:B:45:PHE:HE1 | 17 | 1.29 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 16 | 1.29 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 16 | 1.29 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 16 | 1.29 |
| (1,1753) | 1:B:11:VAL:HG21 | 1:B:45:PHE:HE1 | 4 | 1.29 |
| (1,1753) | 1:B:11:VAL:HG22 | 1:B:45:PHE:HE1 | 4 | 1.29 |
| (1,1753) | 1:B:11:VAL:HG23 | 1:B:45:PHE:HE1 | 4 | 1.29 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 15 | 1.28 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 11 | 1.28 |
| (1,4630) | 1:A:3:ASP:HB2 | 1:A:52:PHE:HD1 | 1 | 1.28 |
| (1,4630) | 1:A:3:ASP:HB2 | 1:A:52:PHE:HD2 | 1 | 1.28 |
| (1,4489) | 1:A:18:MET:HB3 | 1:A:45:PHE:HE1 | 8 | 1.28 |
| (1,4488) | 1:B:18:MET:HB3 | 1:B:45:PHE:HE1 | 12 | 1.28 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 4 | 1.28 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 4 | 1.28 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 4 | 1.28 |
| (1,3370) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HB | 20 | 1.28 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 7 | 1.28 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 7 | 1.28 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 7 | 1.28 |
| (1,1934) | 1:A:18:MET:HE1 | 1:A:45:PHE:HE1 | 17 | 1.28 |
| (1,1934) | 1:A:18:MET:HE2 | 1:A:45:PHE:HE1 | 17 | 1.28 |
| (1,1934) | 1:A:18:MET:HE3 | 1:A:45:PHE:HE1 | 17 | 1.28 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 1 | 1.28 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 20 | 1.27 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 20 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 20 | 1.27 |
| (1,4985) | 1:B:9:ARG:HD2 | 1:B:48:ASN:HD21 | 15 | 1.27 |
| (1,4985) | 1:B:9:ARG:HD3 | 1:B:48:ASN:HD21 | 15 | 1.27 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD2 | 9 | 1.27 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD3 | 9 | 1.27 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 8 | 1.27 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 8 | 1.27 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 8 | 1.27 |
| (1,4489) | 1:A:18:MET:HB3 | 1:A:45:PHE:HE1 | 10 | 1.27 |
| (1,4481) | 1:A:10:ILE:HG21 | 1:A:45:PHE:HE1 | 18 | 1.27 |
| (1,4481) | 1:A:10:ILE:HG22 | 1:A:45:PHE:HE1 | 18 | 1.27 |
| (1,4481) | 1:A:10:ILE:HG23 | 1:A:45:PHE:HE1 | 18 | 1.27 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 6 | 1.27 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 6 | 1.27 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 6 | 1.27 |
| (1,1935) | 1:B:18:MET:HE1 | 1:B:45:PHE:HE1 | 2 | 1.27 |
| (1,1935) | 1:B:18:MET:HE2 | 1:B:45:PHE:HE1 | 2 | 1.27 |
| (1,1935) | 1:B:18:MET:HE3 | 1:B:45:PHE:HE1 | 2 | 1.27 |
| (1,4842) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG12 | 20 | 1.26 |
| (1,4802) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG3 | 11 | 1.26 |
| (1,4686) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HB2 | 7 | 1.26 |
| (1,4686) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HB2 | 7 | 1.26 |
| (1,4475) | 1:A:22:ILE:HD11 | 1:A:45:PHE:HE1 | 19 | 1.26 |
| (1,4475) | 1:A:22:ILE:HD12 | 1:A:45:PHE:HE1 | 19 | 1.26 |
| (1,4475) | 1:A:22:ILE:HD13 | 1:A:45:PHE:HE1 | 19 | 1.26 |
| (1,5174) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HB2 | 3 | 1.25 |
| (1,5174) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HB2 | 3 | 1.25 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD2 | 2 | 1.25 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD3 | 2 | 1.25 |
| (1,5029) | 1:B:20:ASN:HB2 | 1:B:21:GLN:HE21 | 13 | 1.25 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 13 | 1.25 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 13 | 1.25 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 7 | 1.25 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 7 | 1.25 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 7 | 1.25 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 10 | 1.25 |
| (1,4488) | 1:B:18:MET:HB3 | 1:B:45:PHE:HE1 | 18 | 1.25 |
| (1,3370) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HB | 14 | 1.25 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 14 | 1.25 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 14 | 1.25 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 14 | 1.25 |
| (1,1752) | 1:A:11:VAL:HG21 | 1:A:45:PHE:HE1 | 15 | 1.25 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1752) | 1:A:11:VAL:HG22 | 1:A:45:PHE:HE1 | 15 | 1.25 |
| (1,1752) | 1:A:11:VAL:HG23 | 1:A:45:PHE:HE1 | 15 | 1.25 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 10 | 1.24 |
| (1,5166) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HG2 | 8 | 1.24 |
| (1,5166) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HG2 | 8 | 1.24 |
| (1,5166) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HG2 | 8 | 1.24 |
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 20 | 1.24 |
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 20 | 1.24 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 20 | 1.24 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 8 | 1.24 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 8 | 1.24 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 8 | 1.24 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE2 | 9 | 1.24 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE3 | 9 | 1.24 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 5 | 1.24 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 5 | 1.24 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 5 | 1.24 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 15 | 1.24 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 13 | 1.24 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 13 | 1.24 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 13 | 1.24 |
| (1,1935) | 1:B:18:MET:HE1 | 1:B:45:PHE:HE1 | 14 | 1.24 |
| (1,1935) | 1:B:18:MET:HE2 | 1:B:45:PHE:HE1 | 14 | 1.24 |
| (1,1935) | 1:B:18:MET:HE3 | 1:B:45:PHE:HE1 | 14 | 1.24 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 6 | 1.23 |
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 16 | 1.23 |
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 18 | 1.23 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 20 | 1.23 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 20 | 1.23 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 20 | 1.23 |
| (1,4872) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HD21 | 19 | 1.23 |
| (1,4872) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HD21 | 19 | 1.23 |
| (1,4871) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HB2 | 6 | 1.23 |
| (1,4871) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HB2 | 6 | 1.23 |
| (1,4868) | 1:A:54:LYS:HB2 | 1:A:55:ASN:HD21 | 19 | 1.23 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE2 | 3 | 1.23 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE3 | 3 | 1.23 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE2 | 20 | 1.23 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE3 | 20 | 1.23 |
| (1,4820) | 1:A:37:VAL:HG11 | 1:A:39:ASN:HD21 | 2 | 1.23 |
| (1,4820) | 1:A:37:VAL:HG12 | 1:A:39:ASN:HD21 | 2 | 1.23 |
| (1,4820) | 1:A:37:VAL:HG13 | 1:A:39:ASN:HD21 | 2 | 1.23 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 7 | 1.23 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 7 | 1.23 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 7 | 1.23 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 19 | 1.23 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 19 | 1.23 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 19 | 1.23 |
| (1,4630) | 1:A:3:ASP:HB2 | 1:A:52:PHE:HD1 | 17 | 1.23 |
| (1,4630) | 1:A:3:ASP:HB2 | 1:A:52:PHE:HD2 | 17 | 1.23 |
| (1,4566) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HE1 | 6 | 1.23 |
| (1,4566) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HE1 | 6 | 1.23 |
| (1,4566) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HE1 | 6 | 1.23 |
| (1,4548) | 1:B:5:LEU:HB3 | 1:B:52:PHE:HE1 | 11 | 1.23 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 4 | 1.23 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 20 | 1.23 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 5 | 1.23 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 15 | 1.23 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 9 | 1.23 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 9 | 1.23 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 9 | 1.23 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 15 | 1.23 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 15 | 1.23 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 15 | 1.23 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 11 | 1.22 |
| (1,5174) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HB2 | 13 | 1.22 |
| (1,5174) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HB2 | 13 | 1.22 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 7 | 1.22 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 17 | 1.22 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 9 | 1.22 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 7 | 1.22 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 8 | 1.22 |
| (1,4703) | 1:A:17:GLY:HA2 | 1:A:21:GLN:HE22 | 17 | 1.22 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 14 | 1.22 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 14 | 1.22 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 14 | 1.22 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 11 | 1.22 |
| (1,4475) | 1:A:22:ILE:HD11 | 1:A:45:PHE:HE1 | 15 | 1.22 |
| (1,4475) | 1:A:22:ILE:HD12 | 1:A:45:PHE:HE1 | 15 | 1.22 |
| (1,4475) | 1:A:22:ILE:HD13 | 1:A:45:PHE:HE1 | 15 | 1.22 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 1 | 1.22 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 1 | 1.22 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 1 | 1.22 |
| (1,1934) | 1:A:18:MET:HE1 | 1:A:45:PHE:HE1 | 20 | 1.22 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1934) | 1:A:18:MET:HE2 | 1:A:45:PHE:HE1 | 20 | 1.22 |
| (1,1934) | 1:A:18:MET:HE3 | 1:A:45:PHE:HE1 | 20 | 1.22 |
| (1,1066) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:H | 18 | 1.22 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 6 | 1.22 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG21 | 14 | 1.21 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG22 | 14 | 1.21 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG23 | 14 | 1.21 |
| (1,5116) | 1:B:36:ILE:HG21 | 1:B:48:ASN:HB2 | 11 | 1.21 |
| (1,5116) | 1:B:36:ILE:HG22 | 1:B:48:ASN:HB2 | 11 | 1.21 |
| (1,5116) | 1:B:36:ILE:HG23 | 1:B:48:ASN:HB2 | 11 | 1.21 |
| (1,5107) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG3 | 18 | 1.21 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 8 | 1.21 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 9 | 1.21 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 3 | 1.21 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 3 | 1.21 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 3 | 1.21 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 13 | 1.21 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 13 | 1.21 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 13 | 1.21 |
| (1,5029) | 1:B:20:ASN:HB2 | 1:B:21:GLN:HE21 | 4 | 1.21 |
| (1,4868) | 1:A:54:LYS:HB2 | 1:A:55:ASN:HD21 | 18 | 1.21 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG21 | 6 | 1.21 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG22 | 6 | 1.21 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG23 | 6 | 1.21 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 11 | 1.21 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 11 | 1.21 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 11 | 1.21 |
| (1,4488) | 1:B:18:MET:HB3 | 1:B:45:PHE:HE1 | 20 | 1.21 |
| (1,3370) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HB | 17 | 1.21 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 18 | 1.2 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 18 | 1.2 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD2 | 12 | 1.2 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD3 | 12 | 1.2 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB2 | 20 | 1.2 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB3 | 20 | 1.2 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG21 | 17 | 1.2 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG22 | 17 | 1.2 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG23 | 17 | 1.2 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 5 | 1.2 |
| (1,5057) | 1:B:26:ILE:HG12 | 1:B:27:SER:HG | 19 | 1.2 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 19 | 1.2 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE2 | 4 | 1.2 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE3 | 4 | 1.2 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 15 | 1.2 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 9 | 1.2 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 9 | 1.2 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 9 | 1.2 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 10 | 1.2 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 10 | 1.2 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 10 | 1.2 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 15 | 1.2 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 15 | 1.2 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 15 | 1.2 |
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 17 | 1.2 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 8 | 1.2 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 8 | 1.2 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 8 | 1.2 |
| (1,4488) | 1:B:18:MET:HB3 | 1:B:45:PHE:HE1 | 3 | 1.2 |
| (1,4475) | 1:A:22:ILE:HD11 | 1:A:45:PHE:HE1 | 1 | 1.2 |
| (1,4475) | 1:A:22:ILE:HD12 | 1:A:45:PHE:HE1 | 1 | 1.2 |
| (1,4475) | 1:A:22:ILE:HD13 | 1:A:45:PHE:HE1 | 1 | 1.2 |
| (1,5159) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HE2 | 20 | 1.19 |
| (1,5159) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HE2 | 20 | 1.19 |
| (1,5159) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HE2 | 20 | 1.19 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 12 | 1.19 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 12 | 1.19 |
| (1,5106) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG2 | 3 | 1.19 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 5 | 1.19 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 5 | 1.19 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 5 | 1.19 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 6 | 1.19 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 17 | 1.19 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG21 | 8 | 1.19 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG22 | 8 | 1.19 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG23 | 8 | 1.19 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 6 | 1.19 |
| (1,4475) | 1:A:22:ILE:HD11 | 1:A:45:PHE:HE1 | 18 | 1.19 |
| (1,4475) | 1:A:22:ILE:HD12 | 1:A:45:PHE:HE1 | 18 | 1.19 |
| (1,4475) | 1:A:22:ILE:HD13 | 1:A:45:PHE:HE1 | 18 | 1.19 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 19 | 1.19 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 19 | 1.19 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 19 | 1.19 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB2 | 18 | 1.18 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB3 | 18 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG21 | 11 | 1.18 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG22 | 11 | 1.18 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG23 | 11 | 1.18 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG21 | 16 | 1.18 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG22 | 16 | 1.18 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG23 | 16 | 1.18 |
| (1,5106) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG2 | 12 | 1.18 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG21 | 13 | 1.18 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG22 | 13 | 1.18 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG23 | 13 | 1.18 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG21 | 18 | 1.18 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG22 | 18 | 1.18 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG23 | 18 | 1.18 |
| (1,4764) | 1:A:27:SER:HB2 | 1:B:20:ASN:HA | 7 | 1.18 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 3 | 1.18 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 3 | 1.18 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 3 | 1.18 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 6 | 1.18 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 6 | 1.18 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 6 | 1.18 |
| (1,4685) | 1:A:15:LYS:HB2 | 1:A:18:MET:HG2 | 2 | 1.18 |
| (1,4684) | 1:A:15:LYS:HB2 | 1:A:18:MET:HB2 | 16 | 1.18 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 6 | 1.18 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 1 | 1.18 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 1 | 1.18 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 1 | 1.18 |
| (1,2995) | 1:B:8:ILE:HG21 | 1:B:29:PHE:HE1 | 20 | 1.18 |
| (1,2995) | 1:B:8:ILE:HG22 | 1:B:29:PHE:HE1 | 20 | 1.18 |
| (1,2995) | 1:B:8:ILE:HG23 | 1:B:29:PHE:HE1 | 20 | 1.18 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 13 | 1.18 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 13 | 1.18 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 13 | 1.18 |
| (1,1934) | 1:A:18:MET:HE1 | 1:A:45:PHE:HE1 | 5 | 1.18 |
| (1,1934) | 1:A:18:MET:HE2 | 1:A:45:PHE:HE1 | 5 | 1.18 |
| (1,1934) | 1:A:18:MET:HE3 | 1:A:45:PHE:HE1 | 5 | 1.18 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 10 | 1.18 |
| (1,5166) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HG2 | 14 | 1.17 |
| (1,5166) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HG2 | 14 | 1.17 |
| (1,5166) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HG2 | 14 | 1.17 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 7 | 1.17 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 7 | 1.17 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 7 | 1.17 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5145) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG12 | 12 | 1.17 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 19 | 1.17 |
| (1,5057) | 1:B:26:ILE:HG12 | 1:B:27:SER:HG | 17 | 1.17 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE2 | 17 | 1.17 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE3 | 17 | 1.17 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD2 | 20 | 1.17 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD3 | 20 | 1.17 |
| (1,4820) | 1:A:37:VAL:HG11 | 1:A:39:ASN:HD21 | 10 | 1.17 |
| (1,4820) | 1:A:37:VAL:HG12 | 1:A:39:ASN:HD21 | 10 | 1.17 |
| (1,4820) | 1:A:37:VAL:HG13 | 1:A:39:ASN:HD21 | 10 | 1.17 |
| (1,4802) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG3 | 17 | 1.17 |
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 12 | 1.17 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 12 | 1.17 |
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 12 | 1.17 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 18 | 1.17 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 18 | 1.17 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 18 | 1.17 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 7 | 1.17 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 7 | 1.17 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 7 | 1.17 |
| (1,4482) | 1:B:10:ILE:HG21 | 1:B:45:PHE:HE1 | 4 | 1.17 |
| (1,4482) | 1:B:10:ILE:HG22 | 1:B:45:PHE:HE1 | 4 | 1.17 |
| (1,4482) | 1:B:10:ILE:HG23 | 1:B:45:PHE:HE1 | 4 | 1.17 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 4 | 1.17 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 4 | 1.17 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 4 | 1.17 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 18 | 1.17 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 18 | 1.17 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 18 | 1.17 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 3 | 1.17 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 3 | 1.17 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 3 | 1.17 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 7 | 1.17 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 7 | 1.17 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 7 | 1.17 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB2 | 3 | 1.16 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB3 | 3 | 1.16 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG21 | 2 | 1.16 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG22 | 2 | 1.16 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG23 | 2 | 1.16 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG21 | 5 | 1.16 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG22 | 5 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG23 | 5 | 1.16 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 7 | 1.16 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 7 | 1.16 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 7 | 1.16 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 1 | 1.16 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 1 | 1.16 |
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 6 | 1.16 |
| (1,4693) | 1:A:16:ASN:HA | 1:B:32:ASN:HD21 | 4 | 1.16 |
| (1,4629) | 1:A:3:ASP:HB2 | 1:A:52:PHE:HB2 | 19 | 1.16 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 13 | 1.16 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 13 | 1.16 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 13 | 1.16 |
| (1,4566) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HE1 | 15 | 1.16 |
| (1,4566) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HE1 | 15 | 1.16 |
| (1,4566) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HE1 | 15 | 1.16 |
| (1,4566) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HE1 | 20 | 1.16 |
| (1,4566) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HE1 | 20 | 1.16 |
| (1,4566) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HE1 | 20 | 1.16 |
| (1,4488) | 1:B:18:MET:HB3 | 1:B:45:PHE:HE1 | 1 | 1.16 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 10 | 1.16 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 12 | 1.16 |
| (1,3370) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HB | 9 | 1.16 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 11 | 1.15 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 13 | 1.15 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG21 | 15 | 1.15 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG22 | 15 | 1.15 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG23 | 15 | 1.15 |
| (1,4871) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HB2 | 10 | 1.15 |
| (1,4871) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HB2 | 10 | 1.15 |
| (1,4870) | 1:A:54:LYS:HG2 | 1:A:55:ASN:HD21 | 6 | 1.15 |
| (1,4834) | 1:A:39:ASN:HD21 | 1:A:46:THR:HB | 11 | 1.15 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG21 | 1 | 1.15 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG22 | 1 | 1.15 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG23 | 1 | 1.15 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 9 | 1.15 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 9 | 1.15 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 9 | 1.15 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 3 | 1.15 |
| (1,3370) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HB | 1 | 1.15 |
| (1,3370) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HB | 10 | 1.15 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 10 | 1.15 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 10 | 1.15 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 10 | 1.15 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 7 | 1.15 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 7 | 1.15 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 7 | 1.15 |
| (1,5174) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HB2 | 17 | 1.14 |
| (1,5174) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HB2 | 17 | 1.14 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB2 | 2 | 1.14 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB3 | 2 | 1.14 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 7 | 1.14 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 7 | 1.14 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 7 | 1.14 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 13 | 1.14 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 13 | 1.14 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 13 | 1.14 |
| (1,1934) | 1:A:18:MET:HE1 | 1:A:45:PHE:HE1 | 10 | 1.14 |
| (1,1934) | 1:A:18:MET:HE2 | 1:A:45:PHE:HE1 | 10 | 1.14 |
| (1,1934) | 1:A:18:MET:HE3 | 1:A:45:PHE:HE1 | 10 | 1.14 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 19 | 1.14 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 17 | 1.13 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 12 | 1.13 |
| (1,5107) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG3 | 20 | 1.13 |
| (1,5106) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG2 | 15 | 1.13 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 1 | 1.13 |
| (1,5057) | 1:B:26:ILE:HG12 | 1:B:27:SER:HG | 18 | 1.13 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 11 | 1.13 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 11 | 1.13 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 11 | 1.13 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB2 | 9 | 1.13 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB3 | 9 | 1.13 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB2 | 19 | 1.13 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB3 | 19 | 1.13 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB2 | 20 | 1.13 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB3 | 20 | 1.13 |
| (1,4801) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG2 | 7 | 1.13 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 18 | 1.13 |
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 15 | 1.13 |
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 18 | 1.13 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG21 | 5 | 1.13 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG22 | 5 | 1.13 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG23 | 5 | 1.13 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 19 | 1.13 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 20 | 1.13 |

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wwPDB NMR Structure Validation Summary Report

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 20 | 1.13 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 20 | 1.13 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 11 | 1.13 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 11 | 1.13 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 11 | 1.13 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 7 | 1.13 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 7 | 1.13 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 7 | 1.13 |
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 11 | 1.12 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 3 | 1.12 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 15 | 1.12 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 15 | 1.12 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 15 | 1.12 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 15 | 1.12 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG21 | 19 | 1.12 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG22 | 19 | 1.12 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG23 | 19 | 1.12 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 20 | 1.12 |
| (1,4863) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HG2 | 9 | 1.12 |
| (1,4863) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HG2 | 9 | 1.12 |
| (1,4863) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HG2 | 9 | 1.12 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 13 | 1.12 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 13 | 1.12 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 13 | 1.12 |
| (1,4629) | 1:A:3:ASP:HB2 | 1:A:52:PHE:HB2 | 20 | 1.12 |
| (1,4488) | 1:B:18:MET:HB3 | 1:B:45:PHE:HE1 | 14 | 1.12 |
| (1,4488) | 1:B:18:MET:HB3 | 1:B:45:PHE:HE1 | 19 | 1.12 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 19 | 1.12 |
| (1,3370) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HB | 11 | 1.12 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 13 | 1.12 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 13 | 1.12 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 13 | 1.12 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG21 | 2 | 1.12 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG22 | 2 | 1.12 |
| (1,2996) | 1:A:29:PHE:HE1 | 1:A:51:ILE:HG23 | 2 | 1.12 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 16 | 1.12 |
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 17 | 1.11 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG21 | 4 | 1.11 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG22 | 4 | 1.11 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG23 | 4 | 1.11 |
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 2 | 1.11 |
| (1,4868) | 1:A:54:LYS:HB2 | 1:A:55:ASN:HD21 | 4 | 1.11 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB2 | 4 | 1.11 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB3 | 4 | 1.11 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG21 | 19 | 1.11 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG22 | 19 | 1.11 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG23 | 19 | 1.11 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 11 | 1.11 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 15 | 1.11 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 14 | 1.11 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 10 | 1.11 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 10 | 1.11 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 10 | 1.11 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 19 | 1.11 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 19 | 1.11 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 19 | 1.11 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 18 | 1.11 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 18 | 1.11 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 18 | 1.11 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 15 | 1.1 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB2 | 12 | 1.1 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB3 | 12 | 1.1 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG21 | 12 | 1.1 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG22 | 12 | 1.1 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG23 | 12 | 1.1 |
| (1,5031) | 1:B:23:THR:HB | 1:B:26:ILE:HG12 | 18 | 1.1 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 13 | 1.1 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 12 | 1.1 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 12 | 1.1 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 12 | 1.1 |
| (1,3038) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HZ1 | 5 | 1.1 |
| (1,3038) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HZ1 | 5 | 1.1 |
| (1,3038) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HZ1 | 5 | 1.1 |
| (1,1066) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:H | 13 | 1.1 |
| (1,5238) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG11 | 2 | 1.09 |
| (1,5238) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG12 | 2 | 1.09 |
| (1,5238) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG13 | 2 | 1.09 |
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 10 | 1.09 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 3 | 1.09 |
| (1,5173) | 1:B:54:LYS:HG2 | 1:B:55:ASN:HD21 | 3 | 1.09 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 5 | 1.09 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 5 | 1.09 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 5 | 1.09 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD2 | 9 | 1.09 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD3 | 9 | 1.09 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG21 | 13 | 1.09 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG22 | 13 | 1.09 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG23 | 13 | 1.09 |
| (1,5118) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HA | 11 | 1.09 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 4 | 1.09 |
| (1,5057) | 1:B:26:ILE:HG12 | 1:B:27:SER:HG | 16 | 1.09 |
| (1,5031) | 1:B:23:THR:HB | 1:B:26:ILE:HG12 | 12 | 1.09 |
| (1,5007) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HB2 | 2 | 1.09 |
| (1,5007) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HB2 | 2 | 1.09 |
| (1,4856) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HE2 | 12 | 1.09 |
| (1,4856) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HE2 | 12 | 1.09 |
| (1,4856) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HE2 | 12 | 1.09 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB2 | 16 | 1.09 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB3 | 16 | 1.09 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG21 | 5 | 1.09 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG22 | 5 | 1.09 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG23 | 5 | 1.09 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG21 | 16 | 1.09 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG22 | 16 | 1.09 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG23 | 16 | 1.09 |
| (1,4814) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HA | 8 | 1.09 |
| (1,4814) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HA | 18 | 1.09 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 18 | 1.09 |
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 12 | 1.09 |
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 16 | 1.09 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 9 | 1.09 |
| (1,4548) | 1:B:5:LEU:HB3 | 1:B:52:PHE:HE1 | 12 | 1.09 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 15 | 1.09 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 15 | 1.09 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 15 | 1.09 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 5 | 1.09 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 5 | 1.09 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 5 | 1.09 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 8 | 1.09 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 8 | 1.09 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 8 | 1.09 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 5 | 1.09 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 2 | 1.08 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 2 | 1.08 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 2 | 1.08 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 19 | 1.08 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD2 | 1 | 1.08 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD3 | 1 | 1.08 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB2 | 9 | 1.08 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB3 | 9 | 1.08 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG21 | 9 | 1.08 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG22 | 9 | 1.08 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG23 | 9 | 1.08 |
| (1,5118) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HA | 14 | 1.08 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 3 | 1.08 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB2 | 8 | 1.08 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB3 | 8 | 1.08 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 10 | 1.08 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 12 | 1.08 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 12 | 1.08 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 12 | 1.08 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 19 | 1.08 |
| (1,1935) | 1:B:18:MET:HE1 | 1:B:45:PHE:HE1 | 13 | 1.08 |
| (1,1935) | 1:B:18:MET:HE2 | 1:B:45:PHE:HE1 | 13 | 1.08 |
| (1,1935) | 1:B:18:MET:HE3 | 1:B:45:PHE:HE1 | 13 | 1.08 |
| (1,5247) | 1:B:76:GLU:HA | 1:B:77:ARG:HB2 | 8 | 1.07 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 8 | 1.07 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 13 | 1.07 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 13 | 1.07 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 13 | 1.07 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB2 | 7 | 1.07 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB3 | 7 | 1.07 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB2 | 11 | 1.07 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB3 | 11 | 1.07 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 10 | 1.07 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG11 | 13 | 1.07 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG12 | 13 | 1.07 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG13 | 13 | 1.07 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 18 | 1.07 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 18 | 1.07 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 18 | 1.07 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG21 | 17 | 1.07 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG22 | 17 | 1.07 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG23 | 17 | 1.07 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 14 | 1.07 |
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 1 | 1.07 |
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 19 | 1.07 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 18 | 1.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 18 | 1.07 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 18 | 1.07 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 10 | 1.07 |
| (1,3038) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HZ1 | 4 | 1.07 |
| (1,3038) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HZ1 | 4 | 1.07 |
| (1,3038) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HZ1 | 4 | 1.07 |
| (1,5173) | 1:B:54:LYS:HG2 | 1:B:55:ASN:HD21 | 13 | 1.06 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 12 | 1.06 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 12 | 1.06 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 12 | 1.06 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB2 | 14 | 1.06 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB3 | 14 | 1.06 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 6 | 1.06 |
| (1,5088) | 1:B:29:PHE:HZ | 1:B:65:LYS:HD2 | 19 | 1.06 |
| (1,5057) | 1:B:26:ILE:HG12 | 1:B:27:SER:HG | 2 | 1.06 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 6 | 1.06 |
| (1,4870) | 1:A:54:LYS:HG2 | 1:A:55:ASN:HD21 | 11 | 1.06 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG21 | 9 | 1.06 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG22 | 9 | 1.06 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG23 | 9 | 1.06 |
| (1,4814) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HA | 6 | 1.06 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 1 | 1.06 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 3 | 1.06 |
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 4 | 1.06 |
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 8 | 1.06 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 11 | 1.06 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 11 | 1.06 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 11 | 1.06 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 14 | 1.06 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 14 | 1.06 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 14 | 1.06 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 2 | 1.06 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 7 | 1.05 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 3 | 1.05 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 3 | 1.05 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 3 | 1.05 |
| (1,5118) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HA | 16 | 1.05 |
| (1,5106) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG2 | 6 | 1.05 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG11 | 16 | 1.05 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG12 | 16 | 1.05 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG13 | 16 | 1.05 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG21 | 11 | 1.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG22 | 11 | 1.05 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG23 | 11 | 1.05 |
| (1,4801) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG2 | 9 | 1.05 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 5 | 1.05 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 5 | 1.05 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 5 | 1.05 |
| (1,4489) | 1:A:18:MET:HB3 | 1:A:45:PHE:HE1 | 3 | 1.05 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 6 | 1.05 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 6 | 1.05 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 6 | 1.05 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG21 | 20 | 1.05 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG22 | 20 | 1.05 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG23 | 20 | 1.05 |
| (1,3370) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HB | 8 | 1.05 |
| (1,1935) | 1:B:18:MET:HE1 | 1:B:45:PHE:HE1 | 7 | 1.05 |
| (1,1935) | 1:B:18:MET:HE2 | 1:B:45:PHE:HE1 | 7 | 1.05 |
| (1,1935) | 1:B:18:MET:HE3 | 1:B:45:PHE:HE1 | 7 | 1.05 |
| (1,1935) | 1:B:18:MET:HE1 | 1:B:45:PHE:HE1 | 10 | 1.05 |
| (1,1935) | 1:B:18:MET:HE2 | 1:B:45:PHE:HE1 | 10 | 1.05 |
| (1,1935) | 1:B:18:MET:HE3 | 1:B:45:PHE:HE1 | 10 | 1.05 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 13 | 1.04 |
| (1,5118) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HA | 2 | 1.04 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 14 | 1.04 |
| (1,5043) | 1:B:25:VAL:H | 1:B:26:ILE:HG12 | 3 | 1.04 |
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 8 | 1.04 |
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 19 | 1.04 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 1 | 1.04 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE2 | 8 | 1.04 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE3 | 8 | 1.04 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB2 | 5 | 1.04 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB3 | 5 | 1.04 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB2 | 17 | 1.04 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB3 | 17 | 1.04 |
| (1,4814) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HA | 1 | 1.04 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 15 | 1.04 |
| (1,1935) | 1:B:18:MET:HE1 | 1:B:45:PHE:HE1 | 1 | 1.04 |
| (1,1935) | 1:B:18:MET:HE2 | 1:B:45:PHE:HE1 | 1 | 1.04 |
| (1,1935) | 1:B:18:MET:HE3 | 1:B:45:PHE:HE1 | 1 | 1.04 |
| (1,1934) | 1:A:18:MET:HE1 | 1:A:45:PHE:HE1 | 9 | 1.04 |
| (1,1934) | 1:A:18:MET:HE2 | 1:A:45:PHE:HE1 | 9 | 1.04 |
| (1,1934) | 1:A:18:MET:HE3 | 1:A:45:PHE:HE1 | 9 | 1.04 |
| (1,1934) | 1:A:18:MET:HE1 | 1:A:45:PHE:HE1 | 11 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1934) | 1:A:18:MET:HE2 | 1:A:45:PHE:HE1 | 11 | 1.04 |
| (1,1934) | 1:A:18:MET:HE3 | 1:A:45:PHE:HE1 | 11 | 1.04 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 16 | 1.03 |
| (1,5118) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HA | 17 | 1.03 |
| (1,5107) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG3 | 10 | 1.03 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 17 | 1.03 |
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 20 | 1.03 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB2 | 3 | 1.03 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB3 | 3 | 1.03 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 14 | 1.03 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 12 | 1.03 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 15 | 1.03 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 12 | 1.03 |
| (1,4377) | 1:B:4:PHE:H | 1:B:4:PHE:HE1 | 17 | 1.03 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 11 | 1.03 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 11 | 1.03 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 11 | 1.03 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 17 | 1.03 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 17 | 1.03 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 17 | 1.03 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 10 | 1.03 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 10 | 1.03 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 10 | 1.03 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 1 | 1.03 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 1 | 1.03 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 1 | 1.03 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 2 | 1.03 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 2 | 1.03 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 2 | 1.03 |
| (1,1752) | 1:A:11:VAL:HG21 | 1:A:45:PHE:HE1 | 14 | 1.03 |
| (1,1752) | 1:A:11:VAL:HG22 | 1:A:45:PHE:HE1 | 14 | 1.03 |
| (1,1752) | 1:A:11:VAL:HG23 | 1:A:45:PHE:HE1 | 14 | 1.03 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 8 | 1.02 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 8 | 1.02 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 8 | 1.02 |
| (1,5118) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HA | 15 | 1.02 |
| (1,5057) | 1:B:26:ILE:HG12 | 1:B:27:SER:HG | 8 | 1.02 |
| (1,5057) | 1:B:26:ILE:HG12 | 1:B:27:SER:HG | 14 | 1.02 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 7 | 1.02 |
| (1,4863) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HG2 | 10 | 1.02 |
| (1,4863) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HG2 | 10 | 1.02 |
| (1,4863) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HG2 | 10 | 1.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 3 | 1.02 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 2 | 1.02 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 2 | 1.02 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 2 | 1.02 |
| (1,4820) | 1:A:37:VAL:HG11 | 1:A:39:ASN:HD21 | 11 | 1.02 |
| (1,4820) | 1:A:37:VAL:HG12 | 1:A:39:ASN:HD21 | 11 | 1.02 |
| (1,4820) | 1:A:37:VAL:HG13 | 1:A:39:ASN:HD21 | 11 | 1.02 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 18 | 1.02 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 18 | 1.02 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 14 | 1.02 |
| (1,1935) | 1:B:18:MET:HE1 | 1:B:45:PHE:HE1 | 8 | 1.02 |
| (1,1935) | 1:B:18:MET:HE2 | 1:B:45:PHE:HE1 | 8 | 1.02 |
| (1,1935) | 1:B:18:MET:HE3 | 1:B:45:PHE:HE1 | 8 | 1.02 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 3 | 1.02 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 3 | 1.02 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 3 | 1.02 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 4 | 1.01 |
| (1,5162) | 1:B:53:VAL:HA | 1:B:54:LYS:HB2 | 4 | 1.01 |
| (1,5118) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HA | 5 | 1.01 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 16 | 1.01 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 10 | 1.01 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 5 | 1.01 |
| (1,4376) | 1:A:4:PHE:H | 1:A:4:PHE:HE1 | 15 | 1.01 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 17 | 1.01 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 17 | 1.01 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 17 | 1.01 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 12 | 1.01 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 12 | 1.01 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 12 | 1.01 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 18 | 1.01 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 18 | 1.01 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 18 | 1.01 |
| (1,1066) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:H | 8 | 1.01 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 12 | 1.0 |
| (1,5173) | 1:B:54:LYS:HG2 | 1:B:55:ASN:HD21 | 1 | 1.0 |
| (1,5173) | 1:B:54:LYS:HG2 | 1:B:55:ASN:HD21 | 17 | 1.0 |
| (1,5162) | 1:B:53:VAL:HA | 1:B:54:LYS:HB2 | 15 | 1.0 |
| (1,5162) | 1:B:53:VAL:HA | 1:B:54:LYS:HB2 | 18 | 1.0 |
| (1,5107) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG3 | 3 | 1.0 |
| (1,5099) | 1:B:32:ASN:HD21 | 1:B:33:ILE:HB | 2 | 1.0 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 14 | 1.0 |
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 4 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5057) | 1:B:26:ILE:HG12 | 1:B:27:SER:HG | 6 | 1.0 |
| (1,5043) | 1:B:25:VAL:H | 1:B:26:ILE:HG12 | 15 | 1.0 |
| (1,5031) | 1:B:23:THR:HB | 1:B:26:ILE:HG12 | 1 | 1.0 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 2 | 1.0 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 17 | 1.0 |
| (1,4870) | 1:A:54:LYS:HG2 | 1:A:55:ASN:HD21 | 5 | 1.0 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 15 | 1.0 |
| (1,4814) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HA | 13 | 1.0 |
| (1,4788) | 1:A:29:PHE:HZ | 1:A:65:LYS:HD2 | 20 | 1.0 |
| (1,4773) | 1:A:28:LYS:HA | 1:A:28:LYS:HD2 | 14 | 1.0 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD11 | 7 | 1.0 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD12 | 7 | 1.0 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD13 | 7 | 1.0 |
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 5 | 1.0 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 11 | 1.0 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 11 | 1.0 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 11 | 1.0 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 1 | 1.0 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 9 | 1.0 |
| (1,4685) | 1:A:15:LYS:HB2 | 1:A:18:MET:HG2 | 4 | 1.0 |
| (1,4684) | 1:A:15:LYS:HB2 | 1:A:18:MET:HB2 | 4 | 1.0 |
| (1,4489) | 1:A:18:MET:HB3 | 1:A:45:PHE:HE1 | 5 | 1.0 |
| (1,4489) | 1:A:18:MET:HB3 | 1:A:45:PHE:HE1 | 13 | 1.0 |
| (1,4368) | 1:A:4:PHE:HE1 | 1:A:56:THR:HA | 5 | 1.0 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 17 | 1.0 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 4 | 1.0 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 18 | 0.99 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 17 | 0.99 |
| (1,5174) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HB2 | 1 | 0.99 |
| (1,5174) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HB2 | 1 | 0.99 |
| (1,5118) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HA | 4 | 0.99 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 3 | 0.99 |
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 7 | 0.99 |
| (1,4814) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HA | 19 | 0.99 |
| (1,4795) | 1:A:32:ASN:HB2 | 1:B:20:ASN:H | 20 | 0.99 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 5 | 0.99 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 8 | 0.99 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 14 | 0.99 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 9 | 0.99 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 9 | 0.99 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 9 | 0.99 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 11 | 0.99 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4566) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HE1 | 19 | 0.99 |
| (1,4566) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HE1 | 19 | 0.99 |
| (1,4566) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HE1 | 19 | 0.99 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 2 | 0.99 |
| (1,4489) | 1:A:18:MET:HB3 | 1:A:45:PHE:HE1 | 20 | 0.99 |
| (1,4369) | 1:B:4:PHE:HE1 | 1:B:56:THR:HA | 3 | 0.99 |
| (1,3038) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HZ1 | 2 | 0.99 |
| (1,3038) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HZ1 | 2 | 0.99 |
| (1,3038) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HZ1 | 2 | 0.99 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 18 | 0.98 |
| (1,5162) | 1:B:53:VAL:HA | 1:B:54:LYS:HB2 | 11 | 0.98 |
| (1,5162) | 1:B:53:VAL:HA | 1:B:54:LYS:HB2 | 16 | 0.98 |
| (1,5162) | 1:B:53:VAL:HA | 1:B:54:LYS:HB2 | 19 | 0.98 |
| (1,5057) | 1:B:26:ILE:HG12 | 1:B:27:SER:HG | 10 | 0.98 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 8 | 0.98 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 18 | 0.98 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG11 | 18 | 0.98 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG12 | 18 | 0.98 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG13 | 18 | 0.98 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 1 | 0.98 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 1 | 0.98 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 1 | 0.98 |
| (1,4368) | 1:A:4:PHE:HE1 | 1:A:56:THR:HA | 10 | 0.98 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG21 | 2 | 0.98 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG22 | 2 | 0.98 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG23 | 2 | 0.98 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 17 | 0.98 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 17 | 0.98 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 17 | 0.98 |
| (1,3095) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HZ1 | 3 | 0.98 |
| (1,3095) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HZ1 | 3 | 0.98 |
| (1,3095) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HZ1 | 3 | 0.98 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 20 | 0.98 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 20 | 0.98 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 20 | 0.98 |
| (1,2994) | 1:A:8:ILE:HG21 | 1:A:29:PHE:HE1 | 4 | 0.98 |
| (1,2994) | 1:A:8:ILE:HG22 | 1:A:29:PHE:HE1 | 4 | 0.98 |
| (1,2994) | 1:A:8:ILE:HG23 | 1:A:29:PHE:HE1 | 4 | 0.98 |
| (1,2549) | 1:A:38:LEU:HD21 | 1:A:45:PHE:HE1 | 18 | 0.98 |
| (1,2549) | 1:A:38:LEU:HD22 | 1:A:45:PHE:HE1 | 18 | 0.98 |
| (1,2549) | 1:A:38:LEU:HD23 | 1:A:45:PHE:HE1 | 18 | 0.98 |
| (1,1935) | 1:B:18:MET:HE1 | 1:B:45:PHE:HE1 | 12 | 0.98 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1935) | 1:B:18:MET:HE2 | 1:B:45:PHE:HE1 | 12 | 0.98 |
| (1,1935) | 1:B:18:MET:HE3 | 1:B:45:PHE:HE1 | 12 | 0.98 |
| (1,1935) | 1:B:18:MET:HE1 | 1:B:45:PHE:HE1 | 20 | 0.98 |
| (1,1935) | 1:B:18:MET:HE2 | 1:B:45:PHE:HE1 | 20 | 0.98 |
| (1,1935) | 1:B:18:MET:HE3 | 1:B:45:PHE:HE1 | 20 | 0.98 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 3 | 0.98 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 3 | 0.98 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 3 | 0.98 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 6 | 0.98 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 6 | 0.98 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 6 | 0.98 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 20 | 0.97 |
| (1,5173) | 1:B:54:LYS:HG2 | 1:B:55:ASN:HD21 | 6 | 0.97 |
| (1,5166) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HG2 | 11 | 0.97 |
| (1,5166) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HG2 | 11 | 0.97 |
| (1,5166) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HG2 | 11 | 0.97 |
| (1,5162) | 1:B:53:VAL:HA | 1:B:54:LYS:HB2 | 7 | 0.97 |
| (1,5118) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HA | 19 | 0.97 |
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 15 | 0.97 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB2 | 18 | 0.97 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB3 | 18 | 0.97 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 8 | 0.97 |
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 3 | 0.97 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 3 | 0.97 |
| (1,4659) | 1:A:9:ARG:HG2 | 1:A:47:CYS:H | 9 | 0.97 |
| (1,4377) | 1:B:4:PHE:H | 1:B:4:PHE:HE1 | 14 | 0.97 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 15 | 0.97 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 15 | 0.97 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 15 | 0.97 |
| (1,1935) | 1:B:18:MET:HE1 | 1:B:45:PHE:HE1 | 5 | 0.97 |
| (1,1935) | 1:B:18:MET:HE2 | 1:B:45:PHE:HE1 | 5 | 0.97 |
| (1,1935) | 1:B:18:MET:HE3 | 1:B:45:PHE:HE1 | 5 | 0.97 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 6 | 0.97 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 6 | 0.97 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 6 | 0.97 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 16 | 0.97 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 16 | 0.97 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 16 | 0.97 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 5 | 0.96 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 5 | 0.96 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 5 | 0.96 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 6 | 0.96 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 6 | 0.96 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 6 | 0.96 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 9 | 0.96 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 9 | 0.96 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 9 | 0.96 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB2 | 1 | 0.96 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB3 | 1 | 0.96 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 7 | 0.96 |
| (1,4964) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HG2 | 16 | 0.96 |
| (1,4964) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HG2 | 16 | 0.96 |
| (1,4964) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HG2 | 16 | 0.96 |
| (1,4874) | 1:A:55:ASN:H | 1:A:58:LYS:HB2 | 6 | 0.96 |
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 14 | 0.96 |
| (1,4820) | 1:A:37:VAL:HG11 | 1:A:39:ASN:HD21 | 13 | 0.96 |
| (1,4820) | 1:A:37:VAL:HG12 | 1:A:39:ASN:HD21 | 13 | 0.96 |
| (1,4820) | 1:A:37:VAL:HG13 | 1:A:39:ASN:HD21 | 13 | 0.96 |
| (1,4814) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HA | 5 | 0.96 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE2 | 1 | 0.96 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE3 | 1 | 0.96 |
| (1,4703) | 1:A:17:GLY:HA2 | 1:A:21:GLN:HE22 | 6 | 0.96 |
| (1,4684) | 1:A:15:LYS:HB2 | 1:A:18:MET:HB2 | 17 | 0.96 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 19 | 0.96 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 19 | 0.96 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 19 | 0.96 |
| (1,4475) | 1:A:22:ILE:HD11 | 1:A:45:PHE:HE1 | 14 | 0.96 |
| (1,4475) | 1:A:22:ILE:HD12 | 1:A:45:PHE:HE1 | 14 | 0.96 |
| (1,4475) | 1:A:22:ILE:HD13 | 1:A:45:PHE:HE1 | 14 | 0.96 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 20 | 0.96 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 20 | 0.96 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 20 | 0.96 |
| (1,3370) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HB | 19 | 0.96 |
| (1,1934) | 1:A:18:MET:HE1 | 1:A:45:PHE:HE1 | 16 | 0.96 |
| (1,1934) | 1:A:18:MET:HE2 | 1:A:45:PHE:HE1 | 16 | 0.96 |
| (1,1934) | 1:A:18:MET:HE3 | 1:A:45:PHE:HE1 | 16 | 0.96 |
| (1,1066) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:H | 11 | 0.96 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 5 | 0.95 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 14 | 0.95 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 10 | 0.95 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 17 | 0.95 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 17 | 0.95 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 17 | 0.95 |
| (1,5162) | 1:B:53:VAL:HA | 1:B:54:LYS:HB2 | 2 | 0.95 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5162) | 1:B:53:VAL:HA | 1:B:54:LYS:HB2 | 5 | 0.95 |
| (1,5118) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HA | 13 | 0.95 |
| (1,5057) | 1:B:26:ILE:HG12 | 1:B:27:SER:HG | 3 | 0.95 |
| (1,5057) | 1:B:26:ILE:HG12 | 1:B:27:SER:HG | 11 | 0.95 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 9 | 0.95 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 19 | 0.95 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 15 | 0.95 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 16 | 0.95 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE2 | 16 | 0.95 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE3 | 16 | 0.95 |
| (1,5031) | 1:B:23:THR:HB | 1:B:26:ILE:HG12 | 19 | 0.95 |
| (1,4952) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HB2 | 8 | 0.95 |
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 5 | 0.95 |
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 16 | 0.95 |
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 18 | 0.95 |
| (1,4801) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG2 | 19 | 0.95 |
| (1,4774) | 1:A:28:LYS:HB2 | 1:A:28:LYS:HD2 | 13 | 0.95 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 10 | 0.95 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 13 | 0.95 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 8 | 0.95 |
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 8 | 0.95 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 8 | 0.95 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE2 | 7 | 0.95 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE3 | 7 | 0.95 |
| (1,4703) | 1:A:17:GLY:HA2 | 1:A:21:GLN:HE22 | 2 | 0.95 |
| (1,4377) | 1:B:4:PHE:H | 1:B:4:PHE:HE1 | 13 | 0.95 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG21 | 16 | 0.95 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG22 | 16 | 0.95 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG23 | 16 | 0.95 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 18 | 0.95 |
| (1,2549) | 1:A:38:LEU:HD21 | 1:A:45:PHE:HE1 | 1 | 0.95 |
| (1,2549) | 1:A:38:LEU:HD22 | 1:A:45:PHE:HE1 | 1 | 0.95 |
| (1,2549) | 1:A:38:LEU:HD23 | 1:A:45:PHE:HE1 | 1 | 0.95 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 3 | 0.95 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 3 | 0.95 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 3 | 0.95 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 13 | 0.95 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 13 | 0.95 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 13 | 0.95 |
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 13 | 0.94 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 10 | 0.94 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 10 | 0.94 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 10 | 0.94 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 13 | 0.94 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 13 | 0.94 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 13 | 0.94 |
| (1,5162) | 1:B:53:VAL:HA | 1:B:54:LYS:HB2 | 9 | 0.94 |
| (1,5162) | 1:B:53:VAL:HA | 1:B:54:LYS:HB2 | 20 | 0.94 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 16 | 0.94 |
| (1,5043) | 1:B:25:VAL:H | 1:B:26:ILE:HG12 | 18 | 0.94 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 11 | 0.94 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 11 | 0.94 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 11 | 0.94 |
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 7 | 0.94 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 9 | 0.94 |
| (1,4720) | 1:A:20:ASN:H | 1:B:32:ASN:HB2 | 4 | 0.94 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 3 | 0.94 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 3 | 0.94 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 3 | 0.94 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 17 | 0.94 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 17 | 0.94 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 17 | 0.94 |
| (1,4377) | 1:B:4:PHE:H | 1:B:4:PHE:HE1 | 10 | 0.94 |
| (1,3038) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HZ1 | 15 | 0.94 |
| (1,3038) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HZ1 | 15 | 0.94 |
| (1,3038) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HZ1 | 15 | 0.94 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 6 | 0.93 |
| (1,5247) | 1:B:76:GLU:HA | 1:B:77:ARG:HB2 | 16 | 0.93 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 8 | 0.93 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 13 | 0.93 |
| (1,5118) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HA | 12 | 0.93 |
| (1,5107) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG3 | 15 | 0.93 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 16 | 0.93 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 16 | 0.93 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 16 | 0.93 |
| (1,5031) | 1:B:23:THR:HB | 1:B:26:ILE:HG12 | 10 | 0.93 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 2 | 0.93 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 6 | 0.93 |
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 12 | 0.93 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 2 | 0.93 |
| (1,4682) | 1:A:15:LYS:HB2 | 1:A:16:ASN:HB2 | 8 | 0.93 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 18 | 0.93 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 18 | 0.93 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 18 | 0.93 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 3 | 0.93 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 3 | 0.93 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 3 | 0.93 |
| (1,4488) | 1:B:18:MET:HB3 | 1:B:45:PHE:HE1 | 15 | 0.93 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG21 | 13 | 0.93 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG22 | 13 | 0.93 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG23 | 13 | 0.93 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 12 | 0.93 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 12 | 0.93 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 12 | 0.93 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 1 | 0.93 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 1 | 0.93 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 1 | 0.93 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 14 | 0.93 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 14 | 0.93 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 14 | 0.93 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 14 | 0.93 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 20 | 0.92 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 20 | 0.92 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 20 | 0.92 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 15 | 0.92 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 15 | 0.92 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 15 | 0.92 |
| (1,5124) | 1:B:37:VAL:HG11 | 1:B:39:ASN:HD21 | 16 | 0.92 |
| (1,5124) | 1:B:37:VAL:HG12 | 1:B:39:ASN:HD21 | 16 | 0.92 |
| (1,5124) | 1:B:37:VAL:HG13 | 1:B:39:ASN:HD21 | 16 | 0.92 |
| (1,5124) | 1:B:37:VAL:HG11 | 1:B:39:ASN:HD21 | 17 | 0.92 |
| (1,5124) | 1:B:37:VAL:HG12 | 1:B:39:ASN:HD21 | 17 | 0.92 |
| (1,5124) | 1:B:37:VAL:HG13 | 1:B:39:ASN:HD21 | 17 | 0.92 |
| (1,5118) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HA | 9 | 0.92 |
| (1,5099) | 1:B:32:ASN:HD21 | 1:B:33:ILE:HB | 15 | 0.92 |
| (1,5031) | 1:B:23:THR:HB | 1:B:26:ILE:HG12 | 8 | 0.92 |
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 2 | 0.92 |
| (1,4814) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HA | 16 | 0.92 |
| (1,4814) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HA | 17 | 0.92 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 10 | 0.92 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 11 | 0.92 |
| (1,4684) | 1:A:15:LYS:HB2 | 1:A:18:MET:HB2 | 2 | 0.92 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 20 | 0.92 |
| (1,4566) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HE1 | 17 | 0.92 |
| (1,4566) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HE1 | 17 | 0.92 |
| (1,4566) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HE1 | 17 | 0.92 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 5 | 0.92 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 19 | 0.92 |
| (1,4363) | 1:B:29:PHE:HE1 | 1:B:66:LEU:HG | 15 | 0.92 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 5 | 0.92 |
| (1,3094) | 1:A:53:VAL:HG11 | 1:A:58:LYS:HZ1 | 10 | 0.92 |
| (1,3094) | 1:A:53:VAL:HG12 | 1:A:58:LYS:HZ1 | 10 | 0.92 |
| (1,3094) | 1:A:53:VAL:HG13 | 1:A:58:LYS:HZ1 | 10 | 0.92 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG21 | 18 | 0.92 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG22 | 18 | 0.92 |
| (1,2997) | 1:B:29:PHE:HE1 | 1:B:51:ILE:HG23 | 18 | 0.92 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 19 | 0.92 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 19 | 0.92 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 19 | 0.92 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 11 | 0.92 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 11 | 0.92 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 11 | 0.92 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 15 | 0.92 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 15 | 0.92 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 15 | 0.92 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 17 | 0.92 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 2 | 0.91 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 2 | 0.91 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 2 | 0.91 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 18 | 0.91 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 18 | 0.91 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 18 | 0.91 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 15 | 0.91 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 11 | 0.91 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 11 | 0.91 |
| (1,5107) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG3 | 6 | 0.91 |
| (1,5107) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG3 | 12 | 0.91 |
| (1,5057) | 1:B:26:ILE:HG12 | 1:B:27:SER:HG | 7 | 0.91 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 10 | 0.91 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 15 | 0.91 |
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 15 | 0.91 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 15 | 0.91 |
| (1,5043) | 1:B:25:VAL:H | 1:B:26:ILE:HG12 | 12 | 0.91 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 6 | 0.91 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 6 | 0.91 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG11 | 5 | 0.91 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG12 | 5 | 0.91 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG13 | 5 | 0.91 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 15 | 0.91 |
| (1,4871) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HB2 | 17 | 0.91 |
| (1,4871) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HB2 | 17 | 0.91 |
| (1,4870) | 1:A:54:LYS:HG2 | 1:A:55:ASN:HD21 | 1 | 0.91 |
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 13 | 0.91 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 17 | 0.91 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 17 | 0.91 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 17 | 0.91 |
| (1,4820) | 1:A:37:VAL:HG11 | 1:A:39:ASN:HD21 | 14 | 0.91 |
| (1,4820) | 1:A:37:VAL:HG12 | 1:A:39:ASN:HD21 | 14 | 0.91 |
| (1,4820) | 1:A:37:VAL:HG13 | 1:A:39:ASN:HD21 | 14 | 0.91 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 20 | 0.91 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 20 | 0.91 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 20 | 0.91 |
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 10 | 0.91 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE2 | 5 | 0.91 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE3 | 5 | 0.91 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 11 | 0.91 |
| (1,4566) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HE1 | 13 | 0.91 |
| (1,4566) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HE1 | 13 | 0.91 |
| (1,4566) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HE1 | 13 | 0.91 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 9 | 0.91 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 9 | 0.91 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 9 | 0.91 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 5 | 0.91 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 5 | 0.91 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 5 | 0.91 |
| (1,4376) | 1:A:4:PHE:H | 1:A:4:PHE:HE1 | 19 | 0.91 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 14 | 0.91 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 3 | 0.91 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 3 | 0.91 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 3 | 0.91 |
| (1,1935) | 1:B:18:MET:HE1 | 1:B:45:PHE:HE1 | 18 | 0.91 |
| (1,1935) | 1:B:18:MET:HE2 | 1:B:45:PHE:HE1 | 18 | 0.91 |
| (1,1935) | 1:B:18:MET:HE3 | 1:B:45:PHE:HE1 | 18 | 0.91 |
| (1,1934) | 1:A:18:MET:HE1 | 1:A:45:PHE:HE1 | 6 | 0.91 |
| (1,1934) | 1:A:18:MET:HE2 | 1:A:45:PHE:HE1 | 6 | 0.91 |
| (1,1934) | 1:A:18:MET:HE3 | 1:A:45:PHE:HE1 | 6 | 0.91 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 12 | 0.91 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 2 | 0.9 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 16 | 0.9 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 19 | 0.9 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 19 | 0.9 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 19 | 0.9 |
| (1,5095) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG12 | 11 | 0.9 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 4 | 0.9 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 4 | 0.9 |
| (1,5057) | 1:B:26:ILE:HG12 | 1:B:27:SER:HG | 1 | 0.9 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 20 | 0.9 |
| (1,5043) | 1:B:25:VAL:H | 1:B:26:ILE:HG12 | 7 | 0.9 |
| (1,5031) | 1:B:23:THR:HB | 1:B:26:ILE:HG12 | 6 | 0.9 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 5 | 0.9 |
| (1,5008) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD21 | 13 | 0.9 |
| (1,5008) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD21 | 13 | 0.9 |
| (1,5007) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HB2 | 3 | 0.9 |
| (1,5007) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HB2 | 3 | 0.9 |
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 17 | 0.9 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 3 | 0.9 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 11 | 0.9 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 12 | 0.9 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 20 | 0.9 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 3 | 0.9 |
| (1,4703) | 1:A:17:GLY:HA2 | 1:A:21:GLN:HE22 | 16 | 0.9 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 19 | 0.9 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 8 | 0.9 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 8 | 0.9 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 8 | 0.9 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 1 | 0.9 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 1 | 0.9 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 1 | 0.9 |
| (1,4377) | 1:B:4:PHE:H | 1:B:4:PHE:HE1 | 1 | 0.9 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG21 | 3 | 0.9 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG22 | 3 | 0.9 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG23 | 3 | 0.9 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG21 | 10 | 0.9 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG22 | 10 | 0.9 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG23 | 10 | 0.9 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 7 | 0.9 |
| (1,1066) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:H | 9 | 0.9 |
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 7 | 0.89 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 4 | 0.89 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 11 | 0.89 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 11 | 0.89 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 11 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 16 | 0.89 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 16 | 0.89 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 16 | 0.89 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 19 | 0.89 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 19 | 0.89 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 19 | 0.89 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 16 | 0.89 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 16 | 0.89 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 16 | 0.89 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 7 | 0.89 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD2 | 20 | 0.89 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD3 | 20 | 0.89 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 4 | 0.89 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 4 | 0.89 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 4 | 0.89 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 1 | 0.89 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 1 | 0.89 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 2 | 0.89 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 9 | 0.89 |
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 9 | 0.89 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 9 | 0.89 |
| (1,5031) | 1:B:23:THR:HB | 1:B:26:ILE:HG12 | 15 | 0.89 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 1 | 0.89 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 1 | 0.89 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 1 | 0.89 |
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 11 | 0.89 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 3 | 0.89 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE2 | 4 | 0.89 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE3 | 4 | 0.89 |
| (1,4702) | 1:A:17:GLY:HA2 | 1:A:21:GLN:HE21 | 17 | 0.89 |
| (1,4687) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HD21 | 1 | 0.89 |
| (1,4687) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HD21 | 1 | 0.89 |
| (1,4566) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HE1 | 4 | 0.89 |
| (1,4566) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HE1 | 4 | 0.89 |
| (1,4566) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HE1 | 4 | 0.89 |
| (1,4489) | 1:A:18:MET:HB3 | 1:A:45:PHE:HE1 | 16 | 0.89 |
| (1,4376) | 1:A:4:PHE:H | 1:A:4:PHE:HE1 | 6 | 0.89 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 11 | 0.89 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 15 | 0.89 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 15 | 0.89 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 15 | 0.89 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 18 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 18 | 0.89 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 18 | 0.89 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 18 | 0.89 |
| (1,5238) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG11 | 5 | 0.88 |
| (1,5238) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG12 | 5 | 0.88 |
| (1,5238) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG13 | 5 | 0.88 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 2 | 0.88 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 4 | 0.88 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 4 | 0.88 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 4 | 0.88 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 4 | 0.88 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 7 | 0.88 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 7 | 0.88 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 7 | 0.88 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 14 | 0.88 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 14 | 0.88 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 14 | 0.88 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 11 | 0.88 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 11 | 0.88 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 11 | 0.88 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 1 | 0.88 |
| (1,5124) | 1:B:37:VAL:HG11 | 1:B:39:ASN:HD21 | 5 | 0.88 |
| (1,5124) | 1:B:37:VAL:HG12 | 1:B:39:ASN:HD21 | 5 | 0.88 |
| (1,5124) | 1:B:37:VAL:HG13 | 1:B:39:ASN:HD21 | 5 | 0.88 |
| (1,5043) | 1:B:25:VAL:H | 1:B:26:ILE:HG12 | 1 | 0.88 |
| (1,5031) | 1:B:23:THR:HB | 1:B:26:ILE:HG12 | 13 | 0.88 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 3 | 0.88 |
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 3 | 0.88 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 3 | 0.88 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 8 | 0.88 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE2 | 19 | 0.88 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE3 | 19 | 0.88 |
| (1,4721) | 1:A:20:ASN:H | 1:B:32:ASN:HD21 | 2 | 0.88 |
| (1,4721) | 1:A:20:ASN:H | 1:B:32:ASN:HD21 | 15 | 0.88 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 17 | 0.88 |
| (1,4690) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD21 | 16 | 0.88 |
| (1,4690) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD21 | 16 | 0.88 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 1 | 0.88 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 1 | 0.88 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 1 | 0.88 |
| (1,4377) | 1:B:4:PHE:H | 1:B:4:PHE:HE1 | 6 | 0.88 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 13 | 0.88 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1934) | 1:A:18:MET:HE1 | 1:A:45:PHE:HE1 | 7 | 0.88 |
| (1,1934) | 1:A:18:MET:HE2 | 1:A:45:PHE:HE1 | 7 | 0.88 |
| (1,1934) | 1:A:18:MET:HE3 | 1:A:45:PHE:HE1 | 7 | 0.88 |
| (1,1934) | 1:A:18:MET:HE1 | 1:A:45:PHE:HE1 | 8 | 0.88 |
| (1,1934) | 1:A:18:MET:HE2 | 1:A:45:PHE:HE1 | 8 | 0.88 |
| (1,1934) | 1:A:18:MET:HE3 | 1:A:45:PHE:HE1 | 8 | 0.88 |
| (1,5256) | 1:B:77:ARG:HG2 | 1:B:79:SER:HA | 8 | 0.87 |
| (1,5238) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG11 | 6 | 0.87 |
| (1,5238) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG12 | 6 | 0.87 |
| (1,5238) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG13 | 6 | 0.87 |
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 15 | 0.87 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 11 | 0.87 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 11 | 0.87 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 11 | 0.87 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 11 | 0.87 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 12 | 0.87 |
| (1,5057) | 1:B:26:ILE:HG12 | 1:B:27:SER:HG | 15 | 0.87 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 11 | 0.87 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 3 | 0.87 |
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 3 | 0.87 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 3 | 0.87 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 6 | 0.87 |
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 6 | 0.87 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 6 | 0.87 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE2 | 20 | 0.87 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE3 | 20 | 0.87 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 8 | 0.87 |
| (1,5008) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD21 | 20 | 0.87 |
| (1,5008) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD21 | 20 | 0.87 |
| (1,4965) | 1:B:7:GLY:H | 1:B:77:ARG:HG2 | 16 | 0.87 |
| (1,4964) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HG2 | 8 | 0.87 |
| (1,4964) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HG2 | 8 | 0.87 |
| (1,4964) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HG2 | 8 | 0.87 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 7 | 0.87 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 7 | 0.87 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 7 | 0.87 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 12 | 0.87 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 2 | 0.87 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 4 | 0.87 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 4 | 0.87 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 4 | 0.87 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 14 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 14 | 0.87 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 14 | 0.87 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 18 | 0.87 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG21 | 15 | 0.87 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG22 | 15 | 0.87 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG23 | 15 | 0.87 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 9 | 0.87 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 16 | 0.87 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 9 | 0.87 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 9 | 0.87 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 9 | 0.87 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 3 | 0.87 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 3 | 0.87 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 3 | 0.87 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 11 | 0.87 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 11 | 0.87 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 11 | 0.87 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 18 | 0.87 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 18 | 0.87 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 18 | 0.87 |
| (1,5262) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HA | 1 | 0.86 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 9 | 0.86 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 5 | 0.86 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 12 | 0.86 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 12 | 0.86 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 14 | 0.86 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 14 | 0.86 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 19 | 0.86 |
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 19 | 0.86 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 19 | 0.86 |
| (1,5031) | 1:B:23:THR:HB | 1:B:26:ILE:HG12 | 2 | 0.86 |
| (1,4820) | 1:A:37:VAL:HG11 | 1:A:39:ASN:HD21 | 1 | 0.86 |
| (1,4820) | 1:A:37:VAL:HG12 | 1:A:39:ASN:HD21 | 1 | 0.86 |
| (1,4820) | 1:A:37:VAL:HG13 | 1:A:39:ASN:HD21 | 1 | 0.86 |
| (1,4820) | 1:A:37:VAL:HG11 | 1:A:39:ASN:HD21 | 6 | 0.86 |
| (1,4820) | 1:A:37:VAL:HG12 | 1:A:39:ASN:HD21 | 6 | 0.86 |
| (1,4820) | 1:A:37:VAL:HG13 | 1:A:39:ASN:HD21 | 6 | 0.86 |
| (1,4814) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HA | 9 | 0.86 |
| (1,4802) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG3 | 7 | 0.86 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 8 | 0.86 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 8 | 0.86 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 6 | 0.86 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 16 | 0.86 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 14 | 0.86 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 14 | 0.86 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 14 | 0.86 |
| (1,4697) | 1:A:17:GLY:H | 1:A:18:MET:HG2 | 2 | 0.86 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 18 | 0.86 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 18 | 0.86 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 18 | 0.86 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 15 | 0.86 |
| (1,3370) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HB | 3 | 0.86 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 6 | 0.86 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 6 | 0.86 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 6 | 0.86 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 9 | 0.86 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 9 | 0.86 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 9 | 0.86 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 19 | 0.85 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 20 | 0.85 |
| (1,5124) | 1:B:37:VAL:HG11 | 1:B:39:ASN:HD21 | 15 | 0.85 |
| (1,5124) | 1:B:37:VAL:HG12 | 1:B:39:ASN:HD21 | 15 | 0.85 |
| (1,5124) | 1:B:37:VAL:HG13 | 1:B:39:ASN:HD21 | 15 | 0.85 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 5 | 0.85 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 5 | 0.85 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 10 | 0.85 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 10 | 0.85 |
| (1,5005) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HD21 | 13 | 0.85 |
| (1,5005) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HD21 | 13 | 0.85 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG11 | 17 | 0.85 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG12 | 17 | 0.85 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG13 | 17 | 0.85 |
| (1,4873) | 1:A:54:LYS:HE2 | 1:A:55:ASN:HD21 | 19 | 0.85 |
| (1,4873) | 1:A:54:LYS:HE3 | 1:A:55:ASN:HD21 | 19 | 0.85 |
| (1,4834) | 1:A:39:ASN:HD21 | 1:A:46:THR:HB | 17 | 0.85 |
| (1,4802) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG3 | 9 | 0.85 |
| (1,4801) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG2 | 16 | 0.85 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 2 | 0.85 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 2 | 0.85 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 7 | 0.85 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 7 | 0.85 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 14 | 0.85 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 14 | 0.85 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 20 | 0.85 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 2 | 0.85 |
| (1,4689) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HB2 | 3 | 0.85 |
| (1,4689) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HB2 | 3 | 0.85 |
| (1,4684) | 1:A:15:LYS:HB2 | 1:A:18:MET:HB2 | 13 | 0.85 |
| (1,4661) | 1:A:9:ARG:HD2 | 1:A:48:ASN:HD21 | 15 | 0.85 |
| (1,4661) | 1:A:9:ARG:HD3 | 1:A:48:ASN:HD21 | 15 | 0.85 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 2 | 0.85 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 2 | 0.85 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 2 | 0.85 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 2 | 0.85 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 2 | 0.85 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 2 | 0.85 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 16 | 0.85 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 8 | 0.85 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 13 | 0.85 |
| (1,4377) | 1:B:4:PHE:H | 1:B:4:PHE:HE1 | 3 | 0.85 |
| (1,4376) | 1:A:4:PHE:H | 1:A:4:PHE:HE1 | 11 | 0.85 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 1 | 0.85 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG21 | 9 | 0.85 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG22 | 9 | 0.85 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG23 | 9 | 0.85 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 18 | 0.85 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 18 | 0.85 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 18 | 0.85 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 20 | 0.85 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 20 | 0.85 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 20 | 0.85 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 7 | 0.85 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 7 | 0.85 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 7 | 0.85 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 10 | 0.85 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 10 | 0.85 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 10 | 0.85 |
| (1,5263) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HD2 | 6 | 0.84 |
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 4 | 0.84 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 3 | 0.84 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 3 | 0.84 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 3 | 0.84 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 1 | 0.84 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 1 | 0.84 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 1 | 0.84 |
| (1,5126) | 1:B:37:VAL:HG11 | 1:B:48:ASN:HD21 | 20 | 0.84 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5126) | 1:B:37:VAL:HG12 | 1:B:48:ASN:HD21 | 20 | 0.84 |
| (1,5126) | 1:B:37:VAL:HG13 | 1:B:48:ASN:HD21 | 20 | 0.84 |
| (1,5124) | 1:B:37:VAL:HG11 | 1:B:39:ASN:HD21 | 19 | 0.84 |
| (1,5124) | 1:B:37:VAL:HG12 | 1:B:39:ASN:HD21 | 19 | 0.84 |
| (1,5124) | 1:B:37:VAL:HG13 | 1:B:39:ASN:HD21 | 19 | 0.84 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 14 | 0.84 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 14 | 0.84 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 14 | 0.84 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 15 | 0.84 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 15 | 0.84 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 15 | 0.84 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 3 | 0.84 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 3 | 0.84 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 9 | 0.84 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 9 | 0.84 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 11 | 0.84 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 11 | 0.84 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 16 | 0.84 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 16 | 0.84 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 15 | 0.84 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 7 | 0.84 |
| (1,4949) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HD2 | 15 | 0.84 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE2 | 19 | 0.84 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE3 | 19 | 0.84 |
| (1,4822) | 1:A:37:VAL:HG11 | 1:A:48:ASN:HD21 | 12 | 0.84 |
| (1,4822) | 1:A:37:VAL:HG12 | 1:A:48:ASN:HD21 | 12 | 0.84 |
| (1,4822) | 1:A:37:VAL:HG13 | 1:A:48:ASN:HD21 | 12 | 0.84 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 12 | 0.84 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 12 | 0.84 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 12 | 0.84 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 10 | 0.84 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 10 | 0.84 |
| (1,4767) | 1:A:27:SER:HG | 1:A:28:LYS:HD2 | 20 | 0.84 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 11 | 0.84 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 11 | 0.84 |
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 11 | 0.84 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 11 | 0.84 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 8 | 0.84 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 7 | 0.84 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 7 | 0.84 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 7 | 0.84 |
| (1,4376) | 1:A:4:PHE:H | 1:A:4:PHE:HE1 | 2 | 0.84 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4376) | 1:A:4:PHE:H | 1:A:4:PHE:HE1 | 20 | 0.84 |
| (1,4368) | 1:A:4:PHE:HE1 | 1:A:56:THR:HA | 6 | 0.84 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 5 | 0.84 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 5 | 0.84 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 5 | 0.84 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 15 | 0.84 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 15 | 0.84 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 15 | 0.84 |
| (1,5126) | 1:B:37:VAL:HG11 | 1:B:48:ASN:HD21 | 10 | 0.83 |
| (1,5126) | 1:B:37:VAL:HG12 | 1:B:48:ASN:HD21 | 10 | 0.83 |
| (1,5126) | 1:B:37:VAL:HG13 | 1:B:48:ASN:HD21 | 10 | 0.83 |
| (1,5126) | 1:B:37:VAL:HG11 | 1:B:48:ASN:HD21 | 17 | 0.83 |
| (1,5126) | 1:B:37:VAL:HG12 | 1:B:48:ASN:HD21 | 17 | 0.83 |
| (1,5126) | 1:B:37:VAL:HG13 | 1:B:48:ASN:HD21 | 17 | 0.83 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 7 | 0.83 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 7 | 0.83 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 8 | 0.83 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 8 | 0.83 |
| (1,5007) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HB2 | 12 | 0.83 |
| (1,5007) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HB2 | 12 | 0.83 |
| (1,4949) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HD2 | 5 | 0.83 |
| (1,4948) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HA | 9 | 0.83 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 20 | 0.83 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 20 | 0.83 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 20 | 0.83 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 8 | 0.83 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 8 | 0.83 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 8 | 0.83 |
| (1,4822) | 1:A:37:VAL:HG11 | 1:A:48:ASN:HD21 | 2 | 0.83 |
| (1,4822) | 1:A:37:VAL:HG12 | 1:A:48:ASN:HD21 | 2 | 0.83 |
| (1,4822) | 1:A:37:VAL:HG13 | 1:A:48:ASN:HD21 | 2 | 0.83 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 9 | 0.83 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 9 | 0.83 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 19 | 0.83 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 19 | 0.83 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 17 | 0.83 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 16 | 0.83 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE2 | 18 | 0.83 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE3 | 18 | 0.83 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE2 | 20 | 0.83 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE3 | 20 | 0.83 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 12 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4728) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HG12 | 13 | 0.83 |
| (1,4574) | 1:B:44:ILE:HG12 | 1:B:73:PHE:HE1 | 14 | 0.83 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 3 | 0.83 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 3 | 0.83 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 3 | 0.83 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 6 | 0.83 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 6 | 0.83 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 6 | 0.83 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 19 | 0.83 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 19 | 0.83 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 19 | 0.83 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 11 | 0.83 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 16 | 0.83 |
| (1,4376) | 1:A:4:PHE:H | 1:A:4:PHE:HE1 | 9 | 0.83 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 19 | 0.83 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 19 | 0.83 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG21 | 19 | 0.83 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG22 | 19 | 0.83 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG23 | 19 | 0.83 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 4 | 0.83 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 14 | 0.83 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 14 | 0.83 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 14 | 0.83 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 16 | 0.83 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 16 | 0.83 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 16 | 0.83 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 1 | 0.83 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 1 | 0.83 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 1 | 0.83 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 10 | 0.83 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 10 | 0.83 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 10 | 0.83 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 17 | 0.83 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 17 | 0.83 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 17 | 0.83 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 1 | 0.83 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 1 | 0.83 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 1 | 0.83 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 2 | 0.83 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 2 | 0.83 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 2 | 0.83 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 16 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 16 | 0.83 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 16 | 0.83 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 14 | 0.82 |
| (1,5126) | 1:B:37:VAL:HG11 | 1:B:48:ASN:HD21 | 13 | 0.82 |
| (1,5126) | 1:B:37:VAL:HG12 | 1:B:48:ASN:HD21 | 13 | 0.82 |
| (1,5126) | 1:B:37:VAL:HG13 | 1:B:48:ASN:HD21 | 13 | 0.82 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 5 | 0.82 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 5 | 0.82 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 5 | 0.82 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 15 | 0.82 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 15 | 0.82 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 15 | 0.82 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 20 | 0.82 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 20 | 0.82 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 7 | 0.82 |
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 7 | 0.82 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 7 | 0.82 |
| (1,5045) | 1:B:25:VAL:H | 1:B:28:LYS:HD2 | 2 | 0.82 |
| (1,5043) | 1:B:25:VAL:H | 1:B:26:ILE:HG12 | 8 | 0.82 |
| (1,5043) | 1:B:25:VAL:H | 1:B:26:ILE:HG12 | 10 | 0.82 |
| (1,5043) | 1:B:25:VAL:H | 1:B:26:ILE:HG12 | 13 | 0.82 |
| (1,5043) | 1:B:25:VAL:H | 1:B:26:ILE:HG12 | 19 | 0.82 |
| (1,5031) | 1:B:23:THR:HB | 1:B:26:ILE:HG12 | 3 | 0.82 |
| (1,4949) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HD2 | 4 | 0.82 |
| (1,4848) | 1:A:46:THR:HG1 | 1:A:48:ASN:HD21 | 9 | 0.82 |
| (1,4792) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG13 | 15 | 0.82 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 1 | 0.82 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 1 | 0.82 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 13 | 0.82 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 13 | 0.82 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 18 | 0.82 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 18 | 0.82 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 19 | 0.82 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 12 | 0.82 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 13 | 0.82 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 13 | 0.82 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 13 | 0.82 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 16 | 0.82 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 16 | 0.82 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 16 | 0.82 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 8 | 0.82 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 8 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 8 | 0.82 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 17 | 0.82 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 17 | 0.82 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 17 | 0.82 |
| (1,4377) | 1:B:4:PHE:H | 1:B:4:PHE:HE1 | 4 | 0.82 |
| (1,4369) | 1:B:4:PHE:HE1 | 1:B:56:THR:HA | 15 | 0.82 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 10 | 0.82 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 10 | 0.82 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 12 | 0.82 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG21 | 8 | 0.82 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG22 | 8 | 0.82 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG23 | 8 | 0.82 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG21 | 17 | 0.82 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG22 | 17 | 0.82 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG23 | 17 | 0.82 |
| (1,3370) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HB | 13 | 0.82 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 6 | 0.82 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 6 | 0.82 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 6 | 0.82 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 8 | 0.82 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 8 | 0.82 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 8 | 0.82 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 9 | 0.82 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 9 | 0.82 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 9 | 0.82 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 19 | 0.82 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 19 | 0.82 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 19 | 0.82 |
| (1,5255) | 1:B:77:ARG:HG2 | 1:B:78:LEU:HB2 | 8 | 0.81 |
| (1,5208) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HG2 | 12 | 0.81 |
| (1,5208) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HG2 | 12 | 0.81 |
| (1,5208) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HG2 | 12 | 0.81 |
| (1,5192) | 1:B:58:LYS:HE2 | 1:B:59:LEU:HA | 20 | 0.81 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 9 | 0.81 |
| (1,5124) | 1:B:37:VAL:HG11 | 1:B:39:ASN:HD21 | 8 | 0.81 |
| (1,5124) | 1:B:37:VAL:HG12 | 1:B:39:ASN:HD21 | 8 | 0.81 |
| (1,5124) | 1:B:37:VAL:HG13 | 1:B:39:ASN:HD21 | 8 | 0.81 |
| (1,5108) | 1:B:34:ARG:HB2 | 1:B:51:ILE:H | 10 | 0.81 |
| (1,5108) | 1:B:34:ARG:HB2 | 1:B:51:ILE:H | 18 | 0.81 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 17 | 0.81 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 17 | 0.81 |
| (1,5057) | 1:B:26:ILE:HG12 | 1:B:27:SER:HG | 12 | 0.81 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5043) | 1:B:25:VAL:H | 1:B:26:ILE:HG12 | 2 | 0.81 |
| (1,5043) | 1:B:25:VAL:H | 1:B:26:ILE:HG12 | 16 | 0.81 |
| (1,5031) | 1:B:23:THR:HB | 1:B:26:ILE:HG12 | 14 | 0.81 |
| (1,5031) | 1:B:23:THR:HB | 1:B:26:ILE:HG12 | 16 | 0.81 |
| (1,5008) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD21 | 14 | 0.81 |
| (1,5008) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD21 | 14 | 0.81 |
| (1,4948) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HA | 4 | 0.81 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 18 | 0.81 |
| (1,4889) | 1:A:58:LYS:HE2 | 1:A:59:LEU:HA | 12 | 0.81 |
| (1,4867) | 1:A:54:LYS:HB2 | 1:A:55:ASN:HB2 | 4 | 0.81 |
| (1,4820) | 1:A:37:VAL:HG11 | 1:A:39:ASN:HD21 | 12 | 0.81 |
| (1,4820) | 1:A:37:VAL:HG12 | 1:A:39:ASN:HD21 | 12 | 0.81 |
| (1,4820) | 1:A:37:VAL:HG13 | 1:A:39:ASN:HD21 | 12 | 0.81 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 4 | 0.81 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 4 | 0.81 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 4 | 0.81 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 7 | 0.81 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 7 | 0.81 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 7 | 0.81 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 16 | 0.81 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 16 | 0.81 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 16 | 0.81 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 10 | 0.81 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 10 | 0.81 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 10 | 0.81 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 17 | 0.81 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 17 | 0.81 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 17 | 0.81 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 20 | 0.81 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 20 | 0.81 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 6 | 0.81 |
| (1,4733) | 1:A:23:THR:HG21 | 1:A:27:SER:HB2 | 4 | 0.81 |
| (1,4733) | 1:A:23:THR:HG22 | 1:A:27:SER:HB2 | 4 | 0.81 |
| (1,4733) | 1:A:23:THR:HG23 | 1:A:27:SER:HB2 | 4 | 0.81 |
| (1,4690) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD21 | 20 | 0.81 |
| (1,4690) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD21 | 20 | 0.81 |
| (1,4689) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HB2 | 10 | 0.81 |
| (1,4689) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HB2 | 10 | 0.81 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 13 | 0.81 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 3 | 0.81 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 3 | 0.81 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 3 | 0.81 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 6 | 0.81 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 6 | 0.81 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 6 | 0.81 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 4 | 0.81 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 4 | 0.81 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 4 | 0.81 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 15 | 0.81 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 15 | 0.81 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 15 | 0.81 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 8 | 0.81 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 8 | 0.81 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 8 | 0.81 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 14 | 0.81 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 14 | 0.81 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 14 | 0.81 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 1 | 0.81 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 1 | 0.81 |
| (1,4376) | 1:A:4:PHE:H | 1:A:4:PHE:HE1 | 16 | 0.81 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 5 | 0.81 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 5 | 0.81 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 5 | 0.81 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 12 | 0.81 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 12 | 0.81 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 12 | 0.81 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 2 | 0.81 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 2 | 0.81 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 2 | 0.81 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 17 | 0.81 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 17 | 0.81 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 17 | 0.81 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 4 | 0.81 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 4 | 0.81 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 4 | 0.81 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 10 | 0.81 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 10 | 0.81 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 10 | 0.81 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 14 | 0.81 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 14 | 0.81 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 14 | 0.81 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 8 | 0.81 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 8 | 0.81 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 8 | 0.81 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5262) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HA | 10 | 0.8 |
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 8 | 0.8 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 12 | 0.8 |
| (1,5106) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG2 | 1 | 0.8 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 6 | 0.8 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 6 | 0.8 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 6 | 0.8 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 1 | 0.8 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 1 | 0.8 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 1 | 0.8 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 10 | 0.8 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 10 | 0.8 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 10 | 0.8 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 18 | 0.8 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 18 | 0.8 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 3 | 0.8 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 13 | 0.8 |
| (1,5043) | 1:B:25:VAL:H | 1:B:26:ILE:HG12 | 6 | 0.8 |
| (1,5007) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HB2 | 16 | 0.8 |
| (1,5007) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HB2 | 16 | 0.8 |
| (1,4982) | 1:B:9:ARG:HG2 | 1:B:11:VAL:HG21 | 19 | 0.8 |
| (1,4982) | 1:B:9:ARG:HG2 | 1:B:11:VAL:HG22 | 19 | 0.8 |
| (1,4982) | 1:B:9:ARG:HG2 | 1:B:11:VAL:HG23 | 19 | 0.8 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD21 | 10 | 0.8 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD22 | 10 | 0.8 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD23 | 10 | 0.8 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG11 | 9 | 0.8 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG12 | 9 | 0.8 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG13 | 9 | 0.8 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 4 | 0.8 |
| (1,4856) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HE2 | 18 | 0.8 |
| (1,4856) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HE2 | 18 | 0.8 |
| (1,4856) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HE2 | 18 | 0.8 |
| (1,4814) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HA | 11 | 0.8 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 16 | 0.8 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 16 | 0.8 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 16 | 0.8 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 6 | 0.8 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 6 | 0.8 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 11 | 0.8 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 11 | 0.8 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 12 | 0.8 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 12 | 0.8 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 16 | 0.8 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 12 | 0.8 |
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 12 | 0.8 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 12 | 0.8 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 7 | 0.8 |
| (1,4685) | 1:A:15:LYS:HB2 | 1:A:18:MET:HG2 | 17 | 0.8 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 20 | 0.8 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 20 | 0.8 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 20 | 0.8 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 9 | 0.8 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 9 | 0.8 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 9 | 0.8 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 17 | 0.8 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 9 | 0.8 |
| (1,4376) | 1:A:4:PHE:H | 1:A:4:PHE:HE1 | 3 | 0.8 |
| (1,4368) | 1:A:4:PHE:HE1 | 1:A:56:THR:HA | 19 | 0.8 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG21 | 10 | 0.8 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG22 | 10 | 0.8 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG23 | 10 | 0.8 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG21 | 17 | 0.8 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG22 | 17 | 0.8 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG23 | 17 | 0.8 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 13 | 0.8 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 13 | 0.8 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 13 | 0.8 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 16 | 0.8 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 16 | 0.8 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 16 | 0.8 |
| (1,1934) | 1:A:18:MET:HE1 | 1:A:45:PHE:HE1 | 13 | 0.8 |
| (1,1934) | 1:A:18:MET:HE2 | 1:A:45:PHE:HE1 | 13 | 0.8 |
| (1,1934) | 1:A:18:MET:HE3 | 1:A:45:PHE:HE1 | 13 | 0.8 |
| (1,5263) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HD2 | 10 | 0.79 |
| (1,5263) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HD2 | 13 | 0.79 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 12 | 0.79 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 12 | 0.79 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 12 | 0.79 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 9 | 0.79 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 6 | 0.79 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 6 | 0.79 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 6 | 0.79 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 10 | 0.79 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 10 | 0.79 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 10 | 0.79 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 2 | 0.79 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 10 | 0.79 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 10 | 0.79 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 10 | 0.79 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 5 | 0.79 |
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 5 | 0.79 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 5 | 0.79 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE2 | 10 | 0.79 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE3 | 10 | 0.79 |
| (1,4873) | 1:A:54:LYS:HE2 | 1:A:55:ASN:HD21 | 20 | 0.79 |
| (1,4873) | 1:A:54:LYS:HE3 | 1:A:55:ASN:HD21 | 20 | 0.79 |
| (1,4834) | 1:A:39:ASN:HD21 | 1:A:46:THR:HB | 20 | 0.79 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 17 | 0.79 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 17 | 0.79 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 17 | 0.79 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 13 | 0.79 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 13 | 0.79 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 13 | 0.79 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 1 | 0.79 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 1 | 0.79 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 9 | 0.79 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 2 | 0.79 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 2 | 0.79 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 2 | 0.79 |
| (1,4703) | 1:A:17:GLY:HA2 | 1:A:21:GLN:HE22 | 4 | 0.79 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 15 | 0.79 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 15 | 0.79 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 15 | 0.79 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 17 | 0.79 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 17 | 0.79 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 17 | 0.79 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 13 | 0.79 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 13 | 0.79 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 13 | 0.79 |
| (1,4488) | 1:B:18:MET:HB3 | 1:B:45:PHE:HE1 | 11 | 0.79 |
| (1,4377) | 1:B:4:PHE:H | 1:B:4:PHE:HE1 | 12 | 0.79 |
| (1,4376) | 1:A:4:PHE:H | 1:A:4:PHE:HE1 | 5 | 0.79 |
| (1,4369) | 1:B:4:PHE:HE1 | 1:B:56:THR:HA | 11 | 0.79 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG21 | 17 | 0.79 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG22 | 17 | 0.79 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG23 | 17 | 0.79 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 19 | 0.79 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 19 | 0.79 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 19 | 0.79 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 5 | 0.79 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 5 | 0.79 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 5 | 0.79 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 4 | 0.79 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 4 | 0.79 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 4 | 0.79 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 17 | 0.79 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 17 | 0.79 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 17 | 0.79 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 18 | 0.79 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 18 | 0.79 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 18 | 0.79 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 9 | 0.79 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 9 | 0.79 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 9 | 0.79 |
| (1,5262) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HA | 13 | 0.78 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 7 | 0.78 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 5 | 0.78 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 8 | 0.78 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 18 | 0.78 |
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 18 | 0.78 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 18 | 0.78 |
| (1,5009) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD21 | 6 | 0.78 |
| (1,5009) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD21 | 6 | 0.78 |
| (1,4879) | 1:A:55:ASN:HD21 | 1:A:58:LYS:HG3 | 10 | 0.78 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 4 | 0.78 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 4 | 0.78 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 4 | 0.78 |
| (1,4834) | 1:A:39:ASN:HD21 | 1:A:46:THR:HB | 16 | 0.78 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD2 | 4 | 0.78 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD3 | 4 | 0.78 |
| (1,4822) | 1:A:37:VAL:HG11 | 1:A:48:ASN:HD21 | 13 | 0.78 |
| (1,4822) | 1:A:37:VAL:HG12 | 1:A:48:ASN:HD21 | 13 | 0.78 |
| (1,4822) | 1:A:37:VAL:HG13 | 1:A:48:ASN:HD21 | 13 | 0.78 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 8 | 0.78 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 8 | 0.78 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 8 | 0.78 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 3 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 3 | 0.78 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 3 | 0.78 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 19 | 0.78 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 6 | 0.78 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 7 | 0.78 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 18 | 0.78 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 16 | 0.78 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 16 | 0.78 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 16 | 0.78 |
| (1,4691) | 1:A:15:LYS:HE2 | 1:A:16:ASN:HD21 | 7 | 0.78 |
| (1,4691) | 1:A:15:LYS:HE3 | 1:A:16:ASN:HD21 | 7 | 0.78 |
| (1,4690) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD21 | 1 | 0.78 |
| (1,4690) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD21 | 1 | 0.78 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 7 | 0.78 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 7 | 0.78 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 7 | 0.78 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 6 | 0.78 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 6 | 0.78 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 6 | 0.78 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 12 | 0.78 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 12 | 0.78 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 12 | 0.78 |
| (1,4376) | 1:A:4:PHE:H | 1:A:4:PHE:HE1 | 4 | 0.78 |
| (1,4376) | 1:A:4:PHE:H | 1:A:4:PHE:HE1 | 10 | 0.78 |
| (1,4368) | 1:A:4:PHE:HE1 | 1:A:56:THR:HA | 3 | 0.78 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 15 | 0.78 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 10 | 0.78 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 10 | 0.78 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 10 | 0.78 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 19 | 0.78 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 19 | 0.78 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 19 | 0.78 |
| (1,3038) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HZ1 | 7 | 0.78 |
| (1,3038) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HZ1 | 7 | 0.78 |
| (1,3038) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HZ1 | 7 | 0.78 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 1 | 0.78 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 1 | 0.78 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 1 | 0.78 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 7 | 0.78 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 7 | 0.78 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 7 | 0.78 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 20 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 20 | 0.78 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 20 | 0.78 |
| (1,5263) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HD2 | 11 | 0.77 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 9 | 0.77 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 9 | 0.77 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 9 | 0.77 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 16 | 0.77 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 16 | 0.77 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 16 | 0.77 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD11 | 20 | 0.77 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD12 | 20 | 0.77 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD13 | 20 | 0.77 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 8 | 0.77 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 8 | 0.77 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD2 | 14 | 0.77 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD3 | 14 | 0.77 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB2 | 13 | 0.77 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB3 | 13 | 0.77 |
| (1,5126) | 1:B:37:VAL:HG11 | 1:B:48:ASN:HD21 | 19 | 0.77 |
| (1,5126) | 1:B:37:VAL:HG12 | 1:B:48:ASN:HD21 | 19 | 0.77 |
| (1,5126) | 1:B:37:VAL:HG13 | 1:B:48:ASN:HD21 | 19 | 0.77 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 5 | 0.77 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 5 | 0.77 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 5 | 0.77 |
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 6 | 0.77 |
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 6 | 0.77 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 6 | 0.77 |
| (1,5070) | 1:B:28:LYS:HA | 1:B:28:LYS:HG2 | 12 | 0.77 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 2 | 0.77 |
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 2 | 0.77 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 2 | 0.77 |
| (1,5031) | 1:B:23:THR:HB | 1:B:26:ILE:HG12 | 7 | 0.77 |
| (1,5007) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HB2 | 20 | 0.77 |
| (1,5007) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HB2 | 20 | 0.77 |
| (1,4999) | 1:B:15:LYS:H | 1:B:18:MET:HG2 | 14 | 0.77 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 4 | 0.77 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 4 | 0.77 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 4 | 0.77 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 19 | 0.77 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 19 | 0.77 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 19 | 0.77 |
| (1,4879) | 1:A:55:ASN:HD21 | 1:A:58:LYS:HG3 | 19 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 7 | 0.77 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 2 | 0.77 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 2 | 0.77 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 2 | 0.77 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 4 | 0.77 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 4 | 0.77 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 4 | 0.77 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 16 | 0.77 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 16 | 0.77 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 4 | 0.77 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 17 | 0.77 |
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 17 | 0.77 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 17 | 0.77 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 10 | 0.77 |
| (1,4722) | 1:A:20:ASN:HA | 1:B:27:SER:HB2 | 13 | 0.77 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 17 | 0.77 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 17 | 0.77 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 17 | 0.77 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 14 | 0.77 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 16 | 0.77 |
| (1,4671) | 1:A:14:ASP:HB2 | 1:A:43:GLY:H | 4 | 0.77 |
| (1,4628) | 1:A:3:ASP:HB2 | 1:A:4:PHE:H | 17 | 0.77 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 10 | 0.77 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 10 | 0.77 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 10 | 0.77 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 16 | 0.77 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 16 | 0.77 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 16 | 0.77 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 19 | 0.77 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 19 | 0.77 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 19 | 0.77 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 6 | 0.77 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 6 | 0.77 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 6 | 0.77 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 10 | 0.77 |
| (1,4376) | 1:A:4:PHE:H | 1:A:4:PHE:HE1 | 8 | 0.77 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 9 | 0.77 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 13 | 0.77 |
| (1,3038) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HZ1 | 9 | 0.77 |
| (1,3038) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HZ1 | 9 | 0.77 |
| (1,3038) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HZ1 | 9 | 0.77 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 8 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 8 | 0.77 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 8 | 0.77 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 13 | 0.77 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 13 | 0.77 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 13 | 0.77 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 14 | 0.77 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 14 | 0.77 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 14 | 0.77 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 12 | 0.77 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 12 | 0.77 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 12 | 0.77 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 4 | 0.77 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 4 | 0.77 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 4 | 0.77 |
| (1,5253) | 1:B:77:ARG:HG2 | 1:B:78:LEU:H | 8 | 0.76 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD21 | 4 | 0.76 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD22 | 4 | 0.76 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD23 | 4 | 0.76 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 3 | 0.76 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 3 | 0.76 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 3 | 0.76 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 12 | 0.76 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 12 | 0.76 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 12 | 0.76 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 13 | 0.76 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 13 | 0.76 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 13 | 0.76 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 3 | 0.76 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 3 | 0.76 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 3 | 0.76 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 12 | 0.76 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 12 | 0.76 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 12 | 0.76 |
| (1,5035) | 1:B:24:GLY:H | 1:B:26:ILE:HG12 | 12 | 0.76 |
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD21 | 20 | 0.76 |
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD22 | 20 | 0.76 |
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD23 | 20 | 0.76 |
| (1,4806) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HD1 | 17 | 0.76 |
| (1,4806) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HD2 | 17 | 0.76 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 13 | 0.76 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 13 | 0.76 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 13 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 8 | 0.76 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 8 | 0.76 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 8 | 0.76 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 19 | 0.76 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 19 | 0.76 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 19 | 0.76 |
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 16 | 0.76 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 16 | 0.76 |
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 16 | 0.76 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD11 | 13 | 0.76 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD12 | 13 | 0.76 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD13 | 13 | 0.76 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 18 | 0.76 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 14 | 0.76 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 4 | 0.76 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 3 | 0.76 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 3 | 0.76 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 3 | 0.76 |
| (1,4369) | 1:B:4:PHE:HE1 | 1:B:56:THR:HA | 14 | 0.76 |
| (1,4368) | 1:A:4:PHE:HE1 | 1:A:56:THR:HA | 4 | 0.76 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 18 | 0.76 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 18 | 0.76 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 18 | 0.76 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 4 | 0.76 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 4 | 0.76 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 4 | 0.76 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 7 | 0.76 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 7 | 0.76 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 7 | 0.76 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 10 | 0.76 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 10 | 0.76 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 10 | 0.76 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 1 | 0.76 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 1 | 0.76 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 1 | 0.76 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 14 | 0.76 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 14 | 0.76 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 14 | 0.76 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 5 | 0.76 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 5 | 0.76 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 5 | 0.76 |
| (1,1066) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:H | 19 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 5 | 0.75 |
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 12 | 0.75 |
| (1,5217) | 1:B:64:ASP:H | 1:B:65:LYS:HG2 | 1 | 0.75 |
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 19 | 0.75 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 20 | 0.75 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 20 | 0.75 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 20 | 0.75 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 7 | 0.75 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 7 | 0.75 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 7 | 0.75 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 11 | 0.75 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 11 | 0.75 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 11 | 0.75 |
| (1,5060) | 1:B:27:SER:H | 1:B:28:LYS:HB2 | 12 | 0.75 |
| (1,4949) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HD2 | 9 | 0.75 |
| (1,4873) | 1:A:54:LYS:HE2 | 1:A:55:ASN:HD21 | 1 | 0.75 |
| (1,4873) | 1:A:54:LYS:HE3 | 1:A:55:ASN:HD21 | 1 | 0.75 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 4 | 0.75 |
| (1,4820) | 1:A:37:VAL:HG11 | 1:A:39:ASN:HD21 | 15 | 0.75 |
| (1,4820) | 1:A:37:VAL:HG12 | 1:A:39:ASN:HD21 | 15 | 0.75 |
| (1,4820) | 1:A:37:VAL:HG13 | 1:A:39:ASN:HD21 | 15 | 0.75 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 10 | 0.75 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 10 | 0.75 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 10 | 0.75 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 19 | 0.75 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 19 | 0.75 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 19 | 0.75 |
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 14 | 0.75 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 14 | 0.75 |
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 14 | 0.75 |
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 18 | 0.75 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 18 | 0.75 |
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 18 | 0.75 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 1 | 0.75 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 15 | 0.75 |
| (1,4698) | 1:A:17:GLY:H | 1:B:32:ASN:HD21 | 15 | 0.75 |
| (1,4691) | 1:A:15:LYS:HE2 | 1:A:16:ASN:HD21 | 1 | 0.75 |
| (1,4691) | 1:A:15:LYS:HE3 | 1:A:16:ASN:HD21 | 1 | 0.75 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 19 | 0.75 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 19 | 0.75 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 19 | 0.75 |
| (1,4377) | 1:B:4:PHE:H | 1:B:4:PHE:HE1 | 11 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 6 | 0.75 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 13 | 0.75 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 14 | 0.75 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 14 | 0.75 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 14 | 0.75 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 11 | 0.75 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 11 | 0.75 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 11 | 0.75 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 11 | 0.75 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 11 | 0.75 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 11 | 0.75 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 12 | 0.75 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 12 | 0.75 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 12 | 0.75 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 6 | 0.75 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 6 | 0.75 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 6 | 0.75 |
| (1,1934) | 1:A:18:MET:HE1 | 1:A:45:PHE:HE1 | 3 | 0.75 |
| (1,1934) | 1:A:18:MET:HE2 | 1:A:45:PHE:HE1 | 3 | 0.75 |
| (1,1934) | 1:A:18:MET:HE3 | 1:A:45:PHE:HE1 | 3 | 0.75 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 12 | 0.75 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 12 | 0.75 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 12 | 0.75 |
| (1,5256) | 1:B:77:ARG:HG2 | 1:B:79:SER:HA | 16 | 0.74 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 13 | 0.74 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 13 | 0.74 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 13 | 0.74 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD11 | 3 | 0.74 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD12 | 3 | 0.74 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD13 | 3 | 0.74 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD11 | 18 | 0.74 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD12 | 18 | 0.74 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD13 | 18 | 0.74 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 8 | 0.74 |
| (1,5124) | 1:B:37:VAL:HG11 | 1:B:39:ASN:HD21 | 6 | 0.74 |
| (1,5124) | 1:B:37:VAL:HG12 | 1:B:39:ASN:HD21 | 6 | 0.74 |
| (1,5124) | 1:B:37:VAL:HG13 | 1:B:39:ASN:HD21 | 6 | 0.74 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 7 | 0.74 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 7 | 0.74 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 7 | 0.74 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 13 | 0.74 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 13 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 13 | 0.74 |
| (1,5060) | 1:B:27:SER:H | 1:B:28:LYS:HB2 | 4 | 0.74 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 16 | 0.74 |
| (1,5046) | 1:B:25:VAL:HA | 1:B:28:LYS:HB2 | 12 | 0.74 |
| (1,5031) | 1:B:23:THR:HB | 1:B:26:ILE:HG12 | 11 | 0.74 |
| (1,5031) | 1:B:23:THR:HB | 1:B:26:ILE:HG12 | 17 | 0.74 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 13 | 0.74 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD21 | 17 | 0.74 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD22 | 17 | 0.74 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD23 | 17 | 0.74 |
| (1,4925) | 1:A:67:ARG:HG2 | 1:A:75:VAL:H | 7 | 0.74 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD11 | 12 | 0.74 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD12 | 12 | 0.74 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD13 | 12 | 0.74 |
| (1,4856) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HE2 | 1 | 0.74 |
| (1,4856) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HE2 | 1 | 0.74 |
| (1,4856) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HE2 | 1 | 0.74 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 10 | 0.74 |
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 10 | 0.74 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 10 | 0.74 |
| (1,4574) | 1:B:44:ILE:HG12 | 1:B:73:PHE:HE1 | 11 | 0.74 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 20 | 0.74 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 20 | 0.74 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 20 | 0.74 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 19 | 0.74 |
| (1,4369) | 1:B:4:PHE:HE1 | 1:B:56:THR:HA | 2 | 0.74 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 5 | 0.74 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 5 | 0.74 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 5 | 0.74 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 15 | 0.74 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 15 | 0.74 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 15 | 0.74 |
| (1,3038) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HZ1 | 11 | 0.74 |
| (1,3038) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HZ1 | 11 | 0.74 |
| (1,3038) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HZ1 | 11 | 0.74 |
| (1,3038) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HZ1 | 20 | 0.74 |
| (1,3038) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HZ1 | 20 | 0.74 |
| (1,3038) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HZ1 | 20 | 0.74 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 1 | 0.74 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 1 | 0.74 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 1 | 0.74 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 9 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|---------|---------|-------|---------------|
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 9 | 0.74 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 9 | 0.74 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 20 | 0.74 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 20 | 0.74 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 20 | 0.74 |
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 16 | 0.73 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 8 | 0.73 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 8 | 0.73 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 8 | 0.73 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD11 | 14 | 0.73 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD12 | 14 | 0.73 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD13 | 14 | 0.73 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 2 | 0.73 |
| (1,5176) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD21 | 12 | 0.73 |
| (1,5176) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD21 | 12 | 0.73 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 19 | 0.73 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 19 | 0.73 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 19 | 0.73 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 2 | 0.73 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 2 | 0.73 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 2 | 0.73 |
| (1,5061) | 1:B:27:SER:H | 1:B:33:ILE:HG12 | 16 | 0.73 |
| (1,5009) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD21 | 1 | 0.73 |
| (1,5009) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD21 | 1 | 0.73 |
| (1,5009) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD21 | 19 | 0.73 |
| (1,5009) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD21 | 19 | 0.73 |
| (1,5007) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HB2 | 1 | 0.73 |
| (1,5007) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HB2 | 1 | 0.73 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG11 | 7 | 0.73 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG12 | 7 | 0.73 |
| (1,4926) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG13 | 7 | 0.73 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 17 | 0.73 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 17 | 0.73 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 17 | 0.73 |
| (1,4879) | 1:A:55:ASN:HD21 | 1:A:58:LYS:HG3 | 15 | 0.73 |
| (1,4870) | 1:A:54:LYS:HG2 | 1:A:55:ASN:HD21 | 10 | 0.73 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 2 | 0.73 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 2 | 0.73 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 2 | 0.73 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD11 | 17 | 0.73 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD12 | 17 | 0.73 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD13 | 17 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 9 | 0.73 |
| (1,4691) | 1:A:15:LYS:HE2 | 1:A:16:ASN:HD21 | 11 | 0.73 |
| (1,4691) | 1:A:15:LYS:HE3 | 1:A:16:ASN:HD21 | 11 | 0.73 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 18 | 0.73 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 18 | 0.73 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 18 | 0.73 |
| (1,4376) | 1:A:4:PHE:H | 1:A:4:PHE:HE1 | 17 | 0.73 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG21 | 1 | 0.73 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG22 | 1 | 0.73 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG23 | 1 | 0.73 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 11 | 0.73 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 20 | 0.73 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 9 | 0.73 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 9 | 0.73 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 9 | 0.73 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 10 | 0.73 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 10 | 0.73 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 10 | 0.73 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 5 | 0.73 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 5 | 0.73 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 5 | 0.73 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 15 | 0.73 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 15 | 0.73 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 15 | 0.73 |
| (1,1935) | 1:B:18:MET:HE1 | 1:B:45:PHE:HE1 | 3 | 0.73 |
| (1,1935) | 1:B:18:MET:HE2 | 1:B:45:PHE:HE1 | 3 | 0.73 |
| (1,1935) | 1:B:18:MET:HE3 | 1:B:45:PHE:HE1 | 3 | 0.73 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 19 | 0.73 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 19 | 0.73 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 19 | 0.73 |
| (1,5253) | 1:B:77:ARG:HG2 | 1:B:78:LEU:H | 16 | 0.72 |
| (1,5176) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD21 | 8 | 0.72 |
| (1,5176) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD21 | 8 | 0.72 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 11 | 0.72 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 2 | 0.72 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 2 | 0.72 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 2 | 0.72 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 8 | 0.72 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 8 | 0.72 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 8 | 0.72 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 18 | 0.72 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 10 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 10 | 0.72 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 10 | 0.72 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 11 | 0.72 |
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 11 | 0.72 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 11 | 0.72 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE2 | 6 | 0.72 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE3 | 6 | 0.72 |
| (1,4950) | 1:B:3:ASP:HA | 1:B:54:LYS:HB2 | 17 | 0.72 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD21 | 5 | 0.72 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD22 | 5 | 0.72 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD23 | 5 | 0.72 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 12 | 0.72 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 12 | 0.72 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 12 | 0.72 |
| (1,4863) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HG2 | 1 | 0.72 |
| (1,4863) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HG2 | 1 | 0.72 |
| (1,4863) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HG2 | 1 | 0.72 |
| (1,4848) | 1:A:46:THR:HG1 | 1:A:48:ASN:HD21 | 14 | 0.72 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 14 | 0.72 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 14 | 0.72 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 14 | 0.72 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 8 | 0.72 |
| (1,4834) | 1:A:39:ASN:HD21 | 1:A:46:THR:HB | 8 | 0.72 |
| (1,4803) | 1:A:34:ARG:HB2 | 1:A:51:ILE:H | 11 | 0.72 |
| (1,4801) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG2 | 4 | 0.72 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 18 | 0.72 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 18 | 0.72 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 18 | 0.72 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 7 | 0.72 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 7 | 0.72 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 7 | 0.72 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 1 | 0.72 |
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 1 | 0.72 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 1 | 0.72 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 15 | 0.72 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 15 | 0.72 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 15 | 0.72 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 15 | 0.72 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 15 | 0.72 |
| (1,4693) | 1:A:16:ASN:HA | 1:B:32:ASN:HD21 | 2 | 0.72 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 16 | 0.72 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 16 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 16 | 0.72 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 8 | 0.72 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 8 | 0.72 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 8 | 0.72 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 7 | 0.72 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 7 | 0.72 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 7 | 0.72 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 10 | 0.72 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 10 | 0.72 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 10 | 0.72 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 4 | 0.72 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 9 | 0.72 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 9 | 0.72 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG21 | 1 | 0.72 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG22 | 1 | 0.72 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG23 | 1 | 0.72 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 1 | 0.72 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 7 | 0.72 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 7 | 0.72 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 7 | 0.72 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 12 | 0.72 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 12 | 0.72 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 12 | 0.72 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 11 | 0.72 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 11 | 0.72 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 11 | 0.72 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG21 | 11 | 0.72 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG22 | 11 | 0.72 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG23 | 11 | 0.72 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 2 | 0.72 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 2 | 0.72 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 2 | 0.72 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 19 | 0.72 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 19 | 0.72 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 19 | 0.72 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 14 | 0.72 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 14 | 0.72 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 14 | 0.72 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 11 | 0.72 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 11 | 0.72 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 11 | 0.72 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 17 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 17 | 0.72 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 17 | 0.72 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 19 | 0.71 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 19 | 0.71 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 19 | 0.71 |
| (1,5182) | 1:B:55:ASN:HD21 | 1:B:58:LYS:HG3 | 1 | 0.71 |
| (1,5176) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD21 | 14 | 0.71 |
| (1,5176) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD21 | 14 | 0.71 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 13 | 0.71 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 1 | 0.71 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 1 | 0.71 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 1 | 0.71 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 13 | 0.71 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 13 | 0.71 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 10 | 0.71 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 10 | 0.71 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 10 | 0.71 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 8 | 0.71 |
| (1,4870) | 1:A:54:LYS:HG2 | 1:A:55:ASN:HD21 | 9 | 0.71 |
| (1,4848) | 1:A:46:THR:HG1 | 1:A:48:ASN:HD21 | 1 | 0.71 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 13 | 0.71 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 13 | 0.71 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 13 | 0.71 |
| (1,4834) | 1:A:39:ASN:HD21 | 1:A:46:THR:HB | 3 | 0.71 |
| (1,4834) | 1:A:39:ASN:HD21 | 1:A:46:THR:HB | 7 | 0.71 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 9 | 0.71 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 9 | 0.71 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 9 | 0.71 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 5 | 0.71 |
| (1,4745) | 1:A:25:VAL:H | 1:A:28:LYS:HG2 | 2 | 0.71 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 5 | 0.71 |
| (1,4727) | 1:A:20:ASN:HD21 | 1:B:33:ILE:HG12 | 13 | 0.71 |
| (1,4691) | 1:A:15:LYS:HE2 | 1:A:16:ASN:HD21 | 12 | 0.71 |
| (1,4691) | 1:A:15:LYS:HE3 | 1:A:16:ASN:HD21 | 12 | 0.71 |
| (1,4689) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HB2 | 12 | 0.71 |
| (1,4689) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HB2 | 12 | 0.71 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 5 | 0.71 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 5 | 0.71 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 5 | 0.71 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 15 | 0.71 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 15 | 0.71 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 15 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 10 | 0.71 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 10 | 0.71 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 10 | 0.71 |
| (1,4377) | 1:B:4:PHE:H | 1:B:4:PHE:HE1 | 2 | 0.71 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 4 | 0.71 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 4 | 0.71 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 4 | 0.71 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 12 | 0.71 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 12 | 0.71 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 12 | 0.71 |
| (1,2550) | 1:B:38:LEU:HD21 | 1:B:45:PHE:HE1 | 16 | 0.71 |
| (1,2550) | 1:B:38:LEU:HD22 | 1:B:45:PHE:HE1 | 16 | 0.71 |
| (1,2550) | 1:B:38:LEU:HD23 | 1:B:45:PHE:HE1 | 16 | 0.71 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 3 | 0.71 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 3 | 0.71 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 3 | 0.71 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 14 | 0.7 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 14 | 0.7 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 14 | 0.7 |
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 1 | 0.7 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 20 | 0.7 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 20 | 0.7 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 20 | 0.7 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 20 | 0.7 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 20 | 0.7 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 20 | 0.7 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 10 | 0.7 |
| (1,4983) | 1:B:9:ARG:HG2 | 1:B:47:CYS:H | 8 | 0.7 |
| (1,4948) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HA | 15 | 0.7 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 4 | 0.7 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 4 | 0.7 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 4 | 0.7 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 3 | 0.7 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 3 | 0.7 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 3 | 0.7 |
| (1,4834) | 1:A:39:ASN:HD21 | 1:A:46:THR:HB | 19 | 0.7 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD2 | 7 | 0.7 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD3 | 7 | 0.7 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 3 | 0.7 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 3 | 0.7 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 3 | 0.7 |
| (1,4761) | 1:A:27:SER:H | 1:A:28:LYS:HB2 | 20 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4661) | 1:A:9:ARG:HD2 | 1:A:48:ASN:HD21 | 10 | 0.7 |
| (1,4661) | 1:A:9:ARG:HD3 | 1:A:48:ASN:HD21 | 10 | 0.7 |
| (1,4573) | 1:A:44:ILE:HG12 | 1:A:73:PHE:HE1 | 15 | 0.7 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 13 | 0.7 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 4 | 0.7 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 4 | 0.7 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 4 | 0.7 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 9 | 0.7 |
| (1,4477) | 1:A:19:THR:HG21 | 1:A:45:PHE:HE1 | 9 | 0.7 |
| (1,4477) | 1:A:19:THR:HG22 | 1:A:45:PHE:HE1 | 9 | 0.7 |
| (1,4477) | 1:A:19:THR:HG23 | 1:A:45:PHE:HE1 | 9 | 0.7 |
| (1,4377) | 1:B:4:PHE:H | 1:B:4:PHE:HE1 | 20 | 0.7 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 17 | 0.7 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 17 | 0.7 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 18 | 0.7 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 11 | 0.7 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 8 | 0.7 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 8 | 0.7 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 8 | 0.7 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 10 | 0.7 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 10 | 0.7 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 10 | 0.7 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 8 | 0.7 |
| (1,3038) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HZ1 | 19 | 0.7 |
| (1,3038) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HZ1 | 19 | 0.7 |
| (1,3038) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HZ1 | 19 | 0.7 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 8 | 0.7 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 8 | 0.7 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 8 | 0.7 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD11 | 16 | 0.7 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD12 | 16 | 0.7 |
| (1,2326) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HD13 | 16 | 0.7 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD11 | 2 | 0.7 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD12 | 2 | 0.7 |
| (1,2325) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HD13 | 2 | 0.7 |
| (1,1779) | 1:B:11:VAL:HG11 | 1:B:73:PHE:HE1 | 6 | 0.7 |
| (1,1779) | 1:B:11:VAL:HG12 | 1:B:73:PHE:HE1 | 6 | 0.7 |
| (1,1779) | 1:B:11:VAL:HG13 | 1:B:73:PHE:HE1 | 6 | 0.7 |
| (1,1778) | 1:A:11:VAL:HG11 | 1:A:73:PHE:HE1 | 10 | 0.7 |
| (1,1778) | 1:A:11:VAL:HG12 | 1:A:73:PHE:HE1 | 10 | 0.7 |
| (1,1778) | 1:A:11:VAL:HG13 | 1:A:73:PHE:HE1 | 10 | 0.7 |
| (1,5262) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HA | 6 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5212) | 1:B:63:MET:H | 1:B:65:LYS:HG2 | 1 | 0.69 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 10 | 0.69 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 20 | 0.69 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD2 | 18 | 0.69 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD3 | 18 | 0.69 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 9 | 0.69 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 9 | 0.69 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 9 | 0.69 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 17 | 0.69 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 17 | 0.69 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 17 | 0.69 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 18 | 0.69 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 18 | 0.69 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 18 | 0.69 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD11 | 13 | 0.69 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD12 | 13 | 0.69 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD13 | 13 | 0.69 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 5 | 0.69 |
| (1,5043) | 1:B:25:VAL:H | 1:B:26:ILE:HG12 | 17 | 0.69 |
| (1,5009) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD21 | 16 | 0.69 |
| (1,5009) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD21 | 16 | 0.69 |
| (1,4950) | 1:B:3:ASP:HA | 1:B:54:LYS:HB2 | 1 | 0.69 |
| (1,4948) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HA | 5 | 0.69 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 8 | 0.69 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 8 | 0.69 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 8 | 0.69 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD11 | 10 | 0.69 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD12 | 10 | 0.69 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD13 | 10 | 0.69 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 12 | 0.69 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 3 | 0.69 |
| (1,4792) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG13 | 6 | 0.69 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 1 | 0.69 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 1 | 0.69 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 1 | 0.69 |
| (1,4767) | 1:A:27:SER:HG | 1:A:28:LYS:HD2 | 8 | 0.69 |
| (1,4752) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HD2 | 20 | 0.69 |
| (1,4752) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HD2 | 20 | 0.69 |
| (1,4752) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HD2 | 20 | 0.69 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 14 | 0.69 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 6 | 0.69 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 6 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|---------|---------|-------|---------------|
| (1,4691) | 1:A:15:LYS:HE2 | 1:A:16:ASN:HD21 | 5 | 0.69 |
| (1,4691) | 1:A:15:LYS:HE3 | 1:A:16:ASN:HD21 | 5 | 0.69 |
| (1,4628) | 1:A:3:ASP:HB2 | 1:A:4:PHE:H | 1 | 0.69 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 1 | 0.69 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 1 | 0.69 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 1 | 0.69 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 10 | 0.69 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 10 | 0.69 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 10 | 0.69 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 18 | 0.69 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 17 | 0.69 |
| (1,4377) | 1:B:4:PHE:H | 1:B:4:PHE:HE1 | 15 | 0.69 |
| (1,4376) | 1:A:4:PHE:H | 1:A:4:PHE:HE1 | 1 | 0.69 |
| (1,4368) | 1:A:4:PHE:HE1 | 1:A:56:THR:HA | 17 | 0.69 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 14 | 0.69 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 1 | 0.69 |
| (1,3038) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HZ1 | 17 | 0.69 |
| (1,3038) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HZ1 | 17 | 0.69 |
| (1,3038) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HZ1 | 17 | 0.69 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 4 | 0.69 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 4 | 0.69 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 4 | 0.69 |
| (1,1778) | 1:A:11:VAL:HG11 | 1:A:73:PHE:HE1 | 11 | 0.69 |
| (1,1778) | 1:A:11:VAL:HG12 | 1:A:73:PHE:HE1 | 11 | 0.69 |
| (1,1778) | 1:A:11:VAL:HG13 | 1:A:73:PHE:HE1 | 11 | 0.69 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 11 | 0.68 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 13 | 0.68 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 2 | 0.68 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 2 | 0.68 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 2 | 0.68 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 14 | 0.68 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 14 | 0.68 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 14 | 0.68 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 17 | 0.68 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 17 | 0.68 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 17 | 0.68 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 20 | 0.68 |
| (1,4952) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HB2 | 18 | 0.68 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 2 | 0.68 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB2 | 7 | 0.68 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB3 | 7 | 0.68 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 5 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 5 | 0.68 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 5 | 0.68 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 5 | 0.68 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 5 | 0.68 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 5 | 0.68 |
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 1 | 0.68 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 1 | 0.68 |
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 1 | 0.68 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 19 | 0.68 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 9 | 0.68 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 19 | 0.68 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 10 | 0.68 |
| (1,4689) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HB2 | 5 | 0.68 |
| (1,4689) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HB2 | 5 | 0.68 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 13 | 0.68 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 13 | 0.68 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 13 | 0.68 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 7 | 0.68 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 11 | 0.68 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 12 | 0.68 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 12 | 0.68 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 20 | 0.68 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 20 | 0.68 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 20 | 0.68 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 20 | 0.68 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 6 | 0.67 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 10 | 0.67 |
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 19 | 0.67 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 12 | 0.67 |
| (1,5173) | 1:B:54:LYS:HG2 | 1:B:55:ASN:HD21 | 7 | 0.67 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 2 | 0.67 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD2 | 3 | 0.67 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD3 | 3 | 0.67 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 17 | 0.67 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 17 | 0.67 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 17 | 0.67 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 16 | 0.67 |
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 16 | 0.67 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 16 | 0.67 |
| (1,5045) | 1:B:25:VAL:H | 1:B:28:LYS:HD2 | 9 | 0.67 |
| (1,5043) | 1:B:25:VAL:H | 1:B:26:ILE:HG12 | 11 | 0.67 |
| (1,5035) | 1:B:24:GLY:H | 1:B:26:ILE:HG12 | 1 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4985) | 1:B:9:ARG:HD2 | 1:B:48:ASN:HD21 | 2 | 0.67 |
| (1,4985) | 1:B:9:ARG:HD3 | 1:B:48:ASN:HD21 | 2 | 0.67 |
| (1,4982) | 1:B:9:ARG:HG2 | 1:B:11:VAL:HG21 | 6 | 0.67 |
| (1,4982) | 1:B:9:ARG:HG2 | 1:B:11:VAL:HG22 | 6 | 0.67 |
| (1,4982) | 1:B:9:ARG:HG2 | 1:B:11:VAL:HG23 | 6 | 0.67 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 3 | 0.67 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 4 | 0.67 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 5 | 0.67 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 15 | 0.67 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 1 | 0.67 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 1 | 0.67 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 1 | 0.67 |
| (1,4856) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HE2 | 14 | 0.67 |
| (1,4856) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HE2 | 14 | 0.67 |
| (1,4856) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HE2 | 14 | 0.67 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 20 | 0.67 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 9 | 0.67 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 9 | 0.67 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 9 | 0.67 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 14 | 0.67 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 14 | 0.67 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 14 | 0.67 |
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 3 | 0.67 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 3 | 0.67 |
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 3 | 0.67 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG21 | 4 | 0.67 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG22 | 4 | 0.67 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG23 | 4 | 0.67 |
| (1,4761) | 1:A:27:SER:H | 1:A:28:LYS:HB2 | 14 | 0.67 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 15 | 0.67 |
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 15 | 0.67 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 15 | 0.67 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 16 | 0.67 |
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 16 | 0.67 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 16 | 0.67 |
| (1,4703) | 1:A:17:GLY:HA2 | 1:A:21:GLN:HE22 | 15 | 0.67 |
| (1,4703) | 1:A:17:GLY:HA2 | 1:A:21:GLN:HE22 | 20 | 0.67 |
| (1,4689) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HB2 | 6 | 0.67 |
| (1,4689) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HB2 | 6 | 0.67 |
| (1,4678) | 1:A:15:LYS:H | 1:A:18:MET:HG2 | 2 | 0.67 |
| (1,4573) | 1:A:44:ILE:HG12 | 1:A:73:PHE:HE1 | 5 | 0.67 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 2 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 2 | 0.67 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 2 | 0.67 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 11 | 0.67 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 11 | 0.67 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 11 | 0.67 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 20 | 0.67 |
| (1,4377) | 1:B:4:PHE:H | 1:B:4:PHE:HE1 | 19 | 0.67 |
| (1,4376) | 1:A:4:PHE:H | 1:A:4:PHE:HE1 | 18 | 0.67 |
| (1,4369) | 1:B:4:PHE:HE1 | 1:B:56:THR:HA | 17 | 0.67 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 16 | 0.67 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 16 | 0.67 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG21 | 10 | 0.67 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG22 | 10 | 0.67 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG23 | 10 | 0.67 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 1 | 0.67 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 1 | 0.67 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 1 | 0.67 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 16 | 0.67 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 16 | 0.67 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 16 | 0.67 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 17 | 0.67 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 17 | 0.67 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 17 | 0.67 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 11 | 0.67 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 11 | 0.67 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 11 | 0.67 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 7 | 0.67 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 7 | 0.67 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 7 | 0.67 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 13 | 0.67 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 13 | 0.67 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 13 | 0.67 |
| (1,2549) | 1:A:38:LEU:HD21 | 1:A:45:PHE:HE1 | 19 | 0.67 |
| (1,2549) | 1:A:38:LEU:HD22 | 1:A:45:PHE:HE1 | 19 | 0.67 |
| (1,2549) | 1:A:38:LEU:HD23 | 1:A:45:PHE:HE1 | 19 | 0.67 |
| (1,5238) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG11 | 3 | 0.66 |
| (1,5238) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG12 | 3 | 0.66 |
| (1,5238) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG13 | 3 | 0.66 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 19 | 0.66 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 5 | 0.66 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 17 | 0.66 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 7 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 18 | 0.66 |
| (1,5127) | 1:B:37:VAL:HG21 | 1:B:48:ASN:HB2 | 11 | 0.66 |
| (1,5127) | 1:B:37:VAL:HG22 | 1:B:48:ASN:HB2 | 11 | 0.66 |
| (1,5127) | 1:B:37:VAL:HG23 | 1:B:48:ASN:HB2 | 11 | 0.66 |
| (1,5108) | 1:B:34:ARG:HB2 | 1:B:51:ILE:H | 20 | 0.66 |
| (1,5106) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG2 | 17 | 0.66 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 4 | 0.66 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 9 | 0.66 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 12 | 0.66 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 19 | 0.66 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 19 | 0.66 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 19 | 0.66 |
| (1,4864) | 1:A:53:VAL:HG21 | 1:A:58:LYS:HB2 | 6 | 0.66 |
| (1,4864) | 1:A:53:VAL:HG22 | 1:A:58:LYS:HB2 | 6 | 0.66 |
| (1,4864) | 1:A:53:VAL:HG23 | 1:A:58:LYS:HB2 | 6 | 0.66 |
| (1,4834) | 1:A:39:ASN:HD21 | 1:A:46:THR:HB | 4 | 0.66 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 1 | 0.66 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 1 | 0.66 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 1 | 0.66 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD11 | 20 | 0.66 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD12 | 20 | 0.66 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD13 | 20 | 0.66 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 7 | 0.66 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 2 | 0.66 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 5 | 0.66 |
| (1,4728) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HG12 | 18 | 0.66 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 20 | 0.66 |
| (1,4690) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD21 | 11 | 0.66 |
| (1,4690) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD21 | 11 | 0.66 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 17 | 0.66 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 17 | 0.66 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 17 | 0.66 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 8 | 0.66 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 12 | 0.66 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 15 | 0.66 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 15 | 0.66 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG21 | 11 | 0.66 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG22 | 11 | 0.66 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG23 | 11 | 0.66 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG21 | 14 | 0.66 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG22 | 14 | 0.66 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG23 | 14 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 3 | 0.66 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 8 | 0.66 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG21 | 1 | 0.66 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG22 | 1 | 0.66 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG23 | 1 | 0.66 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 14 | 0.66 |
| (1,3370) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HB | 7 | 0.66 |
| (1,3095) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HZ1 | 2 | 0.66 |
| (1,3095) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HZ1 | 2 | 0.66 |
| (1,3095) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HZ1 | 2 | 0.66 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 17 | 0.66 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 17 | 0.66 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 17 | 0.66 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 20 | 0.66 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 20 | 0.66 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 20 | 0.66 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 12 | 0.66 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 12 | 0.66 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 12 | 0.66 |
| (1,1935) | 1:B:18:MET:HE1 | 1:B:45:PHE:HE1 | 15 | 0.66 |
| (1,1935) | 1:B:18:MET:HE2 | 1:B:45:PHE:HE1 | 15 | 0.66 |
| (1,1935) | 1:B:18:MET:HE3 | 1:B:45:PHE:HE1 | 15 | 0.66 |
| (1,1935) | 1:B:18:MET:HE1 | 1:B:45:PHE:HE1 | 19 | 0.66 |
| (1,1935) | 1:B:18:MET:HE2 | 1:B:45:PHE:HE1 | 19 | 0.66 |
| (1,1935) | 1:B:18:MET:HE3 | 1:B:45:PHE:HE1 | 19 | 0.66 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 19 | 0.66 |
| (1,1066) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:H | 1 | 0.66 |
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 14 | 0.65 |
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 18 | 0.65 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 5 | 0.65 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 5 | 0.65 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 5 | 0.65 |
| (1,5168) | 1:B:54:LYS:H | 1:B:54:LYS:HG2 | 8 | 0.65 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 15 | 0.65 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 15 | 0.65 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 9 | 0.65 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 9 | 0.65 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 9 | 0.65 |
| (1,5008) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD21 | 19 | 0.65 |
| (1,5008) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD21 | 19 | 0.65 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD21 | 6 | 0.65 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD22 | 6 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD23 | 6 | 0.65 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 13 | 0.65 |
| (1,4801) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG2 | 13 | 0.65 |
| (1,4734) | 1:A:23:THR:HG21 | 1:B:27:SER:HB2 | 20 | 0.65 |
| (1,4734) | 1:A:23:THR:HG22 | 1:B:27:SER:HB2 | 20 | 0.65 |
| (1,4734) | 1:A:23:THR:HG23 | 1:B:27:SER:HB2 | 20 | 0.65 |
| (1,4703) | 1:A:17:GLY:HA2 | 1:A:21:GLN:HE22 | 18 | 0.65 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 4 | 0.65 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 4 | 0.65 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 4 | 0.65 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 11 | 0.65 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 11 | 0.65 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 11 | 0.65 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 18 | 0.65 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 18 | 0.65 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 18 | 0.65 |
| (1,4481) | 1:A:10:ILE:HG21 | 1:A:45:PHE:HE1 | 14 | 0.65 |
| (1,4481) | 1:A:10:ILE:HG22 | 1:A:45:PHE:HE1 | 14 | 0.65 |
| (1,4481) | 1:A:10:ILE:HG23 | 1:A:45:PHE:HE1 | 14 | 0.65 |
| (1,4477) | 1:A:19:THR:HG21 | 1:A:45:PHE:HE1 | 17 | 0.65 |
| (1,4477) | 1:A:19:THR:HG22 | 1:A:45:PHE:HE1 | 17 | 0.65 |
| (1,4477) | 1:A:19:THR:HG23 | 1:A:45:PHE:HE1 | 17 | 0.65 |
| (1,4369) | 1:B:4:PHE:HE1 | 1:B:56:THR:HA | 13 | 0.65 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 3 | 0.65 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 3 | 0.65 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 3 | 0.65 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 15 | 0.65 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 15 | 0.65 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 15 | 0.65 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 7 | 0.65 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 7 | 0.65 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 7 | 0.65 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 10 | 0.65 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 10 | 0.65 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 10 | 0.65 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 5 | 0.65 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 5 | 0.65 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 5 | 0.65 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG11 | 19 | 0.65 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG12 | 19 | 0.65 |
| (1,1789) | 1:B:12:GLY:HA2 | 1:B:69:VAL:HG13 | 19 | 0.65 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 1 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 18 | 0.65 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 4 | 0.64 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 4 | 0.64 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 4 | 0.64 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 20 | 0.64 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 20 | 0.64 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 20 | 0.64 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 9 | 0.64 |
| (1,5175) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HD21 | 10 | 0.64 |
| (1,5175) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HD21 | 10 | 0.64 |
| (1,5173) | 1:B:54:LYS:HG2 | 1:B:55:ASN:HD21 | 2 | 0.64 |
| (1,5171) | 1:B:54:LYS:HB2 | 1:B:55:ASN:HD21 | 16 | 0.64 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD11 | 8 | 0.64 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD12 | 8 | 0.64 |
| (1,5096) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HD13 | 8 | 0.64 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 20 | 0.64 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 8 | 0.64 |
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 8 | 0.64 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 8 | 0.64 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 13 | 0.64 |
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 13 | 0.64 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 13 | 0.64 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 20 | 0.64 |
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 20 | 0.64 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 20 | 0.64 |
| (1,5035) | 1:B:24:GLY:H | 1:B:26:ILE:HG12 | 2 | 0.64 |
| (1,5035) | 1:B:24:GLY:H | 1:B:26:ILE:HG12 | 15 | 0.64 |
| (1,5009) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD21 | 12 | 0.64 |
| (1,5009) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD21 | 12 | 0.64 |
| (1,4951) | 1:B:3:ASP:HB2 | 1:B:4:PHE:H | 2 | 0.64 |
| (1,4951) | 1:B:3:ASP:HB2 | 1:B:4:PHE:H | 16 | 0.64 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 14 | 0.64 |
| (1,4802) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG3 | 16 | 0.64 |
| (1,4802) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG3 | 19 | 0.64 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD11 | 9 | 0.64 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD12 | 9 | 0.64 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD13 | 9 | 0.64 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 2 | 0.64 |
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 2 | 0.64 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 2 | 0.64 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 12 | 0.64 |
| (1,4697) | 1:A:17:GLY:H | 1:A:18:MET:HG2 | 17 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4678) | 1:A:15:LYS:H | 1:A:18:MET:HG2 | 15 | 0.64 |
| (1,4661) | 1:A:9:ARG:HD2 | 1:A:48:ASN:HD21 | 1 | 0.64 |
| (1,4661) | 1:A:9:ARG:HD3 | 1:A:48:ASN:HD21 | 1 | 0.64 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 17 | 0.64 |
| (1,4568) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HE1 | 6 | 0.64 |
| (1,4568) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HE1 | 6 | 0.64 |
| (1,4568) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HE1 | 6 | 0.64 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 20 | 0.64 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 20 | 0.64 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 20 | 0.64 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 13 | 0.64 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 10 | 0.64 |
| (1,4478) | 1:B:19:THR:HG21 | 1:B:45:PHE:HE1 | 5 | 0.64 |
| (1,4478) | 1:B:19:THR:HG22 | 1:B:45:PHE:HE1 | 5 | 0.64 |
| (1,4478) | 1:B:19:THR:HG23 | 1:B:45:PHE:HE1 | 5 | 0.64 |
| (1,4369) | 1:B:4:PHE:HE1 | 1:B:56:THR:HA | 19 | 0.64 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 10 | 0.64 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 10 | 0.64 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 1 | 0.64 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 1 | 0.64 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG21 | 12 | 0.64 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG22 | 12 | 0.64 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG23 | 12 | 0.64 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG21 | 8 | 0.64 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG22 | 8 | 0.64 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG23 | 8 | 0.64 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 16 | 0.64 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 6 | 0.64 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 6 | 0.64 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 6 | 0.64 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 10 | 0.64 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 18 | 0.64 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 18 | 0.64 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 18 | 0.64 |
| (1,2550) | 1:B:38:LEU:HD21 | 1:B:45:PHE:HE1 | 17 | 0.64 |
| (1,2550) | 1:B:38:LEU:HD22 | 1:B:45:PHE:HE1 | 17 | 0.64 |
| (1,2550) | 1:B:38:LEU:HD23 | 1:B:45:PHE:HE1 | 17 | 0.64 |
| (1,1066) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:H | 14 | 0.64 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 6 | 0.63 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 6 | 0.63 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 6 | 0.63 |
| (1,5243) | 1:B:68:LYS:HA | 1:B:68:LYS:HD2 | 15 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 18 | 0.63 |
| (1,5171) | 1:B:54:LYS:HB2 | 1:B:55:ASN:HD21 | 19 | 0.63 |
| (1,5166) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HG2 | 3 | 0.63 |
| (1,5166) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HG2 | 3 | 0.63 |
| (1,5166) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HG2 | 3 | 0.63 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 1 | 0.63 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 1 | 0.63 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 1 | 0.63 |
| (1,5065) | 1:B:27:SER:HG | 1:B:28:LYS:HD2 | 9 | 0.63 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD11 | 5 | 0.63 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD12 | 5 | 0.63 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD13 | 5 | 0.63 |
| (1,5035) | 1:B:24:GLY:H | 1:B:26:ILE:HG12 | 10 | 0.63 |
| (1,5035) | 1:B:24:GLY:H | 1:B:26:ILE:HG12 | 18 | 0.63 |
| (1,5035) | 1:B:24:GLY:H | 1:B:26:ILE:HG12 | 19 | 0.63 |
| (1,5008) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD21 | 17 | 0.63 |
| (1,5008) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD21 | 17 | 0.63 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 18 | 0.63 |
| (1,4956) | 1:B:4:PHE:H | 1:B:54:LYS:HB2 | 1 | 0.63 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 11 | 0.63 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 18 | 0.63 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 20 | 0.63 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 3 | 0.63 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 3 | 0.63 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 3 | 0.63 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 9 | 0.63 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 9 | 0.63 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 9 | 0.63 |
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD21 | 10 | 0.63 |
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD22 | 10 | 0.63 |
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD23 | 10 | 0.63 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD11 | 19 | 0.63 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD12 | 19 | 0.63 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD13 | 19 | 0.63 |
| (1,4834) | 1:A:39:ASN:HD21 | 1:A:46:THR:HB | 9 | 0.63 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD11 | 14 | 0.63 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD12 | 14 | 0.63 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD13 | 14 | 0.63 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 4 | 0.63 |
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 4 | 0.63 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 4 | 0.63 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 5 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 5 | 0.63 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 5 | 0.63 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 1 | 0.63 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 8 | 0.63 |
| (1,4730) | 1:A:23:THR:HB | 1:A:26:ILE:HG12 | 13 | 0.63 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 4 | 0.63 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 4 | 0.63 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 4 | 0.63 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG21 | 20 | 0.63 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG22 | 20 | 0.63 |
| (1,4709) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG23 | 20 | 0.63 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 13 | 0.63 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 13 | 0.63 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 13 | 0.63 |
| (1,4477) | 1:A:19:THR:HG21 | 1:A:45:PHE:HE1 | 11 | 0.63 |
| (1,4477) | 1:A:19:THR:HG22 | 1:A:45:PHE:HE1 | 11 | 0.63 |
| (1,4477) | 1:A:19:THR:HG23 | 1:A:45:PHE:HE1 | 11 | 0.63 |
| (1,4377) | 1:B:4:PHE:H | 1:B:4:PHE:HE1 | 16 | 0.63 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 5 | 0.63 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 5 | 0.63 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 14 | 0.63 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 14 | 0.63 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 14 | 0.63 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 6 | 0.63 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 6 | 0.63 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 6 | 0.63 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG21 | 19 | 0.63 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG22 | 19 | 0.63 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG23 | 19 | 0.63 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 12 | 0.63 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 12 | 0.63 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 12 | 0.63 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 14 | 0.63 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 14 | 0.63 |
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 14 | 0.63 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 4 | 0.63 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 4 | 0.63 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 4 | 0.63 |
| (1,2550) | 1:B:38:LEU:HD21 | 1:B:45:PHE:HE1 | 4 | 0.63 |
| (1,2550) | 1:B:38:LEU:HD22 | 1:B:45:PHE:HE1 | 4 | 0.63 |
| (1,2550) | 1:B:38:LEU:HD23 | 1:B:45:PHE:HE1 | 4 | 0.63 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 1 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 17 | 0.62 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 17 | 0.62 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 17 | 0.62 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 2 | 0.62 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 16 | 0.62 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 20 | 0.62 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 9 | 0.62 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 9 | 0.62 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 9 | 0.62 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 5 | 0.62 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 5 | 0.62 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 5 | 0.62 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD21 | 14 | 0.62 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD22 | 14 | 0.62 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD23 | 14 | 0.62 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD11 | 18 | 0.62 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD12 | 18 | 0.62 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD13 | 18 | 0.62 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 1 | 0.62 |
| (1,5060) | 1:B:27:SER:H | 1:B:28:LYS:HB2 | 1 | 0.62 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 13 | 0.62 |
| (1,5043) | 1:B:25:VAL:H | 1:B:26:ILE:HG12 | 14 | 0.62 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 19 | 0.62 |
| (1,4931) | 1:A:68:LYS:HA | 1:A:68:LYS:HD2 | 10 | 0.62 |
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 6 | 0.62 |
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 11 | 0.62 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 3 | 0.62 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 15 | 0.62 |
| (1,4870) | 1:A:54:LYS:HG2 | 1:A:55:ASN:HD21 | 12 | 0.62 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 10 | 0.62 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 11 | 0.62 |
| (1,4708) | 1:A:18:MET:HB2 | 1:A:22:ILE:HB | 4 | 0.62 |
| (1,4665) | 1:A:13:GLU:HG2 | 1:A:15:LYS:HB2 | 13 | 0.62 |
| (1,4665) | 1:A:13:GLU:HG3 | 1:A:15:LYS:HB2 | 13 | 0.62 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 16 | 0.62 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 16 | 0.62 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 16 | 0.62 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 15 | 0.62 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 15 | 0.62 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 15 | 0.62 |
| (1,3039) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HZ1 | 18 | 0.62 |
| (1,3039) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HZ1 | 18 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3039) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HZ1 | 18 | 0.62 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 9 | 0.62 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 9 | 0.62 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 9 | 0.62 |
| (1,1779) | 1:B:11:VAL:HG11 | 1:B:73:PHE:HE1 | 20 | 0.62 |
| (1,1779) | 1:B:11:VAL:HG12 | 1:B:73:PHE:HE1 | 20 | 0.62 |
| (1,1779) | 1:B:11:VAL:HG13 | 1:B:73:PHE:HE1 | 20 | 0.62 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 9 | 0.62 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 14 | 0.62 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 4 | 0.62 |
| (1,5255) | 1:B:77:ARG:HG2 | 1:B:78:LEU:HB2 | 16 | 0.61 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 4 | 0.61 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 13 | 0.61 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 13 | 0.61 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 13 | 0.61 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 4 | 0.61 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 4 | 0.61 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 4 | 0.61 |
| (1,5035) | 1:B:24:GLY:H | 1:B:26:ILE:HG12 | 8 | 0.61 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 12 | 0.61 |
| (1,4952) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HB2 | 16 | 0.61 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 14 | 0.61 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 16 | 0.61 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 16 | 0.61 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 16 | 0.61 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 9 | 0.61 |
| (1,4803) | 1:A:34:ARG:HB2 | 1:A:51:ILE:H | 17 | 0.61 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG21 | 6 | 0.61 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG22 | 6 | 0.61 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG23 | 6 | 0.61 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 9 | 0.61 |
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 9 | 0.61 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 9 | 0.61 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 18 | 0.61 |
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 18 | 0.61 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 18 | 0.61 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 3 | 0.61 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 5 | 0.61 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 11 | 0.61 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 20 | 0.61 |
| (1,4705) | 1:A:18:MET:H | 1:B:32:ASN:HD21 | 4 | 0.61 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 5 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 5 | 0.61 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 5 | 0.61 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 1 | 0.61 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 1 | 0.61 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 1 | 0.61 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 6 | 0.61 |
| (1,4478) | 1:B:19:THR:HG21 | 1:B:45:PHE:HE1 | 7 | 0.61 |
| (1,4478) | 1:B:19:THR:HG22 | 1:B:45:PHE:HE1 | 7 | 0.61 |
| (1,4478) | 1:B:19:THR:HG23 | 1:B:45:PHE:HE1 | 7 | 0.61 |
| (1,4368) | 1:A:4:PHE:HE1 | 1:A:56:THR:HA | 20 | 0.61 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG21 | 15 | 0.61 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG22 | 15 | 0.61 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG23 | 15 | 0.61 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG21 | 19 | 0.61 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG22 | 19 | 0.61 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG23 | 19 | 0.61 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 2 | 0.61 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 12 | 0.61 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 4 | 0.61 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 2 | 0.61 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 2 | 0.61 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 2 | 0.61 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 3 | 0.61 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 3 | 0.61 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 3 | 0.61 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 11 | 0.61 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 9 | 0.61 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG21 | 3 | 0.61 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG22 | 3 | 0.61 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG23 | 3 | 0.61 |
| (1,1935) | 1:B:18:MET:HE1 | 1:B:45:PHE:HE1 | 11 | 0.61 |
| (1,1935) | 1:B:18:MET:HE2 | 1:B:45:PHE:HE1 | 11 | 0.61 |
| (1,1935) | 1:B:18:MET:HE3 | 1:B:45:PHE:HE1 | 11 | 0.61 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 13 | 0.61 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 13 | 0.61 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 13 | 0.61 |
| (1,5232) | 1:B:67:ARG:H | 1:B:67:ARG:HG2 | 6 | 0.6 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 12 | 0.6 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 8 | 0.6 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 8 | 0.6 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 8 | 0.6 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 16 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB2 | 17 | 0.6 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB3 | 17 | 0.6 |
| (1,5166) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HG2 | 1 | 0.6 |
| (1,5166) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HG2 | 1 | 0.6 |
| (1,5166) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HG2 | 1 | 0.6 |
| (1,5166) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HG2 | 17 | 0.6 |
| (1,5166) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HG2 | 17 | 0.6 |
| (1,5166) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HG2 | 17 | 0.6 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 16 | 0.6 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 16 | 0.6 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 16 | 0.6 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 7 | 0.6 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 7 | 0.6 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 13 | 0.6 |
| (1,5065) | 1:B:27:SER:HG | 1:B:28:LYS:HD2 | 2 | 0.6 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 14 | 0.6 |
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 14 | 0.6 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 14 | 0.6 |
| (1,5035) | 1:B:24:GLY:H | 1:B:26:ILE:HG12 | 6 | 0.6 |
| (1,4993) | 1:B:14:ASP:HB2 | 1:B:43:GLY:H | 8 | 0.6 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD21 | 2 | 0.6 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD22 | 2 | 0.6 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD23 | 2 | 0.6 |
| (1,4931) | 1:A:68:LYS:HA | 1:A:68:LYS:HD2 | 6 | 0.6 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD11 | 2 | 0.6 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD12 | 2 | 0.6 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD13 | 2 | 0.6 |
| (1,4720) | 1:A:20:ASN:H | 1:B:32:ASN:HB2 | 11 | 0.6 |
| (1,4720) | 1:A:20:ASN:H | 1:B:32:ASN:HB2 | 19 | 0.6 |
| (1,4678) | 1:A:15:LYS:H | 1:A:18:MET:HG2 | 4 | 0.6 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 20 | 0.6 |
| (1,4565) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HE1 | 13 | 0.6 |
| (1,4565) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HE1 | 13 | 0.6 |
| (1,4565) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HE1 | 13 | 0.6 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 20 | 0.6 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 20 | 0.6 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 20 | 0.6 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 15 | 0.6 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 7 | 0.6 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 19 | 0.6 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD11 | 4 | 0.6 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD12 | 4 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD13 | 4 | 0.6 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 9 | 0.6 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 9 | 0.6 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 9 | 0.6 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 19 | 0.6 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 19 | 0.6 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 19 | 0.6 |
| (1,1779) | 1:B:11:VAL:HG11 | 1:B:73:PHE:HE1 | 14 | 0.6 |
| (1,1779) | 1:B:11:VAL:HG12 | 1:B:73:PHE:HE1 | 14 | 0.6 |
| (1,1779) | 1:B:11:VAL:HG13 | 1:B:73:PHE:HE1 | 14 | 0.6 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 4 | 0.6 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 7 | 0.59 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 18 | 0.59 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 18 | 0.59 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 18 | 0.59 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 4 | 0.59 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 1 | 0.59 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 9 | 0.59 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD21 | 11 | 0.59 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD22 | 11 | 0.59 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD23 | 11 | 0.59 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD11 | 20 | 0.59 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD12 | 20 | 0.59 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD13 | 20 | 0.59 |
| (1,5046) | 1:B:25:VAL:HA | 1:B:28:LYS:HB2 | 4 | 0.59 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE2 | 15 | 0.59 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE3 | 15 | 0.59 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE2 | 18 | 0.59 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE3 | 18 | 0.59 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 20 | 0.59 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG11 | 16 | 0.59 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG12 | 16 | 0.59 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG13 | 16 | 0.59 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 6 | 0.59 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 13 | 0.59 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 13 | 0.59 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 13 | 0.59 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 13 | 0.59 |
| (1,4889) | 1:A:58:LYS:HE2 | 1:A:59:LEU:HA | 18 | 0.59 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 12 | 0.59 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 12 | 0.59 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 12 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4795) | 1:A:32:ASN:HB2 | 1:B:20:ASN:H | 11 | 0.59 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 7 | 0.59 |
| (1,4671) | 1:A:14:ASP:HB2 | 1:A:43:GLY:H | 13 | 0.59 |
| (1,4573) | 1:A:44:ILE:HG12 | 1:A:73:PHE:HE1 | 17 | 0.59 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 17 | 0.59 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG21 | 12 | 0.59 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG22 | 12 | 0.59 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG23 | 12 | 0.59 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 2 | 0.59 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 1 | 0.58 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 7 | 0.58 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 10 | 0.58 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 12 | 0.58 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 12 | 0.58 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 12 | 0.58 |
| (1,5182) | 1:B:55:ASN:HD21 | 1:B:58:LYS:HG3 | 14 | 0.58 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 8 | 0.58 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 8 | 0.58 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 8 | 0.58 |
| (1,5035) | 1:B:24:GLY:H | 1:B:26:ILE:HG12 | 3 | 0.58 |
| (1,4985) | 1:B:9:ARG:HD2 | 1:B:48:ASN:HD21 | 3 | 0.58 |
| (1,4985) | 1:B:9:ARG:HD3 | 1:B:48:ASN:HD21 | 3 | 0.58 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 2 | 0.58 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 7 | 0.58 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 9 | 0.58 |
| (1,4879) | 1:A:55:ASN:HD21 | 1:A:58:LYS:HG3 | 7 | 0.58 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 7 | 0.58 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 7 | 0.58 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 7 | 0.58 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE2 | 11 | 0.58 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE3 | 11 | 0.58 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 9 | 0.58 |
| (1,4752) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HD2 | 17 | 0.58 |
| (1,4752) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HD2 | 17 | 0.58 |
| (1,4752) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HD2 | 17 | 0.58 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 19 | 0.58 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 2 | 0.58 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 2 | 0.58 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 2 | 0.58 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 16 | 0.58 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 16 | 0.58 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 16 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 3 | 0.58 |
| (1,4362) | 1:A:29:PHE:HE1 | 1:A:66:LEU:HG | 10 | 0.58 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG21 | 20 | 0.58 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG22 | 20 | 0.58 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG23 | 20 | 0.58 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 16 | 0.58 |
| (1,3038) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HZ1 | 8 | 0.58 |
| (1,3038) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HZ1 | 8 | 0.58 |
| (1,3038) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HZ1 | 8 | 0.58 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD11 | 19 | 0.58 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD12 | 19 | 0.58 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD13 | 19 | 0.58 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 18 | 0.58 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 18 | 0.58 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 18 | 0.58 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 2 | 0.58 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 2 | 0.58 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 2 | 0.58 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 8 | 0.58 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 8 | 0.58 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 8 | 0.58 |
| (1,2549) | 1:A:38:LEU:HD21 | 1:A:45:PHE:HE1 | 12 | 0.58 |
| (1,2549) | 1:A:38:LEU:HD22 | 1:A:45:PHE:HE1 | 12 | 0.58 |
| (1,2549) | 1:A:38:LEU:HD23 | 1:A:45:PHE:HE1 | 12 | 0.58 |
| (1,2549) | 1:A:38:LEU:HD21 | 1:A:45:PHE:HE1 | 15 | 0.58 |
| (1,2549) | 1:A:38:LEU:HD22 | 1:A:45:PHE:HE1 | 15 | 0.58 |
| (1,2549) | 1:A:38:LEU:HD23 | 1:A:45:PHE:HE1 | 15 | 0.58 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 8 | 0.58 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 16 | 0.58 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 3 | 0.58 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 8 | 0.58 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 17 | 0.58 |
| (1,5262) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HA | 11 | 0.57 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 11 | 0.57 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 14 | 0.57 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 17 | 0.57 |
| (1,5220) | 1:B:64:ASP:HB3 | 1:B:65:LYS:HG2 | 6 | 0.57 |
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 2 | 0.57 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 1 | 0.57 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 2 | 0.57 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 2 | 0.57 |
| (1,5035) | 1:B:24:GLY:H | 1:B:26:ILE:HG12 | 16 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5035) | 1:B:24:GLY:H | 1:B:26:ILE:HG12 | 17 | 0.57 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 6 | 0.57 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 8 | 0.57 |
| (1,4873) | 1:A:54:LYS:HE2 | 1:A:55:ASN:HD21 | 2 | 0.57 |
| (1,4873) | 1:A:54:LYS:HE3 | 1:A:55:ASN:HD21 | 2 | 0.57 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 16 | 0.57 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 16 | 0.57 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 16 | 0.57 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 20 | 0.57 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 20 | 0.57 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 20 | 0.57 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 6 | 0.57 |
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 6 | 0.57 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 6 | 0.57 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 6 | 0.57 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 16 | 0.57 |
| (1,4672) | 1:A:14:ASP:HB2 | 1:A:43:GLY:HA2 | 4 | 0.57 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 8 | 0.57 |
| (1,4573) | 1:A:44:ILE:HG12 | 1:A:73:PHE:HE1 | 1 | 0.57 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 5 | 0.57 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 5 | 0.57 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 5 | 0.57 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 7 | 0.57 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 7 | 0.57 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 7 | 0.57 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 1 | 0.57 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 1 | 0.57 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 6 | 0.57 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 6 | 0.57 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 20 | 0.57 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 20 | 0.57 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 10 | 0.57 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 10 | 0.57 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 15 | 0.57 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 15 | 0.57 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 17 | 0.57 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 17 | 0.57 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 17 | 0.57 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 6 | 0.57 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG21 | 13 | 0.57 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG22 | 13 | 0.57 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG23 | 13 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1778) | 1:A:11:VAL:HG11 | 1:A:73:PHE:HE1 | 5 | 0.57 |
| (1,1778) | 1:A:11:VAL:HG12 | 1:A:73:PHE:HE1 | 5 | 0.57 |
| (1,1778) | 1:A:11:VAL:HG13 | 1:A:73:PHE:HE1 | 5 | 0.57 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 19 | 0.57 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 1 | 0.57 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 2 | 0.57 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 10 | 0.56 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 10 | 0.56 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 10 | 0.56 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 19 | 0.56 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 19 | 0.56 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 19 | 0.56 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 5 | 0.56 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 13 | 0.56 |
| (1,5176) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD21 | 17 | 0.56 |
| (1,5176) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD21 | 17 | 0.56 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 5 | 0.56 |
| (1,5035) | 1:B:24:GLY:H | 1:B:26:ILE:HG12 | 11 | 0.56 |
| (1,5035) | 1:B:24:GLY:H | 1:B:26:ILE:HG12 | 13 | 0.56 |
| (1,5013) | 1:B:16:ASN:HB2 | 1:B:18:MET:H | 2 | 0.56 |
| (1,4931) | 1:A:68:LYS:HA | 1:A:68:LYS:HD2 | 11 | 0.56 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 16 | 0.56 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 19 | 0.56 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 10 | 0.56 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 10 | 0.56 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 10 | 0.56 |
| (1,4883) | 1:A:57:ASP:H | 1:A:58:LYS:HB2 | 6 | 0.56 |
| (1,4834) | 1:A:39:ASN:HD21 | 1:A:46:THR:HB | 5 | 0.56 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD2 | 3 | 0.56 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD3 | 3 | 0.56 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD2 | 8 | 0.56 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD3 | 8 | 0.56 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 7 | 0.56 |
| (1,4733) | 1:A:23:THR:HG21 | 1:A:27:SER:HB2 | 17 | 0.56 |
| (1,4733) | 1:A:23:THR:HG22 | 1:A:27:SER:HB2 | 17 | 0.56 |
| (1,4733) | 1:A:23:THR:HG23 | 1:A:27:SER:HB2 | 17 | 0.56 |
| (1,4697) | 1:A:17:GLY:H | 1:A:18:MET:HG2 | 4 | 0.56 |
| (1,4678) | 1:A:15:LYS:H | 1:A:18:MET:HG2 | 20 | 0.56 |
| (1,4628) | 1:A:3:ASP:HB2 | 1:A:4:PHE:H | 18 | 0.56 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 5 | 0.56 |
| (1,4369) | 1:B:4:PHE:HE1 | 1:B:56:THR:HA | 12 | 0.56 |
| (1,4368) | 1:A:4:PHE:HE1 | 1:A:56:THR:HA | 8 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 4 | 0.56 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 4 | 0.56 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 8 | 0.56 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 18 | 0.56 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 2 | 0.56 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 2 | 0.56 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 2 | 0.56 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 13 | 0.56 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 13 | 0.56 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 13 | 0.56 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 13 | 0.56 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 13 | 0.56 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 13 | 0.56 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 5 | 0.56 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 6 | 0.56 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 15 | 0.56 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 15 | 0.56 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 15 | 0.56 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 15 | 0.56 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 6 | 0.56 |
| (1,1066) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:H | 6 | 0.56 |
| (1,5219) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HG2 | 9 | 0.55 |
| (1,5166) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HG2 | 6 | 0.55 |
| (1,5166) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HG2 | 6 | 0.55 |
| (1,5166) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HG2 | 6 | 0.55 |
| (1,5166) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HG2 | 12 | 0.55 |
| (1,5166) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HG2 | 12 | 0.55 |
| (1,5166) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HG2 | 12 | 0.55 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 6 | 0.55 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 6 | 0.55 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 6 | 0.55 |
| (1,5128) | 1:B:37:VAL:HG21 | 1:B:48:ASN:HD21 | 17 | 0.55 |
| (1,5128) | 1:B:37:VAL:HG22 | 1:B:48:ASN:HD21 | 17 | 0.55 |
| (1,5128) | 1:B:37:VAL:HG23 | 1:B:48:ASN:HD21 | 17 | 0.55 |
| (1,5086) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HD2 | 11 | 0.55 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD11 | 16 | 0.55 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD12 | 16 | 0.55 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD13 | 16 | 0.55 |
| (1,5035) | 1:B:24:GLY:H | 1:B:26:ILE:HG12 | 7 | 0.55 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 1 | 0.55 |
| (1,5007) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HB2 | 13 | 0.55 |
| (1,5007) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HB2 | 13 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 20 | 0.55 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD21 | 3 | 0.55 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD22 | 3 | 0.55 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD23 | 3 | 0.55 |
| (1,4920) | 1:A:67:ARG:H | 1:A:67:ARG:HG2 | 7 | 0.55 |
| (1,4920) | 1:A:67:ARG:H | 1:A:67:ARG:HG2 | 17 | 0.55 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 4 | 0.55 |
| (1,4767) | 1:A:27:SER:HG | 1:A:28:LYS:HD2 | 7 | 0.55 |
| (1,4746) | 1:A:25:VAL:H | 1:A:28:LYS:HD2 | 17 | 0.55 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 13 | 0.55 |
| (1,4678) | 1:A:15:LYS:H | 1:A:18:MET:HG2 | 17 | 0.55 |
| (1,4671) | 1:A:14:ASP:HB2 | 1:A:43:GLY:H | 17 | 0.55 |
| (1,4369) | 1:B:4:PHE:HE1 | 1:B:56:THR:HA | 16 | 0.55 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 9 | 0.55 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 9 | 0.55 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 2 | 0.55 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 2 | 0.55 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 2 | 0.55 |
| (1,3094) | 1:A:53:VAL:HG11 | 1:A:58:LYS:HZ1 | 3 | 0.55 |
| (1,3094) | 1:A:53:VAL:HG12 | 1:A:58:LYS:HZ1 | 3 | 0.55 |
| (1,3094) | 1:A:53:VAL:HG13 | 1:A:58:LYS:HZ1 | 3 | 0.55 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD11 | 10 | 0.55 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD12 | 10 | 0.55 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD13 | 10 | 0.55 |
| (1,1039) | 1:B:58:LYS:HZ1 | 1:B:61:THR:H | 9 | 0.55 |
| (1,5249) | 1:B:77:ARG:H | 1:B:77:ARG:HB2 | 16 | 0.54 |
| (1,5245) | 1:B:69:VAL:HG11 | 1:B:70:GLN:HE21 | 17 | 0.54 |
| (1,5245) | 1:B:69:VAL:HG12 | 1:B:70:GLN:HE21 | 17 | 0.54 |
| (1,5245) | 1:B:69:VAL:HG13 | 1:B:70:GLN:HE21 | 17 | 0.54 |
| (1,5243) | 1:B:68:LYS:HA | 1:B:68:LYS:HD2 | 4 | 0.54 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 3 | 0.54 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 8 | 0.54 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 14 | 0.54 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 14 | 0.54 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 14 | 0.54 |
| (1,5176) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD21 | 19 | 0.54 |
| (1,5176) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD21 | 19 | 0.54 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 6 | 0.54 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 6 | 0.54 |
| (1,5065) | 1:B:27:SER:HG | 1:B:28:LYS:HD2 | 5 | 0.54 |
| (1,5035) | 1:B:24:GLY:H | 1:B:26:ILE:HG12 | 14 | 0.54 |
| (1,5008) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD21 | 11 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5008) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD21 | 11 | 0.54 |
| (1,4999) | 1:B:15:LYS:H | 1:B:18:MET:HG2 | 9 | 0.54 |
| (1,4931) | 1:A:68:LYS:HA | 1:A:68:LYS:HD2 | 19 | 0.54 |
| (1,4920) | 1:A:67:ARG:H | 1:A:67:ARG:HG2 | 5 | 0.54 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 1 | 0.54 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 17 | 0.54 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 6 | 0.54 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 6 | 0.54 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 6 | 0.54 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 5 | 0.54 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 9 | 0.54 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 9 | 0.54 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 9 | 0.54 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD11 | 14 | 0.54 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD12 | 14 | 0.54 |
| (1,4793) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HD13 | 14 | 0.54 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG21 | 7 | 0.54 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG22 | 7 | 0.54 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG23 | 7 | 0.54 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 20 | 0.54 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 20 | 0.54 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 20 | 0.54 |
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 18 | 0.54 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 7 | 0.54 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 1 | 0.54 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 19 | 0.54 |
| (1,4478) | 1:B:19:THR:HG21 | 1:B:45:PHE:HE1 | 8 | 0.54 |
| (1,4478) | 1:B:19:THR:HG22 | 1:B:45:PHE:HE1 | 8 | 0.54 |
| (1,4478) | 1:B:19:THR:HG23 | 1:B:45:PHE:HE1 | 8 | 0.54 |
| (1,4369) | 1:B:4:PHE:HE1 | 1:B:56:THR:HA | 10 | 0.54 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 18 | 0.54 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 18 | 0.54 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG21 | 16 | 0.54 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG22 | 16 | 0.54 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG23 | 16 | 0.54 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 5 | 0.54 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 9 | 0.54 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 9 | 0.54 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 9 | 0.54 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 10 | 0.54 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 10 | 0.54 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 10 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 15 | 0.54 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 13 | 0.54 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 13 | 0.54 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 13 | 0.54 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 20 | 0.54 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 20 | 0.54 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 20 | 0.54 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 15 | 0.54 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 1 | 0.53 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 1 | 0.53 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 1 | 0.53 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 10 | 0.53 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 10 | 0.53 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 10 | 0.53 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 14 | 0.53 |
| (1,5176) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD21 | 18 | 0.53 |
| (1,5176) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD21 | 18 | 0.53 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 10 | 0.53 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD11 | 6 | 0.53 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD12 | 6 | 0.53 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD13 | 6 | 0.53 |
| (1,5046) | 1:B:25:VAL:HA | 1:B:28:LYS:HB2 | 1 | 0.53 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE2 | 7 | 0.53 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE3 | 7 | 0.53 |
| (1,5005) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HD21 | 14 | 0.53 |
| (1,5005) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HD21 | 14 | 0.53 |
| (1,4999) | 1:B:15:LYS:H | 1:B:18:MET:HG2 | 4 | 0.53 |
| (1,4984) | 1:B:9:ARG:HG2 | 1:B:76:GLU:H | 6 | 0.53 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 4 | 0.53 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 2 | 0.53 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 16 | 0.53 |
| (1,4920) | 1:A:67:ARG:H | 1:A:67:ARG:HG2 | 13 | 0.53 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 10 | 0.53 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD11 | 20 | 0.53 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD12 | 20 | 0.53 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD13 | 20 | 0.53 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB2 | 15 | 0.53 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB3 | 15 | 0.53 |
| (1,4801) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG2 | 20 | 0.53 |
| (1,4787) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HD2 | 1 | 0.53 |
| (1,4774) | 1:A:28:LYS:HB2 | 1:A:28:LYS:HD2 | 14 | 0.53 |
| (1,4744) | 1:A:25:VAL:H | 1:A:26:ILE:HG12 | 13 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4735) | 1:A:24:GLY:H | 1:A:26:ILE:HG12 | 15 | 0.53 |
| (1,4665) | 1:A:13:GLU:HG2 | 1:A:15:LYS:HB2 | 2 | 0.53 |
| (1,4665) | 1:A:13:GLU:HG3 | 1:A:15:LYS:HB2 | 2 | 0.53 |
| (1,4661) | 1:A:9:ARG:HD2 | 1:A:48:ASN:HD21 | 14 | 0.53 |
| (1,4661) | 1:A:9:ARG:HD3 | 1:A:48:ASN:HD21 | 14 | 0.53 |
| (1,4633) | 1:A:4:PHE:H | 1:A:54:LYS:HB2 | 16 | 0.53 |
| (1,4368) | 1:A:4:PHE:HE1 | 1:A:56:THR:HA | 9 | 0.53 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 2 | 0.53 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 2 | 0.53 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 14 | 0.53 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 14 | 0.53 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 11 | 0.53 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 11 | 0.53 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 19 | 0.53 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 19 | 0.53 |
| (1,3095) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HZ1 | 16 | 0.53 |
| (1,3095) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HZ1 | 16 | 0.53 |
| (1,3095) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HZ1 | 16 | 0.53 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 3 | 0.53 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 6 | 0.53 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 20 | 0.53 |
| (1,1066) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:H | 7 | 0.53 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 3 | 0.52 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 3 | 0.52 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 3 | 0.52 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 7 | 0.52 |
| (1,5249) | 1:B:77:ARG:H | 1:B:77:ARG:HB2 | 8 | 0.52 |
| (1,5236) | 1:B:67:ARG:HG2 | 1:B:72:VAL:HG11 | 2 | 0.52 |
| (1,5236) | 1:B:67:ARG:HG2 | 1:B:72:VAL:HG12 | 2 | 0.52 |
| (1,5236) | 1:B:67:ARG:HG2 | 1:B:72:VAL:HG13 | 2 | 0.52 |
| (1,5232) | 1:B:67:ARG:H | 1:B:67:ARG:HG2 | 3 | 0.52 |
| (1,5232) | 1:B:67:ARG:H | 1:B:67:ARG:HG2 | 5 | 0.52 |
| (1,5174) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HB2 | 10 | 0.52 |
| (1,5174) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HB2 | 10 | 0.52 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 18 | 0.52 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 18 | 0.52 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 18 | 0.52 |
| (1,5126) | 1:B:37:VAL:HG11 | 1:B:48:ASN:HD21 | 7 | 0.52 |
| (1,5126) | 1:B:37:VAL:HG12 | 1:B:48:ASN:HD21 | 7 | 0.52 |
| (1,5126) | 1:B:37:VAL:HG13 | 1:B:48:ASN:HD21 | 7 | 0.52 |
| (1,5072) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HD2 | 18 | 0.52 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 1 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 2 | 0.52 |
| (1,4956) | 1:B:4:PHE:H | 1:B:54:LYS:HB2 | 17 | 0.52 |
| (1,4920) | 1:A:67:ARG:H | 1:A:67:ARG:HG2 | 16 | 0.52 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 2 | 0.52 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 2 | 0.52 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 2 | 0.52 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 15 | 0.52 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 15 | 0.52 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 15 | 0.52 |
| (1,4873) | 1:A:54:LYS:HE2 | 1:A:55:ASN:HD21 | 14 | 0.52 |
| (1,4873) | 1:A:54:LYS:HE3 | 1:A:55:ASN:HD21 | 14 | 0.52 |
| (1,4869) | 1:A:54:LYS:HG2 | 1:A:55:ASN:H | 10 | 0.52 |
| (1,4868) | 1:A:54:LYS:HB2 | 1:A:55:ASN:HD21 | 3 | 0.52 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 10 | 0.52 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 10 | 0.52 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 10 | 0.52 |
| (1,4822) | 1:A:37:VAL:HG11 | 1:A:48:ASN:HD21 | 3 | 0.52 |
| (1,4822) | 1:A:37:VAL:HG12 | 1:A:48:ASN:HD21 | 3 | 0.52 |
| (1,4822) | 1:A:37:VAL:HG13 | 1:A:48:ASN:HD21 | 3 | 0.52 |
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 20 | 0.52 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 20 | 0.52 |
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 20 | 0.52 |
| (1,4767) | 1:A:27:SER:HG | 1:A:28:LYS:HD2 | 9 | 0.52 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 18 | 0.52 |
| (1,4658) | 1:A:9:ARG:HG2 | 1:A:11:VAL:HG21 | 9 | 0.52 |
| (1,4658) | 1:A:9:ARG:HG2 | 1:A:11:VAL:HG22 | 9 | 0.52 |
| (1,4658) | 1:A:9:ARG:HG2 | 1:A:11:VAL:HG23 | 9 | 0.52 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 18 | 0.52 |
| (1,4573) | 1:A:44:ILE:HG12 | 1:A:73:PHE:HE1 | 9 | 0.52 |
| (1,4567) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HE1 | 5 | 0.52 |
| (1,4567) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HE1 | 5 | 0.52 |
| (1,4567) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HE1 | 5 | 0.52 |
| (1,4567) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HE1 | 10 | 0.52 |
| (1,4567) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HE1 | 10 | 0.52 |
| (1,4567) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HE1 | 10 | 0.52 |
| (1,4510) | 1:B:45:PHE:HZ | 1:B:71:GLY:HA2 | 3 | 0.52 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 4 | 0.52 |
| (1,4477) | 1:A:19:THR:HG21 | 1:A:45:PHE:HE1 | 2 | 0.52 |
| (1,4477) | 1:A:19:THR:HG22 | 1:A:45:PHE:HE1 | 2 | 0.52 |
| (1,4477) | 1:A:19:THR:HG23 | 1:A:45:PHE:HE1 | 2 | 0.52 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 5 | 0.52 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 5 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 11 | 0.52 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 11 | 0.52 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 6 | 0.52 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 6 | 0.52 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 6 | 0.52 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 13 | 0.52 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 7 | 0.51 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 7 | 0.51 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 7 | 0.51 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 10 | 0.51 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 10 | 0.51 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 10 | 0.51 |
| (1,5159) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HE2 | 3 | 0.51 |
| (1,5159) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HE2 | 3 | 0.51 |
| (1,5159) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HE2 | 3 | 0.51 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 14 | 0.51 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 14 | 0.51 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 14 | 0.51 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 3 | 0.51 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 4 | 0.51 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 13 | 0.51 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 5 | 0.51 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 5 | 0.51 |
| (1,5128) | 1:B:37:VAL:HG21 | 1:B:48:ASN:HD21 | 13 | 0.51 |
| (1,5128) | 1:B:37:VAL:HG22 | 1:B:48:ASN:HD21 | 13 | 0.51 |
| (1,5128) | 1:B:37:VAL:HG23 | 1:B:48:ASN:HD21 | 13 | 0.51 |
| (1,5126) | 1:B:37:VAL:HG11 | 1:B:48:ASN:HD21 | 6 | 0.51 |
| (1,5126) | 1:B:37:VAL:HG12 | 1:B:48:ASN:HD21 | 6 | 0.51 |
| (1,5126) | 1:B:37:VAL:HG13 | 1:B:48:ASN:HD21 | 6 | 0.51 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 11 | 0.51 |
| (1,5050) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HG2 | 17 | 0.51 |
| (1,5050) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HG2 | 17 | 0.51 |
| (1,5050) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HG2 | 17 | 0.51 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 11 | 0.51 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 17 | 0.51 |
| (1,4951) | 1:B:3:ASP:HB2 | 1:B:4:PHE:H | 12 | 0.51 |
| (1,4920) | 1:A:67:ARG:H | 1:A:67:ARG:HG2 | 9 | 0.51 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 14 | 0.51 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 14 | 0.51 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 14 | 0.51 |
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD21 | 3 | 0.51 |
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD22 | 3 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD23 | 3 | 0.51 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 1 | 0.51 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 1 | 0.51 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 1 | 0.51 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 14 | 0.51 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 14 | 0.51 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 14 | 0.51 |
| (1,4824) | 1:A:37:VAL:HG21 | 1:A:48:ASN:HD21 | 2 | 0.51 |
| (1,4824) | 1:A:37:VAL:HG22 | 1:A:48:ASN:HD21 | 2 | 0.51 |
| (1,4824) | 1:A:37:VAL:HG23 | 1:A:48:ASN:HD21 | 2 | 0.51 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 9 | 0.51 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 16 | 0.51 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 18 | 0.51 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 9 | 0.51 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 9 | 0.51 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 9 | 0.51 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 7 | 0.51 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 13 | 0.51 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 13 | 0.51 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 8 | 0.51 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD11 | 14 | 0.51 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD12 | 14 | 0.51 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD13 | 14 | 0.51 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 7 | 0.51 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 10 | 0.51 |
| (1,5232) | 1:B:67:ARG:H | 1:B:67:ARG:HG2 | 2 | 0.5 |
| (1,5218) | 1:B:64:ASP:HA | 1:B:67:ARG:HG2 | 6 | 0.5 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 17 | 0.5 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 17 | 0.5 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 17 | 0.5 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 19 | 0.5 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 6 | 0.5 |
| (1,5072) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HD2 | 16 | 0.5 |
| (1,4993) | 1:B:14:ASP:HB2 | 1:B:43:GLY:H | 11 | 0.5 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 5 | 0.5 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 8 | 0.5 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 13 | 0.5 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 15 | 0.5 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG21 | 17 | 0.5 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG22 | 17 | 0.5 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG23 | 17 | 0.5 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 16 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 3 | 0.5 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 3 | 0.5 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 2 | 0.5 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 7 | 0.5 |
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 7 | 0.5 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 7 | 0.5 |
| (1,4728) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HG12 | 7 | 0.5 |
| (1,4696) | 1:A:16:ASN:HB2 | 1:A:18:MET:H | 12 | 0.5 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 12 | 0.5 |
| (1,4628) | 1:A:3:ASP:HB2 | 1:A:4:PHE:H | 13 | 0.5 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 6 | 0.5 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 17 | 0.5 |
| (1,4546) | 1:B:5:LEU:HB2 | 1:B:52:PHE:HE1 | 11 | 0.5 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 9 | 0.5 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 9 | 0.5 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 9 | 0.5 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 12 | 0.5 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 12 | 0.5 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 3 | 0.5 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 3 | 0.5 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 7 | 0.5 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 7 | 0.5 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 8 | 0.5 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 8 | 0.5 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 20 | 0.5 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 7 | 0.5 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 7 | 0.5 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 7 | 0.5 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 16 | 0.5 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 6 | 0.5 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 6 | 0.5 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 6 | 0.5 |
| (1,3095) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HZ1 | 13 | 0.5 |
| (1,3095) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HZ1 | 13 | 0.5 |
| (1,3095) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HZ1 | 13 | 0.5 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 17 | 0.5 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 17 | 0.5 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 17 | 0.5 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 16 | 0.5 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 16 | 0.5 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 16 | 0.5 |
| (1,2549) | 1:A:38:LEU:HD21 | 1:A:45:PHE:HE1 | 4 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2549) | 1:A:38:LEU:HD22 | 1:A:45:PHE:HE1 | 4 | 0.5 |
| (1,2549) | 1:A:38:LEU:HD23 | 1:A:45:PHE:HE1 | 4 | 0.5 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 17 | 0.5 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 18 | 0.5 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 19 | 0.5 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 7 | 0.5 |
| (1,5176) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD21 | 16 | 0.49 |
| (1,5176) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD21 | 16 | 0.49 |
| (1,5098) | 1:B:32:ASN:HD21 | 1:B:33:ILE:H | 2 | 0.49 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD11 | 16 | 0.49 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD12 | 16 | 0.49 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD13 | 16 | 0.49 |
| (1,5065) | 1:B:27:SER:HG | 1:B:28:LYS:HD2 | 13 | 0.49 |
| (1,5051) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HD2 | 9 | 0.49 |
| (1,5051) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HD2 | 9 | 0.49 |
| (1,5051) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HD2 | 9 | 0.49 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 3 | 0.49 |
| (1,5008) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD21 | 9 | 0.49 |
| (1,5008) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD21 | 9 | 0.49 |
| (1,5008) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD21 | 18 | 0.49 |
| (1,5008) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD21 | 18 | 0.49 |
| (1,4993) | 1:B:14:ASP:HB2 | 1:B:43:GLY:H | 6 | 0.49 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG11 | 17 | 0.49 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG12 | 17 | 0.49 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG13 | 17 | 0.49 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 2 | 0.49 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 2 | 0.49 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 2 | 0.49 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 9 | 0.49 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 9 | 0.49 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 9 | 0.49 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 13 | 0.49 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 13 | 0.49 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 13 | 0.49 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 8 | 0.49 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 8 | 0.49 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 8 | 0.49 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD11 | 1 | 0.49 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD12 | 1 | 0.49 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD13 | 1 | 0.49 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 9 | 0.49 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 9 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 9 | 0.49 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 16 | 0.49 |
| (1,4774) | 1:A:28:LYS:HB2 | 1:A:28:LYS:HD2 | 1 | 0.49 |
| (1,4774) | 1:A:28:LYS:HB2 | 1:A:28:LYS:HD2 | 7 | 0.49 |
| (1,4747) | 1:A:25:VAL:HA | 1:A:28:LYS:HB2 | 20 | 0.49 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 8 | 0.49 |
| (1,4684) | 1:A:15:LYS:HB2 | 1:A:18:MET:HB2 | 6 | 0.49 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 4 | 0.49 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 10 | 0.49 |
| (1,4543) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HE1 | 12 | 0.49 |
| (1,4543) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HE1 | 12 | 0.49 |
| (1,4543) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HE1 | 12 | 0.49 |
| (1,4369) | 1:B:4:PHE:HE1 | 1:B:56:THR:HA | 1 | 0.49 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 13 | 0.49 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 13 | 0.49 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 16 | 0.49 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 16 | 0.49 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 17 | 0.49 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 17 | 0.49 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG21 | 3 | 0.49 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG22 | 3 | 0.49 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG23 | 3 | 0.49 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 8 | 0.49 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 8 | 0.49 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 8 | 0.49 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 10 | 0.49 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 3 | 0.48 |
| (1,5185) | 1:B:56:THR:HG21 | 1:B:59:LEU:HB2 | 7 | 0.48 |
| (1,5185) | 1:B:56:THR:HG22 | 1:B:59:LEU:HB2 | 7 | 0.48 |
| (1,5185) | 1:B:56:THR:HG23 | 1:B:59:LEU:HB2 | 7 | 0.48 |
| (1,5159) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HE2 | 18 | 0.48 |
| (1,5159) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HE2 | 18 | 0.48 |
| (1,5159) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HE2 | 18 | 0.48 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 3 | 0.48 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 3 | 0.48 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 3 | 0.48 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD2 | 7 | 0.48 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD3 | 7 | 0.48 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD2 | 11 | 0.48 |
| (1,5136) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HD3 | 11 | 0.48 |
| (1,5126) | 1:B:37:VAL:HG11 | 1:B:48:ASN:HD21 | 1 | 0.48 |
| (1,5126) | 1:B:37:VAL:HG12 | 1:B:48:ASN:HD21 | 1 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5126) | 1:B:37:VAL:HG13 | 1:B:48:ASN:HD21 | 1 | 0.48 |
| (1,5107) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG3 | 1 | 0.48 |
| (1,5098) | 1:B:32:ASN:HD21 | 1:B:33:ILE:H | 15 | 0.48 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 7 | 0.48 |
| (1,5072) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HD2 | 5 | 0.48 |
| (1,5072) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HD2 | 6 | 0.48 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 18 | 0.48 |
| (1,5005) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HD21 | 11 | 0.48 |
| (1,5005) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HD21 | 11 | 0.48 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 12 | 0.48 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 14 | 0.48 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 11 | 0.48 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 6 | 0.48 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 8 | 0.48 |
| (1,4920) | 1:A:67:ARG:H | 1:A:67:ARG:HG2 | 18 | 0.48 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 7 | 0.48 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 7 | 0.48 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 7 | 0.48 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 5 | 0.48 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 5 | 0.48 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 5 | 0.48 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 6 | 0.48 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 6 | 0.48 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 6 | 0.48 |
| (1,4824) | 1:A:37:VAL:HG21 | 1:A:48:ASN:HD21 | 12 | 0.48 |
| (1,4824) | 1:A:37:VAL:HG22 | 1:A:48:ASN:HD21 | 12 | 0.48 |
| (1,4824) | 1:A:37:VAL:HG23 | 1:A:48:ASN:HD21 | 12 | 0.48 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 15 | 0.48 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 15 | 0.48 |
| (1,4774) | 1:A:28:LYS:HB2 | 1:A:28:LYS:HD2 | 5 | 0.48 |
| (1,4728) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HG12 | 14 | 0.48 |
| (1,4691) | 1:A:15:LYS:HE2 | 1:A:16:ASN:HD21 | 10 | 0.48 |
| (1,4691) | 1:A:15:LYS:HE3 | 1:A:16:ASN:HD21 | 10 | 0.48 |
| (1,4682) | 1:A:15:LYS:HB2 | 1:A:16:ASN:HB2 | 6 | 0.48 |
| (1,4665) | 1:A:13:GLU:HG2 | 1:A:15:LYS:HB2 | 6 | 0.48 |
| (1,4665) | 1:A:13:GLU:HG3 | 1:A:15:LYS:HB2 | 6 | 0.48 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 6 | 0.48 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 20 | 0.48 |
| (1,4627) | 1:A:3:ASP:HA | 1:A:54:LYS:HB2 | 16 | 0.48 |
| (1,4368) | 1:A:4:PHE:HE1 | 1:A:56:THR:HA | 11 | 0.48 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 8 | 0.48 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 8 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 18 | 0.48 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 18 | 0.48 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG21 | 4 | 0.48 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG22 | 4 | 0.48 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG23 | 4 | 0.48 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 20 | 0.48 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 20 | 0.48 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 20 | 0.48 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 12 | 0.48 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 16 | 0.48 |
| (1,2550) | 1:B:38:LEU:HD21 | 1:B:45:PHE:HE1 | 6 | 0.48 |
| (1,2550) | 1:B:38:LEU:HD22 | 1:B:45:PHE:HE1 | 6 | 0.48 |
| (1,2550) | 1:B:38:LEU:HD23 | 1:B:45:PHE:HE1 | 6 | 0.48 |
| (1,2550) | 1:B:38:LEU:HD21 | 1:B:45:PHE:HE1 | 9 | 0.48 |
| (1,2550) | 1:B:38:LEU:HD22 | 1:B:45:PHE:HE1 | 9 | 0.48 |
| (1,2550) | 1:B:38:LEU:HD23 | 1:B:45:PHE:HE1 | 9 | 0.48 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 7 | 0.48 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 13 | 0.48 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 12 | 0.47 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 5 | 0.47 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 14 | 0.47 |
| (1,5128) | 1:B:37:VAL:HG21 | 1:B:48:ASN:HD21 | 10 | 0.47 |
| (1,5128) | 1:B:37:VAL:HG22 | 1:B:48:ASN:HD21 | 10 | 0.47 |
| (1,5128) | 1:B:37:VAL:HG23 | 1:B:48:ASN:HD21 | 10 | 0.47 |
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 5 | 0.47 |
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 5 | 0.47 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 5 | 0.47 |
| (1,5072) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HD2 | 10 | 0.47 |
| (1,5072) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HD2 | 13 | 0.47 |
| (1,5072) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HD2 | 15 | 0.47 |
| (1,5072) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HD2 | 20 | 0.47 |
| (1,5066) | 1:B:28:LYS:H | 1:B:28:LYS:HB2 | 12 | 0.47 |
| (1,5012) | 1:B:16:ASN:HB2 | 1:B:17:GLY:H | 18 | 0.47 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 10 | 0.47 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 16 | 0.47 |
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 1 | 0.47 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 16 | 0.47 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 16 | 0.47 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 16 | 0.47 |
| (1,4862) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HB2 | 2 | 0.47 |
| (1,4862) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HB2 | 2 | 0.47 |
| (1,4862) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HB2 | 2 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE2 | 16 | 0.47 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE3 | 16 | 0.47 |
| (1,4774) | 1:A:28:LYS:HB2 | 1:A:28:LYS:HD2 | 9 | 0.47 |
| (1,4774) | 1:A:28:LYS:HB2 | 1:A:28:LYS:HD2 | 18 | 0.47 |
| (1,4774) | 1:A:28:LYS:HB2 | 1:A:28:LYS:HD2 | 19 | 0.47 |
| (1,4768) | 1:A:28:LYS:H | 1:A:28:LYS:HB2 | 14 | 0.47 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG21 | 19 | 0.47 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG22 | 19 | 0.47 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG23 | 19 | 0.47 |
| (1,4751) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HG2 | 19 | 0.47 |
| (1,4751) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HG2 | 19 | 0.47 |
| (1,4751) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HG2 | 19 | 0.47 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE2 | 3 | 0.47 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE3 | 3 | 0.47 |
| (1,4690) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD21 | 7 | 0.47 |
| (1,4690) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD21 | 7 | 0.47 |
| (1,4686) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HB2 | 14 | 0.47 |
| (1,4686) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HB2 | 14 | 0.47 |
| (1,4672) | 1:A:14:ASP:HB2 | 1:A:43:GLY:HA2 | 9 | 0.47 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 7 | 0.47 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 17 | 0.47 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 19 | 0.47 |
| (1,4567) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HE1 | 11 | 0.47 |
| (1,4567) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HE1 | 11 | 0.47 |
| (1,4567) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HE1 | 11 | 0.47 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 14 | 0.47 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 14 | 0.47 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 14 | 0.47 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 2 | 0.47 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 18 | 0.47 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 18 | 0.47 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 18 | 0.47 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 18 | 0.47 |
| (1,3094) | 1:A:53:VAL:HG11 | 1:A:58:LYS:HZ1 | 13 | 0.47 |
| (1,3094) | 1:A:53:VAL:HG12 | 1:A:58:LYS:HZ1 | 13 | 0.47 |
| (1,3094) | 1:A:53:VAL:HG13 | 1:A:58:LYS:HZ1 | 13 | 0.47 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 4 | 0.47 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 4 | 0.47 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 4 | 0.47 |
| (1,1779) | 1:B:11:VAL:HG11 | 1:B:73:PHE:HE1 | 17 | 0.47 |
| (1,1779) | 1:B:11:VAL:HG12 | 1:B:73:PHE:HE1 | 17 | 0.47 |
| (1,1779) | 1:B:11:VAL:HG13 | 1:B:73:PHE:HE1 | 17 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 1 | 0.47 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 5 | 0.47 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 16 | 0.47 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 17 | 0.47 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 11 | 0.46 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 11 | 0.46 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 11 | 0.46 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 18 | 0.46 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 18 | 0.46 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 18 | 0.46 |
| (1,5168) | 1:B:54:LYS:H | 1:B:54:LYS:HG2 | 12 | 0.46 |
| (1,5159) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HE2 | 6 | 0.46 |
| (1,5159) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HE2 | 6 | 0.46 |
| (1,5159) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HE2 | 6 | 0.46 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 15 | 0.46 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 15 | 0.46 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 15 | 0.46 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 8 | 0.46 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 8 | 0.46 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 8 | 0.46 |
| (1,5128) | 1:B:37:VAL:HG21 | 1:B:48:ASN:HD21 | 20 | 0.46 |
| (1,5128) | 1:B:37:VAL:HG22 | 1:B:48:ASN:HD21 | 20 | 0.46 |
| (1,5128) | 1:B:37:VAL:HG23 | 1:B:48:ASN:HD21 | 20 | 0.46 |
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 2 | 0.46 |
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 2 | 0.46 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 2 | 0.46 |
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 11 | 0.46 |
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 11 | 0.46 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 11 | 0.46 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 19 | 0.46 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 19 | 0.46 |
| (1,5072) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HD2 | 4 | 0.46 |
| (1,5072) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HD2 | 7 | 0.46 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE2 | 1 | 0.46 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE3 | 1 | 0.46 |
| (1,5034) | 1:B:23:THR:HG21 | 1:B:27:SER:HB2 | 9 | 0.46 |
| (1,5034) | 1:B:23:THR:HG22 | 1:B:27:SER:HB2 | 9 | 0.46 |
| (1,5034) | 1:B:23:THR:HG23 | 1:B:27:SER:HB2 | 9 | 0.46 |
| (1,5013) | 1:B:16:ASN:HB2 | 1:B:18:MET:H | 16 | 0.46 |
| (1,5012) | 1:B:16:ASN:HB2 | 1:B:17:GLY:H | 2 | 0.46 |
| (1,4984) | 1:B:9:ARG:HG2 | 1:B:76:GLU:H | 19 | 0.46 |
| (1,4913) | 1:A:65:LYS:HA | 1:A:65:LYS:HD2 | 5 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 4 | 0.46 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 13 | 0.46 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD2 | 19 | 0.46 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD3 | 19 | 0.46 |
| (1,4774) | 1:A:28:LYS:HB2 | 1:A:28:LYS:HD2 | 4 | 0.46 |
| (1,4695) | 1:A:16:ASN:HB2 | 1:A:17:GLY:H | 6 | 0.46 |
| (1,4671) | 1:A:14:ASP:HB2 | 1:A:43:GLY:H | 7 | 0.46 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 9 | 0.46 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 20 | 0.46 |
| (1,4568) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HE1 | 14 | 0.46 |
| (1,4568) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HE1 | 14 | 0.46 |
| (1,4568) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HE1 | 14 | 0.46 |
| (1,4541) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HE1 | 15 | 0.46 |
| (1,4541) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HE1 | 15 | 0.46 |
| (1,4541) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HE1 | 15 | 0.46 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 6 | 0.46 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 19 | 0.46 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 19 | 0.46 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 19 | 0.46 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 3 | 0.46 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 3 | 0.46 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 3 | 0.46 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG11 | 15 | 0.46 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG12 | 15 | 0.46 |
| (1,1788) | 1:A:12:GLY:HA2 | 1:A:69:VAL:HG13 | 15 | 0.46 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 11 | 0.46 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 8 | 0.45 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 8 | 0.45 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 8 | 0.45 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 6 | 0.45 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 6 | 0.45 |
| (1,5145) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG12 | 8 | 0.45 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 3 | 0.45 |
| (1,5084) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 6 | 0.45 |
| (1,5084) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 6 | 0.45 |
| (1,5066) | 1:B:28:LYS:H | 1:B:28:LYS:HB2 | 1 | 0.45 |
| (1,4999) | 1:B:15:LYS:H | 1:B:18:MET:HG2 | 6 | 0.45 |
| (1,4984) | 1:B:9:ARG:HG2 | 1:B:76:GLU:H | 15 | 0.45 |
| (1,4951) | 1:B:3:ASP:HB2 | 1:B:4:PHE:H | 4 | 0.45 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 20 | 0.45 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB2 | 16 | 0.45 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB3 | 16 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4871) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HB2 | 16 | 0.45 |
| (1,4871) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HB2 | 16 | 0.45 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 19 | 0.45 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 19 | 0.45 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 19 | 0.45 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD11 | 5 | 0.45 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD12 | 5 | 0.45 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD13 | 5 | 0.45 |
| (1,4774) | 1:A:28:LYS:HB2 | 1:A:28:LYS:HD2 | 3 | 0.45 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 9 | 0.45 |
| (1,4755) | 1:A:26:ILE:H | 1:A:28:LYS:HG2 | 2 | 0.45 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 5 | 0.45 |
| (1,4696) | 1:A:16:ASN:HB2 | 1:A:18:MET:H | 5 | 0.45 |
| (1,4689) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HB2 | 1 | 0.45 |
| (1,4689) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HB2 | 1 | 0.45 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 5 | 0.45 |
| (1,4573) | 1:A:44:ILE:HG12 | 1:A:73:PHE:HE1 | 10 | 0.45 |
| (1,4573) | 1:A:44:ILE:HG12 | 1:A:73:PHE:HE1 | 16 | 0.45 |
| (1,4568) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HE1 | 20 | 0.45 |
| (1,4568) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HE1 | 20 | 0.45 |
| (1,4568) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HE1 | 20 | 0.45 |
| (1,4509) | 1:A:45:PHE:HZ | 1:A:71:GLY:HA2 | 6 | 0.45 |
| (1,4368) | 1:A:4:PHE:HE1 | 1:A:56:THR:HA | 1 | 0.45 |
| (1,3937) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HB3 | 19 | 0.45 |
| (1,3833) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HB3 | 14 | 0.45 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 3 | 0.45 |
| (1,3371) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HB | 2 | 0.45 |
| (1,1779) | 1:B:11:VAL:HG11 | 1:B:73:PHE:HE1 | 13 | 0.45 |
| (1,1779) | 1:B:11:VAL:HG12 | 1:B:73:PHE:HE1 | 13 | 0.45 |
| (1,1779) | 1:B:11:VAL:HG13 | 1:B:73:PHE:HE1 | 13 | 0.45 |
| (1,1779) | 1:B:11:VAL:HG11 | 1:B:73:PHE:HE1 | 19 | 0.45 |
| (1,1779) | 1:B:11:VAL:HG12 | 1:B:73:PHE:HE1 | 19 | 0.45 |
| (1,1779) | 1:B:11:VAL:HG13 | 1:B:73:PHE:HE1 | 19 | 0.45 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 3 | 0.45 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 1 | 0.44 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 1 | 0.44 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 1 | 0.44 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 18 | 0.44 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 18 | 0.44 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 18 | 0.44 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 17 | 0.44 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 17 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 17 | 0.44 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 3 | 0.44 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 9 | 0.44 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 9 | 0.44 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 9 | 0.44 |
| (1,5145) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG12 | 3 | 0.44 |
| (1,5012) | 1:B:16:ASN:HB2 | 1:B:17:GLY:H | 16 | 0.44 |
| (1,5005) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HD21 | 17 | 0.44 |
| (1,5005) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HD21 | 17 | 0.44 |
| (1,4994) | 1:B:14:ASP:HB2 | 1:B:43:GLY:HA2 | 11 | 0.44 |
| (1,4983) | 1:B:9:ARG:HG2 | 1:B:47:CYS:H | 5 | 0.44 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 18 | 0.44 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG21 | 18 | 0.44 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG22 | 18 | 0.44 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG23 | 18 | 0.44 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 3 | 0.44 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 3 | 0.44 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 3 | 0.44 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD11 | 18 | 0.44 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD12 | 18 | 0.44 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD13 | 18 | 0.44 |
| (1,4865) | 1:A:54:LYS:H | 1:A:54:LYS:HG2 | 4 | 0.44 |
| (1,4863) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HG2 | 4 | 0.44 |
| (1,4863) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HG2 | 4 | 0.44 |
| (1,4863) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HG2 | 4 | 0.44 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 6 | 0.44 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 6 | 0.44 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 6 | 0.44 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 11 | 0.44 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 18 | 0.44 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD2 | 16 | 0.44 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD3 | 16 | 0.44 |
| (1,4752) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HD2 | 8 | 0.44 |
| (1,4752) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HD2 | 8 | 0.44 |
| (1,4752) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HD2 | 8 | 0.44 |
| (1,4747) | 1:A:25:VAL:HA | 1:A:28:LYS:HB2 | 14 | 0.44 |
| (1,4686) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HB2 | 15 | 0.44 |
| (1,4686) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HB2 | 15 | 0.44 |
| (1,4633) | 1:A:4:PHE:H | 1:A:54:LYS:HB2 | 13 | 0.44 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 16 | 0.44 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 14 | 0.44 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 14 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,4362) | 1:A:29:PHE:HE1 | 1:A:66:LEU:HG | 20 | 0.44 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 3 | 0.44 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 8 | 0.44 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 13 | 0.44 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 19 | 0.44 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 19 | 0.44 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 19 | 0.44 |
| (1,3095) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HZ1 | 7 | 0.44 |
| (1,3095) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HZ1 | 7 | 0.44 |
| (1,3095) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HZ1 | 7 | 0.44 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD11 | 7 | 0.44 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD12 | 7 | 0.44 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD13 | 7 | 0.44 |
| (1,1779) | 1:B:11:VAL:HG11 | 1:B:73:PHE:HE1 | 11 | 0.44 |
| (1,1779) | 1:B:11:VAL:HG12 | 1:B:73:PHE:HE1 | 11 | 0.44 |
| (1,1779) | 1:B:11:VAL:HG13 | 1:B:73:PHE:HE1 | 11 | 0.44 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 19 | 0.44 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 4 | 0.44 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 5 | 0.44 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 13 | 0.43 |
| (1,5222) | 1:B:65:LYS:H | 1:B:65:LYS:HG2 | 6 | 0.43 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 4 | 0.43 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 4 | 0.43 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 4 | 0.43 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 7 | 0.43 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 7 | 0.43 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 7 | 0.43 |
| (1,5176) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD21 | 5 | 0.43 |
| (1,5176) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD21 | 5 | 0.43 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD11 | 19 | 0.43 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD12 | 19 | 0.43 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD13 | 19 | 0.43 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 18 | 0.43 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD11 | 7 | 0.43 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD12 | 7 | 0.43 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD13 | 7 | 0.43 |
| (1,5009) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD21 | 5 | 0.43 |
| (1,5009) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD21 | 5 | 0.43 |
| (1,5006) | 1:B:15:LYS:HG2 | 1:B:18:MET:HG2 | 8 | 0.43 |
| (1,5006) | 1:B:15:LYS:HG3 | 1:B:18:MET:HG2 | 8 | 0.43 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 5 | 0.43 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 17 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 7 | 0.43 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG21 | 16 | 0.43 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG22 | 16 | 0.43 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG23 | 16 | 0.43 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD11 | 3 | 0.43 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD12 | 3 | 0.43 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD13 | 3 | 0.43 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 18 | 0.43 |
| (1,4882) | 1:A:56:THR:HG21 | 1:A:59:LEU:HB2 | 15 | 0.43 |
| (1,4882) | 1:A:56:THR:HG22 | 1:A:59:LEU:HB2 | 15 | 0.43 |
| (1,4882) | 1:A:56:THR:HG23 | 1:A:59:LEU:HB2 | 15 | 0.43 |
| (1,4824) | 1:A:37:VAL:HG21 | 1:A:48:ASN:HD21 | 13 | 0.43 |
| (1,4824) | 1:A:37:VAL:HG22 | 1:A:48:ASN:HD21 | 13 | 0.43 |
| (1,4824) | 1:A:37:VAL:HG23 | 1:A:48:ASN:HD21 | 13 | 0.43 |
| (1,4746) | 1:A:25:VAL:H | 1:A:28:LYS:HD2 | 8 | 0.43 |
| (1,4720) | 1:A:20:ASN:H | 1:B:32:ASN:HB2 | 6 | 0.43 |
| (1,4720) | 1:A:20:ASN:H | 1:B:32:ASN:HB2 | 14 | 0.43 |
| (1,4703) | 1:A:17:GLY:HA2 | 1:A:21:GLN:HE22 | 5 | 0.43 |
| (1,4695) | 1:A:16:ASN:HB2 | 1:A:17:GLY:H | 5 | 0.43 |
| (1,4693) | 1:A:16:ASN:HA | 1:B:32:ASN:HD21 | 17 | 0.43 |
| (1,4672) | 1:A:14:ASP:HB2 | 1:A:43:GLY:HA2 | 17 | 0.43 |
| (1,4671) | 1:A:14:ASP:HB2 | 1:A:43:GLY:H | 19 | 0.43 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 7 | 0.43 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 16 | 0.43 |
| (1,4573) | 1:A:44:ILE:HG12 | 1:A:73:PHE:HE1 | 11 | 0.43 |
| (1,4363) | 1:B:29:PHE:HE1 | 1:B:66:LEU:HG | 18 | 0.43 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 2 | 0.43 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 4 | 0.43 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 15 | 0.43 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 18 | 0.43 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 19 | 0.43 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 4 | 0.43 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 6 | 0.43 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 8 | 0.43 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 16 | 0.43 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 17 | 0.43 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 4 | 0.43 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 4 | 0.43 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 4 | 0.43 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 4 | 0.43 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 4 | 0.43 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 4 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 17 | 0.43 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 6 | 0.43 |
| (1,3095) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HZ1 | 8 | 0.43 |
| (1,3095) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HZ1 | 8 | 0.43 |
| (1,3095) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HZ1 | 8 | 0.43 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 9 | 0.43 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 17 | 0.42 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 16 | 0.42 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 16 | 0.42 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 16 | 0.42 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD21 | 3 | 0.42 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD22 | 3 | 0.42 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD23 | 3 | 0.42 |
| (1,5176) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD21 | 20 | 0.42 |
| (1,5176) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD21 | 20 | 0.42 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 19 | 0.42 |
| (1,5099) | 1:B:32:ASN:HD21 | 1:B:33:ILE:HB | 1 | 0.42 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 18 | 0.42 |
| (1,5013) | 1:B:16:ASN:HB2 | 1:B:18:MET:H | 18 | 0.42 |
| (1,5012) | 1:B:16:ASN:HB2 | 1:B:17:GLY:H | 8 | 0.42 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 7 | 0.42 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 7 | 0.42 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 15 | 0.42 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 15 | 0.42 |
| (1,4985) | 1:B:9:ARG:HD2 | 1:B:48:ASN:HD21 | 5 | 0.42 |
| (1,4985) | 1:B:9:ARG:HD3 | 1:B:48:ASN:HD21 | 5 | 0.42 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 7 | 0.42 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 8 | 0.42 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 14 | 0.42 |
| (1,4862) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HB2 | 7 | 0.42 |
| (1,4862) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HB2 | 7 | 0.42 |
| (1,4862) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HB2 | 7 | 0.42 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 6 | 0.42 |
| (1,4802) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG3 | 4 | 0.42 |
| (1,4703) | 1:A:17:GLY:HA2 | 1:A:21:GLN:HE22 | 13 | 0.42 |
| (1,4686) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HB2 | 19 | 0.42 |
| (1,4686) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HB2 | 19 | 0.42 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 3 | 0.42 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 5 | 0.42 |
| (1,4573) | 1:A:44:ILE:HG12 | 1:A:73:PHE:HE1 | 6 | 0.42 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 7 | 0.42 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 7 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 2 | 0.42 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 2 | 0.42 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 20 | 0.42 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 20 | 0.42 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 3 | 0.42 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 5 | 0.42 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 6 | 0.42 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 7 | 0.42 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 17 | 0.42 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 2 | 0.42 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 5 | 0.42 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 12 | 0.42 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 13 | 0.42 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 15 | 0.42 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 18 | 0.42 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 19 | 0.42 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG21 | 7 | 0.42 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG22 | 7 | 0.42 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG23 | 7 | 0.42 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD11 | 7 | 0.42 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD12 | 7 | 0.42 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD13 | 7 | 0.42 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 5 | 0.42 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 5 | 0.42 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 5 | 0.42 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 18 | 0.42 |
| (1,5262) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HA | 8 | 0.41 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 6 | 0.41 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 15 | 0.41 |
| (1,5128) | 1:B:37:VAL:HG21 | 1:B:48:ASN:HD21 | 19 | 0.41 |
| (1,5128) | 1:B:37:VAL:HG22 | 1:B:48:ASN:HD21 | 19 | 0.41 |
| (1,5128) | 1:B:37:VAL:HG23 | 1:B:48:ASN:HD21 | 19 | 0.41 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD11 | 1 | 0.41 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD12 | 1 | 0.41 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD13 | 1 | 0.41 |
| (1,5066) | 1:B:28:LYS:H | 1:B:28:LYS:HB2 | 4 | 0.41 |
| (1,5051) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HD2 | 2 | 0.41 |
| (1,5051) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HD2 | 2 | 0.41 |
| (1,5051) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HD2 | 2 | 0.41 |
| (1,5007) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HB2 | 19 | 0.41 |
| (1,5007) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HB2 | 19 | 0.41 |
| (1,4996) | 1:B:14:ASP:HB2 | 1:B:44:ILE:HG21 | 8 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4996) | 1:B:14:ASP:HB2 | 1:B:44:ILE:HG22 | 8 | 0.41 |
| (1,4996) | 1:B:14:ASP:HB2 | 1:B:44:ILE:HG23 | 8 | 0.41 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 13 | 0.41 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 15 | 0.41 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 20 | 0.41 |
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 5 | 0.41 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 20 | 0.41 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 20 | 0.41 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 20 | 0.41 |
| (1,4889) | 1:A:58:LYS:HE2 | 1:A:59:LEU:HA | 14 | 0.41 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB2 | 8 | 0.41 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB3 | 8 | 0.41 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB2 | 11 | 0.41 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB3 | 11 | 0.41 |
| (1,4872) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HD21 | 5 | 0.41 |
| (1,4872) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HD21 | 5 | 0.41 |
| (1,4870) | 1:A:54:LYS:HG2 | 1:A:55:ASN:HD21 | 3 | 0.41 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 5 | 0.41 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 5 | 0.41 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 5 | 0.41 |
| (1,4795) | 1:A:32:ASN:HB2 | 1:B:20:ASN:H | 6 | 0.41 |
| (1,4773) | 1:A:28:LYS:HA | 1:A:28:LYS:HD2 | 4 | 0.41 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG21 | 13 | 0.41 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG22 | 13 | 0.41 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG23 | 13 | 0.41 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD11 | 15 | 0.41 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD12 | 15 | 0.41 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD13 | 15 | 0.41 |
| (1,4686) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HB2 | 18 | 0.41 |
| (1,4686) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HB2 | 18 | 0.41 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 14 | 0.41 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 1 | 0.41 |
| (1,4628) | 1:A:3:ASP:HB2 | 1:A:4:PHE:H | 20 | 0.41 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 7 | 0.41 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD1 | 3 | 0.41 |
| (1,4365) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HD2 | 3 | 0.41 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 6 | 0.41 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 6 | 0.41 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG21 | 11 | 0.41 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG22 | 11 | 0.41 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG23 | 11 | 0.41 |
| (1,3834) | 1:B:12:GLY:HA3 | 1:B:73:PHE:HB3 | 7 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 1 | 0.41 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 16 | 0.41 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 1 | 0.41 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 10 | 0.41 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 18 | 0.41 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD11 | 20 | 0.41 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD12 | 20 | 0.41 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD13 | 20 | 0.41 |
| (1,1778) | 1:A:11:VAL:HG11 | 1:A:73:PHE:HE1 | 15 | 0.41 |
| (1,1778) | 1:A:11:VAL:HG12 | 1:A:73:PHE:HE1 | 15 | 0.41 |
| (1,1778) | 1:A:11:VAL:HG13 | 1:A:73:PHE:HE1 | 15 | 0.41 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 1 | 0.4 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 5 | 0.4 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 9 | 0.4 |
| (1,5244) | 1:B:68:LYS:HD2 | 1:B:69:VAL:H | 4 | 0.4 |
| (1,5224) | 1:B:65:LYS:HA | 1:B:65:LYS:HD2 | 15 | 0.4 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 2 | 0.4 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 2 | 0.4 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 2 | 0.4 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 3 | 0.4 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 3 | 0.4 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 3 | 0.4 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB2 | 10 | 0.4 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB3 | 10 | 0.4 |
| (1,5175) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HD21 | 16 | 0.4 |
| (1,5175) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HD21 | 16 | 0.4 |
| (1,5165) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HB2 | 9 | 0.4 |
| (1,5165) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HB2 | 9 | 0.4 |
| (1,5165) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HB2 | 9 | 0.4 |
| (1,5164) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HE2 | 20 | 0.4 |
| (1,5164) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HE2 | 20 | 0.4 |
| (1,5164) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HE2 | 20 | 0.4 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 8 | 0.4 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 9 | 0.4 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 17 | 0.4 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD11 | 12 | 0.4 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD12 | 12 | 0.4 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD13 | 12 | 0.4 |
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 13 | 0.4 |
| (1,5019) | 1:B:17:GLY:HA2 | 1:B:21:GLN:HE22 | 14 | 0.4 |
| (1,5019) | 1:B:17:GLY:HA2 | 1:B:21:GLN:HE22 | 18 | 0.4 |
| (1,5019) | 1:B:17:GLY:HA2 | 1:B:21:GLN:HE22 | 20 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5013) | 1:B:16:ASN:HB2 | 1:B:18:MET:H | 12 | 0.4 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 14 | 0.4 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 14 | 0.4 |
| (1,4998) | 1:B:14:ASP:HB2 | 1:B:45:PHE:HD1 | 17 | 0.4 |
| (1,4998) | 1:B:14:ASP:HB2 | 1:B:45:PHE:HD2 | 17 | 0.4 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 11 | 0.4 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 2 | 0.4 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 16 | 0.4 |
| (1,4932) | 1:A:68:LYS:HD2 | 1:A:69:VAL:H | 6 | 0.4 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 11 | 0.4 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 11 | 0.4 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 11 | 0.4 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 11 | 0.4 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 19 | 0.4 |
| (1,4882) | 1:A:56:THR:HG21 | 1:A:59:LEU:HB2 | 7 | 0.4 |
| (1,4882) | 1:A:56:THR:HG22 | 1:A:59:LEU:HB2 | 7 | 0.4 |
| (1,4882) | 1:A:56:THR:HG23 | 1:A:59:LEU:HB2 | 7 | 0.4 |
| (1,4863) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HG2 | 11 | 0.4 |
| (1,4863) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HG2 | 11 | 0.4 |
| (1,4863) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HG2 | 11 | 0.4 |
| (1,4862) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HB2 | 13 | 0.4 |
| (1,4862) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HB2 | 13 | 0.4 |
| (1,4862) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HB2 | 13 | 0.4 |
| (1,4842) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG12 | 15 | 0.4 |
| (1,4705) | 1:A:18:MET:H | 1:B:32:ASN:HD21 | 6 | 0.4 |
| (1,4686) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HB2 | 6 | 0.4 |
| (1,4686) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HB2 | 6 | 0.4 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 11 | 0.4 |
| (1,4369) | 1:B:4:PHE:HE1 | 1:B:56:THR:HA | 4 | 0.4 |
| (1,4369) | 1:B:4:PHE:HE1 | 1:B:56:THR:HA | 6 | 0.4 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD1 | 4 | 0.4 |
| (1,4364) | 1:A:12:GLY:HA3 | 1:A:73:PHE:HD2 | 4 | 0.4 |
| (1,4256) | 1:A:41:LYS:HA | 1:A:42:ASP:H | 1 | 0.4 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 9 | 0.4 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 10 | 0.4 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 7 | 0.4 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 11 | 0.4 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 20 | 0.4 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 2 | 0.4 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD11 | 3 | 0.4 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD12 | 3 | 0.4 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD13 | 3 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 16 | 0.4 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 16 | 0.4 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 16 | 0.4 |
| (1,1802) | 1:A:13:GLU:HB3 | 1:A:71:GLY:HA3 | 4 | 0.4 |
| (1,1778) | 1:A:11:VAL:HG11 | 1:A:73:PHE:HE1 | 1 | 0.4 |
| (1,1778) | 1:A:11:VAL:HG12 | 1:A:73:PHE:HE1 | 1 | 0.4 |
| (1,1778) | 1:A:11:VAL:HG13 | 1:A:73:PHE:HE1 | 1 | 0.4 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 20 | 0.4 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 7 | 0.4 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 18 | 0.4 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 15 | 0.4 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 15 | 0.39 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 5 | 0.39 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 5 | 0.39 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 5 | 0.39 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 10 | 0.39 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 17 | 0.39 |
| (1,5166) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HG2 | 13 | 0.39 |
| (1,5166) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HG2 | 13 | 0.39 |
| (1,5166) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HG2 | 13 | 0.39 |
| (1,5108) | 1:B:34:ARG:HB2 | 1:B:51:ILE:H | 3 | 0.39 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 14 | 0.39 |
| (1,5070) | 1:B:28:LYS:HA | 1:B:28:LYS:HG2 | 4 | 0.39 |
| (1,5057) | 1:B:26:ILE:HG12 | 1:B:27:SER:HG | 13 | 0.39 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE2 | 13 | 0.39 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE3 | 13 | 0.39 |
| (1,5019) | 1:B:17:GLY:HA2 | 1:B:21:GLN:HE22 | 10 | 0.39 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 4 | 0.39 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 4 | 0.39 |
| (1,5000) | 1:B:15:LYS:HA | 1:B:16:ASN:HB2 | 3 | 0.39 |
| (1,4994) | 1:B:14:ASP:HB2 | 1:B:43:GLY:HA2 | 18 | 0.39 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 12 | 0.39 |
| (1,4932) | 1:A:68:LYS:HD2 | 1:A:69:VAL:H | 11 | 0.39 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 1 | 0.39 |
| (1,4871) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HB2 | 13 | 0.39 |
| (1,4871) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HB2 | 13 | 0.39 |
| (1,4842) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG12 | 18 | 0.39 |
| (1,4822) | 1:A:37:VAL:HG11 | 1:A:48:ASN:HD21 | 4 | 0.39 |
| (1,4822) | 1:A:37:VAL:HG12 | 1:A:48:ASN:HD21 | 4 | 0.39 |
| (1,4822) | 1:A:37:VAL:HG13 | 1:A:48:ASN:HD21 | 4 | 0.39 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD11 | 18 | 0.39 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD12 | 18 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD13 | 18 | 0.39 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 15 | 0.39 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 2 | 0.39 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 12 | 0.39 |
| (1,4574) | 1:B:44:ILE:HG12 | 1:B:73:PHE:HE1 | 6 | 0.39 |
| (1,4546) | 1:B:5:LEU:HB2 | 1:B:52:PHE:HE1 | 12 | 0.39 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 12 | 0.39 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG21 | 16 | 0.39 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG22 | 16 | 0.39 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG23 | 16 | 0.39 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG21 | 6 | 0.39 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG22 | 6 | 0.39 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG23 | 6 | 0.39 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 12 | 0.39 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 14 | 0.39 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD21 | 17 | 0.39 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD22 | 17 | 0.39 |
| (1,2842) | 1:A:7:GLY:HA3 | 1:A:49:LEU:HD23 | 17 | 0.39 |
| (1,1802) | 1:A:13:GLU:HB3 | 1:A:71:GLY:HA3 | 13 | 0.39 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 1 | 0.39 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 4 | 0.39 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 6 | 0.39 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 15 | 0.39 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 10 | 0.39 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 2 | 0.39 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 18 | 0.38 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 20 | 0.38 |
| (1,5245) | 1:B:69:VAL:HG11 | 1:B:70:GLN:HE21 | 2 | 0.38 |
| (1,5245) | 1:B:69:VAL:HG12 | 1:B:70:GLN:HE21 | 2 | 0.38 |
| (1,5245) | 1:B:69:VAL:HG13 | 1:B:70:GLN:HE21 | 2 | 0.38 |
| (1,5176) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD21 | 4 | 0.38 |
| (1,5176) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD21 | 4 | 0.38 |
| (1,5162) | 1:B:53:VAL:HA | 1:B:54:LYS:HB2 | 14 | 0.38 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 14 | 0.38 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 14 | 0.38 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 14 | 0.38 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 18 | 0.38 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 18 | 0.38 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 18 | 0.38 |
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 4 | 0.38 |
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 4 | 0.38 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 4 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 5 | 0.38 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 16 | 0.38 |
| (1,4999) | 1:B:15:LYS:H | 1:B:18:MET:HG2 | 18 | 0.38 |
| (1,4981) | 1:B:9:ARG:H | 1:B:76:GLU:HB2 | 12 | 0.38 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 15 | 0.38 |
| (1,4943) | 1:A:80:ASN:HB2 | 1:A:80:ASN:HD21 | 3 | 0.38 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD2 | 17 | 0.38 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD3 | 17 | 0.38 |
| (1,4802) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG3 | 13 | 0.38 |
| (1,4773) | 1:A:28:LYS:HA | 1:A:28:LYS:HD2 | 9 | 0.38 |
| (1,4695) | 1:A:16:ASN:HB2 | 1:A:17:GLY:H | 12 | 0.38 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 13 | 0.38 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 3 | 0.38 |
| (1,4573) | 1:A:44:ILE:HG12 | 1:A:73:PHE:HE1 | 20 | 0.38 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 2 | 0.38 |
| (1,4257) | 1:B:41:LYS:HA | 1:B:42:ASP:H | 13 | 0.38 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 11 | 0.38 |
| (1,3743) | 1:A:70:GLN:HA | 1:A:71:GLY:HA3 | 9 | 0.38 |
| (1,3459) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:HD11 | 3 | 0.38 |
| (1,3459) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:HD12 | 3 | 0.38 |
| (1,3459) | 1:A:58:LYS:HZ1 | 1:A:62:LEU:HD13 | 3 | 0.38 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 11 | 0.38 |
| (1,3095) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HZ1 | 11 | 0.38 |
| (1,3095) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HZ1 | 11 | 0.38 |
| (1,3095) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HZ1 | 11 | 0.38 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 14 | 0.38 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 17 | 0.38 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 5 | 0.38 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 13 | 0.38 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 20 | 0.38 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 15 | 0.38 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 1 | 0.38 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 9 | 0.38 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 12 | 0.37 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 12 | 0.37 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 12 | 0.37 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB2 | 6 | 0.37 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB3 | 6 | 0.37 |
| (1,5130) | 1:B:38:LEU:HD21 | 1:B:39:ASN:HD21 | 19 | 0.37 |
| (1,5130) | 1:B:38:LEU:HD22 | 1:B:39:ASN:HD21 | 19 | 0.37 |
| (1,5130) | 1:B:38:LEU:HD23 | 1:B:39:ASN:HD21 | 19 | 0.37 |
| (1,5107) | 1:B:34:ARG:HB2 | 1:B:50:MET:HG3 | 17 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 19 | 0.37 |
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 19 | 0.37 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 19 | 0.37 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 5 | 0.37 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 5 | 0.37 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 11 | 0.37 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 11 | 0.37 |
| (1,5000) | 1:B:15:LYS:HA | 1:B:16:ASN:HB2 | 20 | 0.37 |
| (1,4951) | 1:B:3:ASP:HB2 | 1:B:4:PHE:H | 19 | 0.37 |
| (1,4950) | 1:B:3:ASP:HA | 1:B:54:LYS:HB2 | 13 | 0.37 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD21 | 9 | 0.37 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD22 | 9 | 0.37 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD23 | 9 | 0.37 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 4 | 0.37 |
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 19 | 0.37 |
| (1,4873) | 1:A:54:LYS:HE2 | 1:A:55:ASN:HD21 | 17 | 0.37 |
| (1,4873) | 1:A:54:LYS:HE3 | 1:A:55:ASN:HD21 | 17 | 0.37 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 7 | 0.37 |
| (1,4856) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HE2 | 10 | 0.37 |
| (1,4856) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HE2 | 10 | 0.37 |
| (1,4856) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HE2 | 10 | 0.37 |
| (1,4842) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG12 | 6 | 0.37 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 12 | 0.37 |
| (1,4773) | 1:A:28:LYS:HA | 1:A:28:LYS:HD2 | 3 | 0.37 |
| (1,4773) | 1:A:28:LYS:HA | 1:A:28:LYS:HD2 | 5 | 0.37 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE2 | 9 | 0.37 |
| (1,4743) | 1:A:24:GLY:HA2 | 1:A:28:LYS:HE3 | 9 | 0.37 |
| (1,4633) | 1:A:4:PHE:H | 1:A:54:LYS:HB2 | 17 | 0.37 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 8 | 0.37 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 19 | 0.37 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 19 | 0.37 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 19 | 0.37 |
| (1,4542) | 1:B:5:LEU:HD11 | 1:B:52:PHE:HE1 | 14 | 0.37 |
| (1,4542) | 1:B:5:LEU:HD12 | 1:B:52:PHE:HE1 | 14 | 0.37 |
| (1,4542) | 1:B:5:LEU:HD13 | 1:B:52:PHE:HE1 | 14 | 0.37 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG21 | 9 | 0.37 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG22 | 9 | 0.37 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG23 | 9 | 0.37 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 7 | 0.37 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 4 | 0.37 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 12 | 0.37 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 11 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 12 | 0.36 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 1 | 0.36 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 2 | 0.36 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 9 | 0.36 |
| (1,5182) | 1:B:55:ASN:HD21 | 1:B:58:LYS:HG3 | 2 | 0.36 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 7 | 0.36 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 7 | 0.36 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 7 | 0.36 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 18 | 0.36 |
| (1,5130) | 1:B:38:LEU:HD21 | 1:B:39:ASN:HD21 | 6 | 0.36 |
| (1,5130) | 1:B:38:LEU:HD22 | 1:B:39:ASN:HD21 | 6 | 0.36 |
| (1,5130) | 1:B:38:LEU:HD23 | 1:B:39:ASN:HD21 | 6 | 0.36 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 17 | 0.36 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 12 | 0.36 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 12 | 0.36 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 12 | 0.36 |
| (1,5051) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HD2 | 6 | 0.36 |
| (1,5051) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HD2 | 6 | 0.36 |
| (1,5051) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HD2 | 6 | 0.36 |
| (1,5013) | 1:B:16:ASN:HB2 | 1:B:18:MET:H | 1 | 0.36 |
| (1,5011) | 1:B:16:ASN:HB2 | 1:B:16:ASN:HD21 | 2 | 0.36 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 9 | 0.36 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 5 | 0.36 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 11 | 0.36 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 19 | 0.36 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 14 | 0.36 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 14 | 0.36 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 14 | 0.36 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 18 | 0.36 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 18 | 0.36 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 18 | 0.36 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 3 | 0.36 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 3 | 0.36 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 3 | 0.36 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 5 | 0.36 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 5 | 0.36 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 5 | 0.36 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 11 | 0.36 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 11 | 0.36 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 11 | 0.36 |
| (1,4842) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG12 | 10 | 0.36 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 17 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4822) | 1:A:37:VAL:HG11 | 1:A:48:ASN:HD21 | 7 | 0.36 |
| (1,4822) | 1:A:37:VAL:HG12 | 1:A:48:ASN:HD21 | 7 | 0.36 |
| (1,4822) | 1:A:37:VAL:HG13 | 1:A:48:ASN:HD21 | 7 | 0.36 |
| (1,4801) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG2 | 6 | 0.36 |
| (1,4773) | 1:A:28:LYS:HA | 1:A:28:LYS:HD2 | 7 | 0.36 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG21 | 17 | 0.36 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG22 | 17 | 0.36 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG23 | 17 | 0.36 |
| (1,4758) | 1:A:26:ILE:HG12 | 1:A:27:SER:HG | 20 | 0.36 |
| (1,4694) | 1:A:16:ASN:HB2 | 1:A:16:ASN:HD21 | 12 | 0.36 |
| (1,4694) | 1:A:16:ASN:HB2 | 1:A:16:ASN:HD21 | 16 | 0.36 |
| (1,4690) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD21 | 9 | 0.36 |
| (1,4690) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD21 | 9 | 0.36 |
| (1,4687) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HD21 | 11 | 0.36 |
| (1,4687) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HD21 | 11 | 0.36 |
| (1,4661) | 1:A:9:ARG:HD2 | 1:A:48:ASN:HD21 | 8 | 0.36 |
| (1,4661) | 1:A:9:ARG:HD3 | 1:A:48:ASN:HD21 | 8 | 0.36 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 6 | 0.36 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 1 | 0.36 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 14 | 0.36 |
| (1,4478) | 1:B:19:THR:HG21 | 1:B:45:PHE:HE1 | 1 | 0.36 |
| (1,4478) | 1:B:19:THR:HG22 | 1:B:45:PHE:HE1 | 1 | 0.36 |
| (1,4478) | 1:B:19:THR:HG23 | 1:B:45:PHE:HE1 | 1 | 0.36 |
| (1,4362) | 1:A:29:PHE:HE1 | 1:A:66:LEU:HG | 6 | 0.36 |
| (1,4199) | 1:B:82:GLU:H | 1:B:83:HIS:HB3 | 5 | 0.36 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG21 | 19 | 0.36 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG22 | 19 | 0.36 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG23 | 19 | 0.36 |
| (1,2033) | 1:A:22:ILE:HB | 1:A:45:PHE:HE1 | 19 | 0.36 |
| (1,1802) | 1:A:13:GLU:HB3 | 1:A:71:GLY:HA3 | 7 | 0.36 |
| (1,1779) | 1:B:11:VAL:HG11 | 1:B:73:PHE:HE1 | 15 | 0.36 |
| (1,1779) | 1:B:11:VAL:HG12 | 1:B:73:PHE:HE1 | 15 | 0.36 |
| (1,1779) | 1:B:11:VAL:HG13 | 1:B:73:PHE:HE1 | 15 | 0.36 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 17 | 0.36 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 5 | 0.36 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 4 | 0.35 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 4 | 0.35 |
| (1,5239) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG21 | 5 | 0.35 |
| (1,5239) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG22 | 5 | 0.35 |
| (1,5239) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG23 | 5 | 0.35 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD21 | 15 | 0.35 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD22 | 15 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|-----------------|-----------------|-------|---------------|
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD23 | 15 | 0.35 |
| (1,5185) | 1:B:56:THR:HG21 | 1:B:59:LEU:HB2 | 2 | 0.35 |
| (1,5185) | 1:B:56:THR:HG22 | 1:B:59:LEU:HB2 | 2 | 0.35 |
| (1,5185) | 1:B:56:THR:HG23 | 1:B:59:LEU:HB2 | 2 | 0.35 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB2 | 5 | 0.35 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB3 | 5 | 0.35 |
| (1,5165) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HB2 | 5 | 0.35 |
| (1,5165) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HB2 | 5 | 0.35 |
| (1,5165) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HB2 | 5 | 0.35 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 5 | 0.35 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 5 | 0.35 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 5 | 0.35 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 4 | 0.35 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 16 | 0.35 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 20 | 0.35 |
| (1,5108) | 1:B:34:ARG:HB2 | 1:B:51:ILE:H | 15 | 0.35 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 19 | 0.35 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 19 | 0.35 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 19 | 0.35 |
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 10 | 0.35 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 4 | 0.35 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 4 | 0.35 |
| (1,5013) | 1:B:16:ASN:HB2 | 1:B:18:MET:H | 3 | 0.35 |
| (1,5012) | 1:B:16:ASN:HB2 | 1:B:17:GLY:H | 10 | 0.35 |
| (1,5011) | 1:B:16:ASN:HB2 | 1:B:16:ASN:HD21 | 16 | 0.35 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 8 | 0.35 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 8 | 0.35 |
| (1,4966) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HG12 | 9 | 0.35 |
| (1,4956) | 1:B:4:PHE:H | 1:B:54:LYS:HB2 | 14 | 0.35 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 9 | 0.35 |
| (1,4933) | 1:A:69:VAL:HG11 | 1:A:70:GLN:HE21 | 20 | 0.35 |
| (1,4933) | 1:A:69:VAL:HG12 | 1:A:70:GLN:HE21 | 20 | 0.35 |
| (1,4933) | 1:A:69:VAL:HG13 | 1:A:70:GLN:HE21 | 20 | 0.35 |
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 4 | 0.35 |
| (1,4872) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HD21 | 17 | 0.35 |
| (1,4872) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HD21 | 17 | 0.35 |
| (1,4862) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HB2 | 5 | 0.35 |
| (1,4862) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HB2 | 5 | 0.35 |
| (1,4862) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HB2 | 5 | 0.35 |
| (1,4861) | 1:A:53:VAL:HG11 | 1:A:58:LYS:HE2 | 12 | 0.35 |
| (1,4861) | 1:A:53:VAL:HG12 | 1:A:58:LYS:HE2 | 12 | 0.35 |
| (1,4861) | 1:A:53:VAL:HG13 | 1:A:58:LYS:HE2 | 12 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4856) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HE2 | 16 | 0.35 |
| (1,4856) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HE2 | 16 | 0.35 |
| (1,4856) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HE2 | 16 | 0.35 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 4 | 0.35 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 4 | 0.35 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 4 | 0.35 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 17 | 0.35 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 17 | 0.35 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 17 | 0.35 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 20 | 0.35 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 20 | 0.35 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 20 | 0.35 |
| (1,4842) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG12 | 8 | 0.35 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 3 | 0.35 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE2 | 5 | 0.35 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE3 | 5 | 0.35 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD2 | 1 | 0.35 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD3 | 1 | 0.35 |
| (1,4826) | 1:A:38:LEU:HD21 | 1:A:39:ASN:HD21 | 12 | 0.35 |
| (1,4826) | 1:A:38:LEU:HD22 | 1:A:39:ASN:HD21 | 12 | 0.35 |
| (1,4826) | 1:A:38:LEU:HD23 | 1:A:39:ASN:HD21 | 12 | 0.35 |
| (1,4795) | 1:A:32:ASN:HB2 | 1:B:20:ASN:H | 12 | 0.35 |
| (1,4787) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HD2 | 16 | 0.35 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD11 | 13 | 0.35 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD12 | 13 | 0.35 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD13 | 13 | 0.35 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD11 | 5 | 0.35 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD12 | 5 | 0.35 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD13 | 5 | 0.35 |
| (1,4752) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HD2 | 13 | 0.35 |
| (1,4752) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HD2 | 13 | 0.35 |
| (1,4752) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HD2 | 13 | 0.35 |
| (1,4720) | 1:A:20:ASN:H | 1:B:32:ASN:HB2 | 12 | 0.35 |
| (1,4689) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HB2 | 11 | 0.35 |
| (1,4689) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HB2 | 11 | 0.35 |
| (1,4672) | 1:A:14:ASP:HB2 | 1:A:43:GLY:HA2 | 2 | 0.35 |
| (1,4672) | 1:A:14:ASP:HB2 | 1:A:43:GLY:HA2 | 13 | 0.35 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 4 | 0.35 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 4 | 0.35 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 4 | 0.35 |
| (1,4573) | 1:A:44:ILE:HG12 | 1:A:73:PHE:HE1 | 18 | 0.35 |
| (1,4478) | 1:B:19:THR:HG21 | 1:B:45:PHE:HE1 | 12 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4478) | 1:B:19:THR:HG22 | 1:B:45:PHE:HE1 | 12 | 0.35 |
| (1,4478) | 1:B:19:THR:HG23 | 1:B:45:PHE:HE1 | 12 | 0.35 |
| (1,4368) | 1:A:4:PHE:HE1 | 1:A:56:THR:HA | 16 | 0.35 |
| (1,3937) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HB3 | 7 | 0.35 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD11 | 5 | 0.35 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD12 | 5 | 0.35 |
| (1,3458) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HD13 | 5 | 0.35 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 1 | 0.35 |
| (1,2033) | 1:A:22:ILE:HB | 1:A:45:PHE:HE1 | 1 | 0.35 |
| (1,1802) | 1:A:13:GLU:HB3 | 1:A:71:GLY:HA3 | 15 | 0.35 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 5 | 0.35 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 10 | 0.35 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 2 | 0.35 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 14 | 0.35 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 6 | 0.35 |
| (1,5257) | 1:B:80:ASN:HB2 | 1:B:80:ASN:HD21 | 12 | 0.34 |
| (1,5257) | 1:B:80:ASN:HB2 | 1:B:80:ASN:HD21 | 15 | 0.34 |
| (1,5248) | 1:B:76:GLU:HB2 | 1:B:77:ARG:H | 9 | 0.34 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 20 | 0.34 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 20 | 0.34 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 20 | 0.34 |
| (1,5172) | 1:B:54:LYS:HG2 | 1:B:55:ASN:H | 6 | 0.34 |
| (1,5172) | 1:B:54:LYS:HG2 | 1:B:55:ASN:H | 17 | 0.34 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 10 | 0.34 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB2 | 4 | 0.34 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB3 | 4 | 0.34 |
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 13 | 0.34 |
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 13 | 0.34 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 13 | 0.34 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD11 | 9 | 0.34 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD12 | 9 | 0.34 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD13 | 9 | 0.34 |
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 20 | 0.34 |
| (1,5013) | 1:B:16:ASN:HB2 | 1:B:18:MET:H | 6 | 0.34 |
| (1,4982) | 1:B:9:ARG:HG2 | 1:B:11:VAL:HG21 | 15 | 0.34 |
| (1,4982) | 1:B:9:ARG:HG2 | 1:B:11:VAL:HG22 | 15 | 0.34 |
| (1,4982) | 1:B:9:ARG:HG2 | 1:B:11:VAL:HG23 | 15 | 0.34 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 14 | 0.34 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 17 | 0.34 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 17 | 0.34 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 17 | 0.34 |
| (1,4879) | 1:A:55:ASN:HD21 | 1:A:58:LYS:HG3 | 3 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB2 | 2 | 0.34 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB3 | 2 | 0.34 |
| (1,4872) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HD21 | 9 | 0.34 |
| (1,4872) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HD21 | 9 | 0.34 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 16 | 0.34 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 16 | 0.34 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 16 | 0.34 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 19 | 0.34 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 19 | 0.34 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 19 | 0.34 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 8 | 0.34 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 19 | 0.34 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD2 | 5 | 0.34 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD3 | 5 | 0.34 |
| (1,4773) | 1:A:28:LYS:HA | 1:A:28:LYS:HD2 | 1 | 0.34 |
| (1,4773) | 1:A:28:LYS:HA | 1:A:28:LYS:HD2 | 19 | 0.34 |
| (1,4733) | 1:A:23:THR:HG21 | 1:A:27:SER:HB2 | 16 | 0.34 |
| (1,4733) | 1:A:23:THR:HG22 | 1:A:27:SER:HB2 | 16 | 0.34 |
| (1,4733) | 1:A:23:THR:HG23 | 1:A:27:SER:HB2 | 16 | 0.34 |
| (1,4694) | 1:A:16:ASN:HB2 | 1:A:16:ASN:HD21 | 5 | 0.34 |
| (1,4693) | 1:A:16:ASN:HA | 1:B:32:ASN:HD21 | 6 | 0.34 |
| (1,4477) | 1:A:19:THR:HG21 | 1:A:45:PHE:HE1 | 3 | 0.34 |
| (1,4477) | 1:A:19:THR:HG22 | 1:A:45:PHE:HE1 | 3 | 0.34 |
| (1,4477) | 1:A:19:THR:HG23 | 1:A:45:PHE:HE1 | 3 | 0.34 |
| (1,4368) | 1:A:4:PHE:HE1 | 1:A:56:THR:HA | 2 | 0.34 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 14 | 0.34 |
| (1,3744) | 1:B:70:GLN:HA | 1:B:71:GLY:HA3 | 20 | 0.34 |
| (1,3192) | 1:A:54:LYS:HA | 1:A:54:LYS:HE2 | 18 | 0.34 |
| (1,3192) | 1:A:54:LYS:HA | 1:A:54:LYS:HE3 | 18 | 0.34 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD21 | 13 | 0.34 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD22 | 13 | 0.34 |
| (1,2843) | 1:B:7:GLY:HA3 | 1:B:49:LEU:HD23 | 13 | 0.34 |
| (1,1803) | 1:B:13:GLU:HB3 | 1:B:71:GLY:HA3 | 4 | 0.34 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 12 | 0.34 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 8 | 0.34 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 15 | 0.34 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 20 | 0.34 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 5 | 0.34 |
| (1,1473) | 1:A:5:LEU:HG | 1:A:52:PHE:HE1 | 12 | 0.34 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 4 | 0.34 |
| (1,5257) | 1:B:80:ASN:HB2 | 1:B:80:ASN:HD21 | 1 | 0.33 |
| (1,5257) | 1:B:80:ASN:HB2 | 1:B:80:ASN:HD21 | 14 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5245) | 1:B:69:VAL:HG11 | 1:B:70:GLN:HE21 | 12 | 0.33 |
| (1,5245) | 1:B:69:VAL:HG12 | 1:B:70:GLN:HE21 | 12 | 0.33 |
| (1,5245) | 1:B:69:VAL:HG13 | 1:B:70:GLN:HE21 | 12 | 0.33 |
| (1,5237) | 1:B:67:ARG:HG2 | 1:B:75:VAL:H | 6 | 0.33 |
| (1,5182) | 1:B:55:ASN:HD21 | 1:B:58:LYS:HG3 | 8 | 0.33 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 10 | 0.33 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 10 | 0.33 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 10 | 0.33 |
| (1,5130) | 1:B:38:LEU:HD21 | 1:B:39:ASN:HD21 | 5 | 0.33 |
| (1,5130) | 1:B:38:LEU:HD22 | 1:B:39:ASN:HD21 | 5 | 0.33 |
| (1,5130) | 1:B:38:LEU:HD23 | 1:B:39:ASN:HD21 | 5 | 0.33 |
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 6 | 0.33 |
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 18 | 0.33 |
| (1,5012) | 1:B:16:ASN:HB2 | 1:B:17:GLY:H | 12 | 0.33 |
| (1,5011) | 1:B:16:ASN:HB2 | 1:B:16:ASN:HD21 | 12 | 0.33 |
| (1,5011) | 1:B:16:ASN:HB2 | 1:B:16:ASN:HD21 | 18 | 0.33 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 7 | 0.33 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 7 | 0.33 |
| (1,4943) | 1:A:80:ASN:HB2 | 1:A:80:ASN:HD21 | 12 | 0.33 |
| (1,4943) | 1:A:80:ASN:HB2 | 1:A:80:ASN:HD21 | 13 | 0.33 |
| (1,4943) | 1:A:80:ASN:HB2 | 1:A:80:ASN:HD21 | 15 | 0.33 |
| (1,4943) | 1:A:80:ASN:HB2 | 1:A:80:ASN:HD21 | 16 | 0.33 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 13 | 0.33 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 15 | 0.33 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 15 | 0.33 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 15 | 0.33 |
| (1,4885) | 1:A:58:LYS:H | 1:A:58:LYS:HB2 | 6 | 0.33 |
| (1,4869) | 1:A:54:LYS:HG2 | 1:A:55:ASN:H | 9 | 0.33 |
| (1,4862) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HB2 | 14 | 0.33 |
| (1,4862) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HB2 | 14 | 0.33 |
| (1,4862) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HB2 | 14 | 0.33 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 7 | 0.33 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 7 | 0.33 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 7 | 0.33 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 15 | 0.33 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 15 | 0.33 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 15 | 0.33 |
| (1,4842) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG12 | 3 | 0.33 |
| (1,4842) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG12 | 9 | 0.33 |
| (1,4822) | 1:A:37:VAL:HG11 | 1:A:48:ASN:HD21 | 17 | 0.33 |
| (1,4822) | 1:A:37:VAL:HG12 | 1:A:48:ASN:HD21 | 17 | 0.33 |
| (1,4822) | 1:A:37:VAL:HG13 | 1:A:48:ASN:HD21 | 17 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4802) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG3 | 20 | 0.33 |
| (1,4795) | 1:A:32:ASN:HB2 | 1:B:20:ASN:H | 17 | 0.33 |
| (1,4772) | 1:A:28:LYS:HA | 1:A:28:LYS:HG2 | 14 | 0.33 |
| (1,4734) | 1:A:23:THR:HG21 | 1:B:27:SER:HB2 | 17 | 0.33 |
| (1,4734) | 1:A:23:THR:HG22 | 1:B:27:SER:HB2 | 17 | 0.33 |
| (1,4734) | 1:A:23:THR:HG23 | 1:B:27:SER:HB2 | 17 | 0.33 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 17 | 0.33 |
| (1,4694) | 1:A:16:ASN:HB2 | 1:A:16:ASN:HD21 | 9 | 0.33 |
| (1,4694) | 1:A:16:ASN:HB2 | 1:A:16:ASN:HD21 | 10 | 0.33 |
| (1,4691) | 1:A:15:LYS:HE2 | 1:A:16:ASN:HD21 | 3 | 0.33 |
| (1,4691) | 1:A:15:LYS:HE3 | 1:A:16:ASN:HD21 | 3 | 0.33 |
| (1,4686) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HB2 | 8 | 0.33 |
| (1,4686) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HB2 | 8 | 0.33 |
| (1,4686) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HB2 | 20 | 0.33 |
| (1,4686) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HB2 | 20 | 0.33 |
| (1,4680) | 1:A:15:LYS:HA | 1:A:16:ASN:HD21 | 2 | 0.33 |
| (1,4678) | 1:A:15:LYS:H | 1:A:18:MET:HG2 | 12 | 0.33 |
| (1,4665) | 1:A:13:GLU:HG2 | 1:A:15:LYS:HB2 | 17 | 0.33 |
| (1,4665) | 1:A:13:GLU:HG3 | 1:A:15:LYS:HB2 | 17 | 0.33 |
| (1,4643) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HG12 | 2 | 0.33 |
| (1,4636) | 1:A:5:LEU:HD11 | 1:A:34:ARG:HG2 | 17 | 0.33 |
| (1,4636) | 1:A:5:LEU:HD12 | 1:A:34:ARG:HG2 | 17 | 0.33 |
| (1,4636) | 1:A:5:LEU:HD13 | 1:A:34:ARG:HG2 | 17 | 0.33 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 5 | 0.33 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 5 | 0.33 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 5 | 0.33 |
| (1,4573) | 1:A:44:ILE:HG12 | 1:A:73:PHE:HE1 | 19 | 0.33 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 12 | 0.33 |
| (1,4568) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HE1 | 19 | 0.33 |
| (1,4568) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HE1 | 19 | 0.33 |
| (1,4568) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HE1 | 19 | 0.33 |
| (1,4477) | 1:A:19:THR:HG21 | 1:A:45:PHE:HE1 | 6 | 0.33 |
| (1,4477) | 1:A:19:THR:HG22 | 1:A:45:PHE:HE1 | 6 | 0.33 |
| (1,4477) | 1:A:19:THR:HG23 | 1:A:45:PHE:HE1 | 6 | 0.33 |
| (1,4242) | 1:A:15:LYS:HA | 1:A:17:GLY:H | 18 | 0.33 |
| (1,3937) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HB3 | 6 | 0.33 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 7 | 0.33 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 7 | 0.33 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 7 | 0.33 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE2 | 1 | 0.33 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE3 | 1 | 0.33 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE2 | 19 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE3 | 19 | 0.33 |
| (1,3192) | 1:A:54:LYS:HA | 1:A:54:LYS:HE2 | 15 | 0.33 |
| (1,3192) | 1:A:54:LYS:HA | 1:A:54:LYS:HE3 | 15 | 0.33 |
| (1,2033) | 1:A:22:ILE:HB | 1:A:45:PHE:HE1 | 15 | 0.33 |
| (1,1779) | 1:B:11:VAL:HG11 | 1:B:73:PHE:HE1 | 4 | 0.33 |
| (1,1779) | 1:B:11:VAL:HG12 | 1:B:73:PHE:HE1 | 4 | 0.33 |
| (1,1779) | 1:B:11:VAL:HG13 | 1:B:73:PHE:HE1 | 4 | 0.33 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 6 | 0.33 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 16 | 0.33 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 19 | 0.33 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 16 | 0.33 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 10 | 0.33 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 11 | 0.32 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 19 | 0.32 |
| (1,5239) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG21 | 2 | 0.32 |
| (1,5239) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG22 | 2 | 0.32 |
| (1,5239) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG23 | 2 | 0.32 |
| (1,5172) | 1:B:54:LYS:HG2 | 1:B:55:ASN:H | 14 | 0.32 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 2 | 0.32 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 2 | 0.32 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 2 | 0.32 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 9 | 0.32 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 9 | 0.32 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 9 | 0.32 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 13 | 0.32 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 13 | 0.32 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 13 | 0.32 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 19 | 0.32 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 19 | 0.32 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 19 | 0.32 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 20 | 0.32 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 20 | 0.32 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 20 | 0.32 |
| (1,5099) | 1:B:32:ASN:HD21 | 1:B:33:ILE:HB | 16 | 0.32 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 2 | 0.32 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 16 | 0.32 |
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 15 | 0.32 |
| (1,5019) | 1:B:17:GLY:HA2 | 1:B:21:GLN:HE22 | 17 | 0.32 |
| (1,5012) | 1:B:16:ASN:HB2 | 1:B:17:GLY:H | 6 | 0.32 |
| (1,5011) | 1:B:16:ASN:HB2 | 1:B:16:ASN:HD21 | 3 | 0.32 |
| (1,5011) | 1:B:16:ASN:HB2 | 1:B:16:ASN:HD21 | 9 | 0.32 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 10 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 10 | 0.32 |
| (1,4981) | 1:B:9:ARG:H | 1:B:76:GLU:HB2 | 4 | 0.32 |
| (1,4882) | 1:A:56:THR:HG21 | 1:A:59:LEU:HB2 | 13 | 0.32 |
| (1,4882) | 1:A:56:THR:HG22 | 1:A:59:LEU:HB2 | 13 | 0.32 |
| (1,4882) | 1:A:56:THR:HG23 | 1:A:59:LEU:HB2 | 13 | 0.32 |
| (1,4882) | 1:A:56:THR:HG21 | 1:A:59:LEU:HB2 | 16 | 0.32 |
| (1,4882) | 1:A:56:THR:HG22 | 1:A:59:LEU:HB2 | 16 | 0.32 |
| (1,4882) | 1:A:56:THR:HG23 | 1:A:59:LEU:HB2 | 16 | 0.32 |
| (1,4872) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HD21 | 6 | 0.32 |
| (1,4872) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HD21 | 6 | 0.32 |
| (1,4869) | 1:A:54:LYS:HG2 | 1:A:55:ASN:H | 11 | 0.32 |
| (1,4863) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HG2 | 6 | 0.32 |
| (1,4863) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HG2 | 6 | 0.32 |
| (1,4863) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HG2 | 6 | 0.32 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 2 | 0.32 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 2 | 0.32 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 2 | 0.32 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 8 | 0.32 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 8 | 0.32 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 8 | 0.32 |
| (1,4768) | 1:A:28:LYS:H | 1:A:28:LYS:HB2 | 20 | 0.32 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 16 | 0.32 |
| (1,4694) | 1:A:16:ASN:HB2 | 1:A:16:ASN:HD21 | 3 | 0.32 |
| (1,4694) | 1:A:16:ASN:HB2 | 1:A:16:ASN:HD21 | 6 | 0.32 |
| (1,4633) | 1:A:4:PHE:H | 1:A:54:LYS:HB2 | 14 | 0.32 |
| (1,4628) | 1:A:3:ASP:HB2 | 1:A:4:PHE:H | 4 | 0.32 |
| (1,4574) | 1:B:44:ILE:HG12 | 1:B:73:PHE:HE1 | 18 | 0.32 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 4 | 0.32 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 16 | 0.32 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 16 | 0.32 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 16 | 0.32 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD11 | 2 | 0.32 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD12 | 2 | 0.32 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD13 | 2 | 0.32 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD11 | 3 | 0.32 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD12 | 3 | 0.32 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD13 | 3 | 0.32 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD11 | 8 | 0.32 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD12 | 8 | 0.32 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD13 | 8 | 0.32 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 11 | 0.32 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 13 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 11 | 0.32 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 1 | 0.31 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 1 | 0.31 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 1 | 0.31 |
| (1,5257) | 1:B:80:ASN:HB2 | 1:B:80:ASN:HD21 | 6 | 0.31 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 10 | 0.31 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 8 | 0.31 |
| (1,5182) | 1:B:55:ASN:HD21 | 1:B:58:LYS:HG3 | 3 | 0.31 |
| (1,5176) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD21 | 15 | 0.31 |
| (1,5176) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD21 | 15 | 0.31 |
| (1,5174) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HB2 | 9 | 0.31 |
| (1,5174) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HB2 | 9 | 0.31 |
| (1,5165) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HB2 | 11 | 0.31 |
| (1,5165) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HB2 | 11 | 0.31 |
| (1,5165) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HB2 | 11 | 0.31 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 15 | 0.31 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 20 | 0.31 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 1 | 0.31 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 1 | 0.31 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 1 | 0.31 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 12 | 0.31 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 12 | 0.31 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 12 | 0.31 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 16 | 0.31 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 16 | 0.31 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 16 | 0.31 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 14 | 0.31 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB2 | 10 | 0.31 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB3 | 10 | 0.31 |
| (1,5118) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HA | 3 | 0.31 |
| (1,5116) | 1:B:36:ILE:HG21 | 1:B:48:ASN:HB2 | 16 | 0.31 |
| (1,5116) | 1:B:36:ILE:HG22 | 1:B:48:ASN:HB2 | 16 | 0.31 |
| (1,5116) | 1:B:36:ILE:HG23 | 1:B:48:ASN:HB2 | 16 | 0.31 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 16 | 0.31 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 16 | 0.31 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 16 | 0.31 |
| (1,5093) | 1:B:32:ASN:HB2 | 1:B:32:ASN:HD21 | 4 | 0.31 |
| (1,5093) | 1:B:32:ASN:HB2 | 1:B:32:ASN:HD21 | 6 | 0.31 |
| (1,5093) | 1:B:32:ASN:HB2 | 1:B:32:ASN:HD21 | 19 | 0.31 |
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 16 | 0.31 |
| (1,5070) | 1:B:28:LYS:HA | 1:B:28:LYS:HG2 | 1 | 0.31 |
| (1,5034) | 1:B:23:THR:HG21 | 1:B:27:SER:HB2 | 20 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5034) | 1:B:23:THR:HG22 | 1:B:27:SER:HB2 | 20 | 0.31 |
| (1,5034) | 1:B:23:THR:HG23 | 1:B:27:SER:HB2 | 20 | 0.31 |
| (1,5012) | 1:B:16:ASN:HB2 | 1:B:17:GLY:H | 13 | 0.31 |
| (1,5004) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HB2 | 17 | 0.31 |
| (1,5004) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HB2 | 17 | 0.31 |
| (1,4950) | 1:B:3:ASP:HA | 1:B:54:LYS:HB2 | 6 | 0.31 |
| (1,4943) | 1:A:80:ASN:HB2 | 1:A:80:ASN:HD21 | 11 | 0.31 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 3 | 0.31 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG21 | 13 | 0.31 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG22 | 13 | 0.31 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG23 | 13 | 0.31 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 11 | 0.31 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 11 | 0.31 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 11 | 0.31 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 10 | 0.31 |
| (1,4814) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HA | 10 | 0.31 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 11 | 0.31 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 11 | 0.31 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 11 | 0.31 |
| (1,4787) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HD2 | 6 | 0.31 |
| (1,4776) | 1:A:28:LYS:HB2 | 1:A:29:PHE:H | 14 | 0.31 |
| (1,4727) | 1:A:20:ASN:HD21 | 1:B:33:ILE:HG12 | 2 | 0.31 |
| (1,4636) | 1:A:5:LEU:HD11 | 1:A:34:ARG:HG2 | 16 | 0.31 |
| (1,4636) | 1:A:5:LEU:HD12 | 1:A:34:ARG:HG2 | 16 | 0.31 |
| (1,4636) | 1:A:5:LEU:HD13 | 1:A:34:ARG:HG2 | 16 | 0.31 |
| (1,4627) | 1:A:3:ASP:HA | 1:A:54:LYS:HB2 | 6 | 0.31 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 17 | 0.31 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 17 | 0.31 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 17 | 0.31 |
| (1,4574) | 1:B:44:ILE:HG12 | 1:B:73:PHE:HE1 | 1 | 0.31 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 13 | 0.31 |
| (1,4567) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HE1 | 1 | 0.31 |
| (1,4567) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HE1 | 1 | 0.31 |
| (1,4567) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HE1 | 1 | 0.31 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG21 | 18 | 0.31 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG22 | 18 | 0.31 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG23 | 18 | 0.31 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 14 | 0.31 |
| (1,1802) | 1:A:13:GLU:HB3 | 1:A:71:GLY:HA3 | 6 | 0.31 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 2 | 0.31 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 8 | 0.31 |
| (1,5245) | 1:B:69:VAL:HG11 | 1:B:70:GLN:HE21 | 14 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5245) | 1:B:69:VAL:HG12 | 1:B:70:GLN:HE21 | 14 | 0.3 |
| (1,5245) | 1:B:69:VAL:HG13 | 1:B:70:GLN:HE21 | 14 | 0.3 |
| (1,5182) | 1:B:55:ASN:HD21 | 1:B:58:LYS:HG3 | 18 | 0.3 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 3 | 0.3 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 3 | 0.3 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 3 | 0.3 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 11 | 0.3 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 11 | 0.3 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 11 | 0.3 |
| (1,5130) | 1:B:38:LEU:HD21 | 1:B:39:ASN:HD21 | 8 | 0.3 |
| (1,5130) | 1:B:38:LEU:HD22 | 1:B:39:ASN:HD21 | 8 | 0.3 |
| (1,5130) | 1:B:38:LEU:HD23 | 1:B:39:ASN:HD21 | 8 | 0.3 |
| (1,5108) | 1:B:34:ARG:HB2 | 1:B:51:ILE:H | 1 | 0.3 |
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 7 | 0.3 |
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 7 | 0.3 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 7 | 0.3 |
| (1,5001) | 1:B:15:LYS:HA | 1:B:16:ASN:HD21 | 13 | 0.3 |
| (1,4981) | 1:B:9:ARG:H | 1:B:76:GLU:HB2 | 20 | 0.3 |
| (1,4956) | 1:B:4:PHE:H | 1:B:54:LYS:HB2 | 5 | 0.3 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG21 | 9 | 0.3 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG22 | 9 | 0.3 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG23 | 9 | 0.3 |
| (1,4896) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 6 | 0.3 |
| (1,4896) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 6 | 0.3 |
| (1,4896) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 6 | 0.3 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD11 | 16 | 0.3 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD12 | 16 | 0.3 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD13 | 16 | 0.3 |
| (1,4879) | 1:A:55:ASN:HD21 | 1:A:58:LYS:HG3 | 2 | 0.3 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 1 | 0.3 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 7 | 0.3 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 20 | 0.3 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 20 | 0.3 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 20 | 0.3 |
| (1,4679) | 1:A:15:LYS:HA | 1:A:16:ASN:HB2 | 11 | 0.3 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 15 | 0.3 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 11 | 0.3 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 11 | 0.3 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 11 | 0.3 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 16 | 0.3 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 16 | 0.3 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 16 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 2 | 0.3 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 2 | 0.3 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 2 | 0.3 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 3 | 0.3 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 3 | 0.3 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 3 | 0.3 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 15 | 0.3 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 15 | 0.3 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 15 | 0.3 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 5 | 0.3 |
| (1,4568) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HE1 | 11 | 0.3 |
| (1,4568) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HE1 | 11 | 0.3 |
| (1,4568) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HE1 | 11 | 0.3 |
| (1,4568) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HE1 | 17 | 0.3 |
| (1,4568) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HE1 | 17 | 0.3 |
| (1,4568) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HE1 | 17 | 0.3 |
| (1,4478) | 1:B:19:THR:HG21 | 1:B:45:PHE:HE1 | 2 | 0.3 |
| (1,4478) | 1:B:19:THR:HG22 | 1:B:45:PHE:HE1 | 2 | 0.3 |
| (1,4478) | 1:B:19:THR:HG23 | 1:B:45:PHE:HE1 | 2 | 0.3 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 2 | 0.3 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 2 | 0.3 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 2 | 0.3 |
| (1,4363) | 1:B:29:PHE:HE1 | 1:B:66:LEU:HG | 8 | 0.3 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE2 | 10 | 0.3 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE3 | 10 | 0.3 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG21 | 12 | 0.3 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG22 | 12 | 0.3 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG23 | 12 | 0.3 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 1 | 0.3 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 15 | 0.3 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 13 | 0.3 |
| (1,5236) | 1:B:67:ARG:HG2 | 1:B:72:VAL:HG11 | 5 | 0.29 |
| (1,5236) | 1:B:67:ARG:HG2 | 1:B:72:VAL:HG12 | 5 | 0.29 |
| (1,5236) | 1:B:67:ARG:HG2 | 1:B:72:VAL:HG13 | 5 | 0.29 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD21 | 13 | 0.29 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD22 | 13 | 0.29 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD23 | 13 | 0.29 |
| (1,5185) | 1:B:56:THR:HG21 | 1:B:59:LEU:HB2 | 17 | 0.29 |
| (1,5185) | 1:B:56:THR:HG22 | 1:B:59:LEU:HB2 | 17 | 0.29 |
| (1,5185) | 1:B:56:THR:HG23 | 1:B:59:LEU:HB2 | 17 | 0.29 |
| (1,5175) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HD21 | 13 | 0.29 |
| (1,5175) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HD21 | 13 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5172) | 1:B:54:LYS:HG2 | 1:B:55:ASN:H | 10 | 0.29 |
| (1,5171) | 1:B:54:LYS:HB2 | 1:B:55:ASN:HD21 | 7 | 0.29 |
| (1,5165) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HB2 | 7 | 0.29 |
| (1,5165) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HB2 | 7 | 0.29 |
| (1,5165) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HB2 | 7 | 0.29 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 10 | 0.29 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 17 | 0.29 |
| (1,5159) | 1:B:51:ILE:HD11 | 1:B:58:LYS:HE2 | 14 | 0.29 |
| (1,5159) | 1:B:51:ILE:HD12 | 1:B:58:LYS:HE2 | 14 | 0.29 |
| (1,5159) | 1:B:51:ILE:HD13 | 1:B:58:LYS:HE2 | 14 | 0.29 |
| (1,5146) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG13 | 1 | 0.29 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 4 | 0.29 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 4 | 0.29 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 4 | 0.29 |
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 7 | 0.29 |
| (1,5065) | 1:B:27:SER:HG | 1:B:28:LYS:HD2 | 12 | 0.29 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 6 | 0.29 |
| (1,5019) | 1:B:17:GLY:HA2 | 1:B:21:GLN:HE22 | 3 | 0.29 |
| (1,5008) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD21 | 8 | 0.29 |
| (1,5008) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD21 | 8 | 0.29 |
| (1,4992) | 1:B:14:ASP:HB2 | 1:B:40:ALA:HB1 | 17 | 0.29 |
| (1,4992) | 1:B:14:ASP:HB2 | 1:B:40:ALA:HB2 | 17 | 0.29 |
| (1,4992) | 1:B:14:ASP:HB2 | 1:B:40:ALA:HB3 | 17 | 0.29 |
| (1,4932) | 1:A:68:LYS:HD2 | 1:A:69:VAL:H | 19 | 0.29 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 18 | 0.29 |
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 18 | 0.29 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 18 | 0.29 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB2 | 13 | 0.29 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB3 | 13 | 0.29 |
| (1,4862) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HB2 | 15 | 0.29 |
| (1,4862) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HB2 | 15 | 0.29 |
| (1,4862) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HB2 | 15 | 0.29 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 12 | 0.29 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 15 | 0.29 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD11 | 13 | 0.29 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD12 | 13 | 0.29 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD13 | 13 | 0.29 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 9 | 0.29 |
| (1,4773) | 1:A:28:LYS:HA | 1:A:28:LYS:HD2 | 18 | 0.29 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD11 | 18 | 0.29 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD12 | 18 | 0.29 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD13 | 18 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD11 | 19 | 0.29 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD12 | 19 | 0.29 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD13 | 19 | 0.29 |
| (1,4671) | 1:A:14:ASP:HB2 | 1:A:43:GLY:H | 2 | 0.29 |
| (1,4568) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HE1 | 13 | 0.29 |
| (1,4568) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HE1 | 13 | 0.29 |
| (1,4568) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HE1 | 13 | 0.29 |
| (1,4565) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HE1 | 4 | 0.29 |
| (1,4565) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HE1 | 4 | 0.29 |
| (1,4565) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HE1 | 4 | 0.29 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 9 | 0.29 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 19 | 0.29 |
| (1,4477) | 1:A:19:THR:HG21 | 1:A:45:PHE:HE1 | 16 | 0.29 |
| (1,4477) | 1:A:19:THR:HG22 | 1:A:45:PHE:HE1 | 16 | 0.29 |
| (1,4477) | 1:A:19:THR:HG23 | 1:A:45:PHE:HE1 | 16 | 0.29 |
| (1,4362) | 1:A:29:PHE:HE1 | 1:A:66:LEU:HG | 14 | 0.29 |
| (1,4242) | 1:A:15:LYS:HA | 1:A:17:GLY:H | 20 | 0.29 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE2 | 8 | 0.29 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE3 | 8 | 0.29 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD11 | 17 | 0.29 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD12 | 17 | 0.29 |
| (1,3457) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HD13 | 17 | 0.29 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 3 | 0.29 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD11 | 8 | 0.29 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD12 | 8 | 0.29 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD13 | 8 | 0.29 |
| (1,1802) | 1:A:13:GLU:HB3 | 1:A:71:GLY:HA3 | 10 | 0.29 |
| (1,1802) | 1:A:13:GLU:HB3 | 1:A:71:GLY:HA3 | 16 | 0.29 |
| (1,1753) | 1:B:11:VAL:HG21 | 1:B:45:PHE:HE1 | 15 | 0.29 |
| (1,1753) | 1:B:11:VAL:HG22 | 1:B:45:PHE:HE1 | 15 | 0.29 |
| (1,1753) | 1:B:11:VAL:HG23 | 1:B:45:PHE:HE1 | 15 | 0.29 |
| (1,1753) | 1:B:11:VAL:HG21 | 1:B:45:PHE:HE1 | 19 | 0.29 |
| (1,1753) | 1:B:11:VAL:HG22 | 1:B:45:PHE:HE1 | 19 | 0.29 |
| (1,1753) | 1:B:11:VAL:HG23 | 1:B:45:PHE:HE1 | 19 | 0.29 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 3 | 0.29 |
| (1,1555) | 1:A:7:GLY:HA3 | 1:A:8:ILE:HB | 9 | 0.29 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 11 | 0.28 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 11 | 0.28 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 11 | 0.28 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 14 | 0.28 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 2 | 0.28 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 15 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 9 | 0.28 |
| (1,5165) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HB2 | 19 | 0.28 |
| (1,5165) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HB2 | 19 | 0.28 |
| (1,5165) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HB2 | 19 | 0.28 |
| (1,5130) | 1:B:38:LEU:HD21 | 1:B:39:ASN:HD21 | 17 | 0.28 |
| (1,5130) | 1:B:38:LEU:HD22 | 1:B:39:ASN:HD21 | 17 | 0.28 |
| (1,5130) | 1:B:38:LEU:HD23 | 1:B:39:ASN:HD21 | 17 | 0.28 |
| (1,5093) | 1:B:32:ASN:HB2 | 1:B:32:ASN:HD21 | 11 | 0.28 |
| (1,5086) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HD2 | 4 | 0.28 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD11 | 19 | 0.28 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD12 | 19 | 0.28 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD13 | 19 | 0.28 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 6 | 0.28 |
| (1,5012) | 1:B:16:ASN:HB2 | 1:B:17:GLY:H | 1 | 0.28 |
| (1,5000) | 1:B:15:LYS:HA | 1:B:16:ASN:HB2 | 13 | 0.28 |
| (1,4956) | 1:B:4:PHE:H | 1:B:54:LYS:HB2 | 6 | 0.28 |
| (1,4956) | 1:B:4:PHE:H | 1:B:54:LYS:HB2 | 9 | 0.28 |
| (1,4956) | 1:B:4:PHE:H | 1:B:54:LYS:HB2 | 13 | 0.28 |
| (1,4948) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HA | 6 | 0.28 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 1 | 0.28 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG11 | 7 | 0.28 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG12 | 7 | 0.28 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG13 | 7 | 0.28 |
| (1,4910) | 1:A:64:ASP:HA | 1:A:67:ARG:HG2 | 7 | 0.28 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 15 | 0.28 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD11 | 14 | 0.28 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD12 | 14 | 0.28 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD13 | 14 | 0.28 |
| (1,4890) | 1:A:58:LYS:HE2 | 1:A:62:LEU:H | 10 | 0.28 |
| (1,4889) | 1:A:58:LYS:HE2 | 1:A:59:LEU:HA | 1 | 0.28 |
| (1,4879) | 1:A:55:ASN:HD21 | 1:A:58:LYS:HG3 | 14 | 0.28 |
| (1,4879) | 1:A:55:ASN:HD21 | 1:A:58:LYS:HG3 | 17 | 0.28 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 9 | 0.28 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 12 | 0.28 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 12 | 0.28 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 12 | 0.28 |
| (1,4826) | 1:A:38:LEU:HD21 | 1:A:39:ASN:HD21 | 6 | 0.28 |
| (1,4826) | 1:A:38:LEU:HD22 | 1:A:39:ASN:HD21 | 6 | 0.28 |
| (1,4826) | 1:A:38:LEU:HD23 | 1:A:39:ASN:HD21 | 6 | 0.28 |
| (1,4812) | 1:A:36:ILE:HG21 | 1:A:48:ASN:HB2 | 1 | 0.28 |
| (1,4812) | 1:A:36:ILE:HG22 | 1:A:48:ASN:HB2 | 1 | 0.28 |
| (1,4812) | 1:A:36:ILE:HG23 | 1:A:48:ASN:HB2 | 1 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4803) | 1:A:34:ARG:HB2 | 1:A:51:ILE:H | 13 | 0.28 |
| (1,4720) | 1:A:20:ASN:H | 1:B:32:ASN:HB2 | 3 | 0.28 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 3 | 0.28 |
| (1,4696) | 1:A:16:ASN:HB2 | 1:A:18:MET:H | 11 | 0.28 |
| (1,4695) | 1:A:16:ASN:HB2 | 1:A:17:GLY:H | 1 | 0.28 |
| (1,4690) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD21 | 3 | 0.28 |
| (1,4690) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD21 | 3 | 0.28 |
| (1,4641) | 1:A:6:ALA:HB1 | 1:A:77:ARG:HG2 | 7 | 0.28 |
| (1,4641) | 1:A:6:ALA:HB2 | 1:A:77:ARG:HG2 | 7 | 0.28 |
| (1,4641) | 1:A:6:ALA:HB3 | 1:A:77:ARG:HG2 | 7 | 0.28 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 3 | 0.28 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 3 | 0.28 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 3 | 0.28 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 20 | 0.28 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 20 | 0.28 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 20 | 0.28 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 17 | 0.28 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 17 | 0.28 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 17 | 0.28 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 20 | 0.28 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 20 | 0.28 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 20 | 0.28 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 18 | 0.28 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 10 | 0.28 |
| (1,3192) | 1:A:54:LYS:HA | 1:A:54:LYS:HE2 | 8 | 0.28 |
| (1,3192) | 1:A:54:LYS:HA | 1:A:54:LYS:HE3 | 8 | 0.28 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD11 | 15 | 0.28 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD12 | 15 | 0.28 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD13 | 15 | 0.28 |
| (1,1803) | 1:B:13:GLU:HB3 | 1:B:71:GLY:HA3 | 7 | 0.28 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 9 | 0.28 |
| (1,5206) | 1:B:62:LEU:HA | 1:B:65:LYS:HG2 | 15 | 0.27 |
| (1,5197) | 1:B:59:LEU:HB2 | 1:B:60:THR:HG21 | 3 | 0.27 |
| (1,5197) | 1:B:59:LEU:HB2 | 1:B:60:THR:HG22 | 3 | 0.27 |
| (1,5197) | 1:B:59:LEU:HB2 | 1:B:60:THR:HG23 | 3 | 0.27 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD11 | 4 | 0.27 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD12 | 4 | 0.27 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD13 | 4 | 0.27 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD11 | 11 | 0.27 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD12 | 11 | 0.27 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD13 | 11 | 0.27 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB2 | 12 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB3 | 12 | 0.27 |
| (1,5175) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HD21 | 3 | 0.27 |
| (1,5175) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HD21 | 3 | 0.27 |
| (1,5172) | 1:B:54:LYS:HG2 | 1:B:55:ASN:H | 3 | 0.27 |
| (1,5165) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HB2 | 15 | 0.27 |
| (1,5165) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HB2 | 15 | 0.27 |
| (1,5165) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HB2 | 15 | 0.27 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 3 | 0.27 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 5 | 0.27 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 18 | 0.27 |
| (1,5126) | 1:B:37:VAL:HG11 | 1:B:48:ASN:HD21 | 18 | 0.27 |
| (1,5126) | 1:B:37:VAL:HG12 | 1:B:48:ASN:HD21 | 18 | 0.27 |
| (1,5126) | 1:B:37:VAL:HG13 | 1:B:48:ASN:HD21 | 18 | 0.27 |
| (1,5116) | 1:B:36:ILE:HG21 | 1:B:48:ASN:HB2 | 4 | 0.27 |
| (1,5116) | 1:B:36:ILE:HG22 | 1:B:48:ASN:HB2 | 4 | 0.27 |
| (1,5116) | 1:B:36:ILE:HG23 | 1:B:48:ASN:HB2 | 4 | 0.27 |
| (1,5099) | 1:B:32:ASN:HD21 | 1:B:33:ILE:HB | 14 | 0.27 |
| (1,5093) | 1:B:32:ASN:HB2 | 1:B:32:ASN:HD21 | 14 | 0.27 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 1 | 0.27 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 8 | 0.27 |
| (1,5074) | 1:B:28:LYS:HB2 | 1:B:29:PHE:H | 1 | 0.27 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 7 | 0.27 |
| (1,5045) | 1:B:25:VAL:H | 1:B:28:LYS:HD2 | 12 | 0.27 |
| (1,5034) | 1:B:23:THR:HG21 | 1:B:27:SER:HB2 | 11 | 0.27 |
| (1,5034) | 1:B:23:THR:HG22 | 1:B:27:SER:HB2 | 11 | 0.27 |
| (1,5034) | 1:B:23:THR:HG23 | 1:B:27:SER:HB2 | 11 | 0.27 |
| (1,5034) | 1:B:23:THR:HG21 | 1:B:27:SER:HB2 | 13 | 0.27 |
| (1,5034) | 1:B:23:THR:HG22 | 1:B:27:SER:HB2 | 13 | 0.27 |
| (1,5034) | 1:B:23:THR:HG23 | 1:B:27:SER:HB2 | 13 | 0.27 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 20 | 0.27 |
| (1,4950) | 1:B:3:ASP:HA | 1:B:54:LYS:HB2 | 3 | 0.27 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 20 | 0.27 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 19 | 0.27 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 10 | 0.27 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG11 | 5 | 0.27 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG12 | 5 | 0.27 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG13 | 5 | 0.27 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD11 | 15 | 0.27 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD12 | 15 | 0.27 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD13 | 15 | 0.27 |
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 15 | 0.27 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 15 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 15 | 0.27 |
| (1,4778) | 1:A:28:LYS:HG2 | 1:A:29:PHE:H | 18 | 0.27 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD11 | 4 | 0.27 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD12 | 4 | 0.27 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD13 | 4 | 0.27 |
| (1,4760) | 1:A:27:SER:H | 1:A:27:SER:HB2 | 11 | 0.27 |
| (1,4760) | 1:A:27:SER:H | 1:A:27:SER:HB2 | 15 | 0.27 |
| (1,4679) | 1:A:15:LYS:HA | 1:A:16:ASN:HB2 | 3 | 0.27 |
| (1,4665) | 1:A:13:GLU:HG2 | 1:A:15:LYS:HB2 | 4 | 0.27 |
| (1,4665) | 1:A:13:GLU:HG3 | 1:A:15:LYS:HB2 | 4 | 0.27 |
| (1,4628) | 1:A:3:ASP:HB2 | 1:A:4:PHE:H | 10 | 0.27 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 2 | 0.27 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 2 | 0.27 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 2 | 0.27 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 10 | 0.27 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 10 | 0.27 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 10 | 0.27 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 9 | 0.27 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 9 | 0.27 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 9 | 0.27 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 11 | 0.27 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 11 | 0.27 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 11 | 0.27 |
| (1,4574) | 1:B:44:ILE:HG12 | 1:B:73:PHE:HE1 | 3 | 0.27 |
| (1,4574) | 1:B:44:ILE:HG12 | 1:B:73:PHE:HE1 | 7 | 0.27 |
| (1,4478) | 1:B:19:THR:HG21 | 1:B:45:PHE:HE1 | 10 | 0.27 |
| (1,4478) | 1:B:19:THR:HG22 | 1:B:45:PHE:HE1 | 10 | 0.27 |
| (1,4478) | 1:B:19:THR:HG23 | 1:B:45:PHE:HE1 | 10 | 0.27 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 7 | 0.27 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 7 | 0.27 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 7 | 0.27 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG21 | 4 | 0.27 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG22 | 4 | 0.27 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG23 | 4 | 0.27 |
| (1,4242) | 1:A:15:LYS:HA | 1:A:17:GLY:H | 1 | 0.27 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE2 | 16 | 0.27 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE3 | 16 | 0.27 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE2 | 1 | 0.27 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE3 | 1 | 0.27 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD11 | 5 | 0.27 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD12 | 5 | 0.27 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD13 | 5 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2034) | 1:B:22:ILE:HB | 1:B:45:PHE:HE1 | 16 | 0.27 |
| (1,5260) | 1:B:82:GLU:H | 1:B:82:GLU:HG2 | 6 | 0.26 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 19 | 0.26 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 20 | 0.26 |
| (1,5246) | 1:B:76:GLU:H | 1:B:76:GLU:HB2 | 12 | 0.26 |
| (1,5209) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HD2 | 19 | 0.26 |
| (1,5209) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HD2 | 19 | 0.26 |
| (1,5209) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HD2 | 19 | 0.26 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 7 | 0.26 |
| (1,5192) | 1:B:58:LYS:HE2 | 1:B:59:LEU:HA | 18 | 0.26 |
| (1,5185) | 1:B:56:THR:HG21 | 1:B:59:LEU:HB2 | 5 | 0.26 |
| (1,5185) | 1:B:56:THR:HG22 | 1:B:59:LEU:HB2 | 5 | 0.26 |
| (1,5185) | 1:B:56:THR:HG23 | 1:B:59:LEU:HB2 | 5 | 0.26 |
| (1,5151) | 1:B:46:THR:HG1 | 1:B:48:ASN:HD21 | 11 | 0.26 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 2 | 0.26 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 9 | 0.26 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 10 | 0.26 |
| (1,5130) | 1:B:38:LEU:HD21 | 1:B:39:ASN:HD21 | 16 | 0.26 |
| (1,5130) | 1:B:38:LEU:HD22 | 1:B:39:ASN:HD21 | 16 | 0.26 |
| (1,5130) | 1:B:38:LEU:HD23 | 1:B:39:ASN:HD21 | 16 | 0.26 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 6 | 0.26 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 6 | 0.26 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 6 | 0.26 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD11 | 14 | 0.26 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD12 | 14 | 0.26 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD13 | 14 | 0.26 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 7 | 0.26 |
| (1,5074) | 1:B:28:LYS:HB2 | 1:B:29:PHE:H | 4 | 0.26 |
| (1,5074) | 1:B:28:LYS:HB2 | 1:B:29:PHE:H | 12 | 0.26 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 1 | 0.26 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 3 | 0.26 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 6 | 0.26 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 10 | 0.26 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 15 | 0.26 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE2 | 5 | 0.26 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE3 | 5 | 0.26 |
| (1,5019) | 1:B:17:GLY:HA2 | 1:B:21:GLN:HE22 | 6 | 0.26 |
| (1,4950) | 1:B:3:ASP:HA | 1:B:54:LYS:HB2 | 14 | 0.26 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 12 | 0.26 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG21 | 5 | 0.26 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG22 | 5 | 0.26 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG23 | 5 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG21 | 7 | 0.26 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG22 | 7 | 0.26 |
| (1,4927) | 1:A:67:ARG:HG2 | 1:A:75:VAL:HG23 | 7 | 0.26 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 1 | 0.26 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 18 | 0.26 |
| (1,4871) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HB2 | 8 | 0.26 |
| (1,4871) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HB2 | 8 | 0.26 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 6 | 0.26 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 16 | 0.26 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 19 | 0.26 |
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 2 | 0.26 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 2 | 0.26 |
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 2 | 0.26 |
| (1,4760) | 1:A:27:SER:H | 1:A:27:SER:HB2 | 12 | 0.26 |
| (1,4760) | 1:A:27:SER:H | 1:A:27:SER:HB2 | 13 | 0.26 |
| (1,4760) | 1:A:27:SER:H | 1:A:27:SER:HB2 | 18 | 0.26 |
| (1,4752) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HD2 | 2 | 0.26 |
| (1,4752) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HD2 | 2 | 0.26 |
| (1,4752) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HD2 | 2 | 0.26 |
| (1,4720) | 1:A:20:ASN:H | 1:B:32:ASN:HB2 | 5 | 0.26 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 1 | 0.26 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 2 | 0.26 |
| (1,4679) | 1:A:15:LYS:HA | 1:A:16:ASN:HB2 | 6 | 0.26 |
| (1,4679) | 1:A:15:LYS:HA | 1:A:16:ASN:HB2 | 9 | 0.26 |
| (1,4678) | 1:A:15:LYS:H | 1:A:18:MET:HG2 | 5 | 0.26 |
| (1,4633) | 1:A:4:PHE:H | 1:A:54:LYS:HB2 | 7 | 0.26 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 17 | 0.26 |
| (1,4627) | 1:A:3:ASP:HA | 1:A:54:LYS:HB2 | 17 | 0.26 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 12 | 0.26 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 12 | 0.26 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 12 | 0.26 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 19 | 0.26 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 19 | 0.26 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 19 | 0.26 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 8 | 0.26 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 8 | 0.26 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 8 | 0.26 |
| (1,4568) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HE1 | 4 | 0.26 |
| (1,4568) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HE1 | 4 | 0.26 |
| (1,4568) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HE1 | 4 | 0.26 |
| (1,4567) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HE1 | 15 | 0.26 |
| (1,4567) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HE1 | 15 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4567) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HE1 | 15 | 0.26 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 18 | 0.26 |
| (1,4369) | 1:B:4:PHE:HE1 | 1:B:56:THR:HA | 20 | 0.26 |
| (1,4363) | 1:B:29:PHE:HE1 | 1:B:66:LEU:HG | 16 | 0.26 |
| (1,4363) | 1:B:29:PHE:HE1 | 1:B:66:LEU:HG | 17 | 0.26 |
| (1,4362) | 1:A:29:PHE:HE1 | 1:A:66:LEU:HG | 11 | 0.26 |
| (1,4243) | 1:B:15:LYS:HA | 1:B:17:GLY:H | 8 | 0.26 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 13 | 0.26 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 13 | 0.26 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 13 | 0.26 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG21 | 4 | 0.26 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG22 | 4 | 0.26 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG23 | 4 | 0.26 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG11 | 15 | 0.26 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG12 | 15 | 0.26 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG13 | 15 | 0.26 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG11 | 15 | 0.26 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG12 | 15 | 0.26 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG13 | 15 | 0.26 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE2 | 3 | 0.26 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE3 | 3 | 0.26 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE2 | 10 | 0.26 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE3 | 10 | 0.26 |
| (1,3494) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:HD21 | 4 | 0.26 |
| (1,3494) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:HD22 | 4 | 0.26 |
| (1,3494) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:HD23 | 4 | 0.26 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 4 | 0.26 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 12 | 0.26 |
| (1,2034) | 1:B:22:ILE:HB | 1:B:45:PHE:HE1 | 17 | 0.26 |
| (1,1803) | 1:B:13:GLU:HB3 | 1:B:71:GLY:HA3 | 11 | 0.26 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 10 | 0.26 |
| (1,5250) | 1:B:77:ARG:H | 1:B:77:ARG:HG2 | 15 | 0.25 |
| (1,5245) | 1:B:69:VAL:HG11 | 1:B:70:GLN:HE21 | 1 | 0.25 |
| (1,5245) | 1:B:69:VAL:HG12 | 1:B:70:GLN:HE21 | 1 | 0.25 |
| (1,5245) | 1:B:69:VAL:HG13 | 1:B:70:GLN:HE21 | 1 | 0.25 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB2 | 1 | 0.25 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB3 | 1 | 0.25 |
| (1,5172) | 1:B:54:LYS:HG2 | 1:B:55:ASN:H | 1 | 0.25 |
| (1,5166) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HG2 | 10 | 0.25 |
| (1,5166) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HG2 | 10 | 0.25 |
| (1,5166) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HG2 | 10 | 0.25 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 1 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5146) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG13 | 14 | 0.25 |
| (1,5116) | 1:B:36:ILE:HG21 | 1:B:48:ASN:HB2 | 15 | 0.25 |
| (1,5116) | 1:B:36:ILE:HG22 | 1:B:48:ASN:HB2 | 15 | 0.25 |
| (1,5116) | 1:B:36:ILE:HG23 | 1:B:48:ASN:HB2 | 15 | 0.25 |
| (1,5093) | 1:B:32:ASN:HB2 | 1:B:32:ASN:HD21 | 16 | 0.25 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 4 | 0.25 |
| (1,5086) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HD2 | 7 | 0.25 |
| (1,5086) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HD2 | 13 | 0.25 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 3 | 0.25 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 8 | 0.25 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 11 | 0.25 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 14 | 0.25 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 16 | 0.25 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 17 | 0.25 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 20 | 0.25 |
| (1,5019) | 1:B:17:GLY:HA2 | 1:B:21:GLN:HE22 | 11 | 0.25 |
| (1,5000) | 1:B:15:LYS:HA | 1:B:16:ASN:HB2 | 9 | 0.25 |
| (1,4986) | 1:B:9:ARG:HD2 | 1:B:76:GLU:HB2 | 12 | 0.25 |
| (1,4986) | 1:B:9:ARG:HD3 | 1:B:76:GLU:HB2 | 12 | 0.25 |
| (1,4956) | 1:B:4:PHE:H | 1:B:54:LYS:HB2 | 3 | 0.25 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 3 | 0.25 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 17 | 0.25 |
| (1,4932) | 1:A:68:LYS:HD2 | 1:A:69:VAL:H | 10 | 0.25 |
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 10 | 0.25 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 3 | 0.25 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 7 | 0.25 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 11 | 0.25 |
| (1,4879) | 1:A:55:ASN:HD21 | 1:A:58:LYS:HG3 | 9 | 0.25 |
| (1,4879) | 1:A:55:ASN:HD21 | 1:A:58:LYS:HG3 | 11 | 0.25 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 18 | 0.25 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 13 | 0.25 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 13 | 0.25 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 13 | 0.25 |
| (1,4822) | 1:A:37:VAL:HG11 | 1:A:48:ASN:HD21 | 20 | 0.25 |
| (1,4822) | 1:A:37:VAL:HG12 | 1:A:48:ASN:HD21 | 20 | 0.25 |
| (1,4822) | 1:A:37:VAL:HG13 | 1:A:48:ASN:HD21 | 20 | 0.25 |
| (1,4803) | 1:A:34:ARG:HB2 | 1:A:51:ILE:H | 7 | 0.25 |
| (1,4778) | 1:A:28:LYS:HG2 | 1:A:29:PHE:H | 10 | 0.25 |
| (1,4769) | 1:A:28:LYS:H | 1:A:28:LYS:HG2 | 15 | 0.25 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG21 | 2 | 0.25 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG22 | 2 | 0.25 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG23 | 2 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4760) | 1:A:27:SER:H | 1:A:27:SER:HB2 | 3 | 0.25 |
| (1,4760) | 1:A:27:SER:H | 1:A:27:SER:HB2 | 8 | 0.25 |
| (1,4760) | 1:A:27:SER:H | 1:A:27:SER:HB2 | 10 | 0.25 |
| (1,4760) | 1:A:27:SER:H | 1:A:27:SER:HB2 | 14 | 0.25 |
| (1,4760) | 1:A:27:SER:H | 1:A:27:SER:HB2 | 16 | 0.25 |
| (1,4760) | 1:A:27:SER:H | 1:A:27:SER:HB2 | 19 | 0.25 |
| (1,4728) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HG12 | 16 | 0.25 |
| (1,4727) | 1:A:20:ASN:HD21 | 1:B:33:ILE:HG12 | 18 | 0.25 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 13 | 0.25 |
| (1,4705) | 1:A:18:MET:H | 1:B:32:ASN:HD21 | 15 | 0.25 |
| (1,4665) | 1:A:13:GLU:HG2 | 1:A:15:LYS:HB2 | 15 | 0.25 |
| (1,4665) | 1:A:13:GLU:HG3 | 1:A:15:LYS:HB2 | 15 | 0.25 |
| (1,4665) | 1:A:13:GLU:HG2 | 1:A:15:LYS:HB2 | 19 | 0.25 |
| (1,4665) | 1:A:13:GLU:HG3 | 1:A:15:LYS:HB2 | 19 | 0.25 |
| (1,4633) | 1:A:4:PHE:H | 1:A:54:LYS:HB2 | 2 | 0.25 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 4 | 0.25 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 4 | 0.25 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 4 | 0.25 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 15 | 0.25 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 15 | 0.25 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 15 | 0.25 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 6 | 0.25 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 6 | 0.25 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 6 | 0.25 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 10 | 0.25 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 10 | 0.25 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 10 | 0.25 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 18 | 0.25 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 18 | 0.25 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 18 | 0.25 |
| (1,4574) | 1:B:44:ILE:HG12 | 1:B:73:PHE:HE1 | 15 | 0.25 |
| (1,4568) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HE1 | 15 | 0.25 |
| (1,4568) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HE1 | 15 | 0.25 |
| (1,4568) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HE1 | 15 | 0.25 |
| (1,4477) | 1:A:19:THR:HG21 | 1:A:45:PHE:HE1 | 13 | 0.25 |
| (1,4477) | 1:A:19:THR:HG22 | 1:A:45:PHE:HE1 | 13 | 0.25 |
| (1,4477) | 1:A:19:THR:HG23 | 1:A:45:PHE:HE1 | 13 | 0.25 |
| (1,4369) | 1:B:4:PHE:HE1 | 1:B:56:THR:HA | 18 | 0.25 |
| (1,4362) | 1:A:29:PHE:HE1 | 1:A:66:LEU:HG | 5 | 0.25 |
| (1,3937) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HB3 | 3 | 0.25 |
| (1,3937) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HB3 | 18 | 0.25 |
| (1,3768) | 1:B:69:VAL:HA | 1:B:70:GLN:HG2 | 7 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3768) | 1:B:69:VAL:HA | 1:B:70:GLN:HG3 | 7 | 0.25 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 2 | 0.25 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 8 | 0.25 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 8 | 0.25 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 8 | 0.25 |
| (1,3095) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HZ1 | 5 | 0.25 |
| (1,3095) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HZ1 | 5 | 0.25 |
| (1,3095) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HZ1 | 5 | 0.25 |
| (1,1556) | 1:B:7:GLY:HA3 | 1:B:8:ILE:HB | 16 | 0.25 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 4 | 0.24 |
| (1,5206) | 1:B:62:LEU:HA | 1:B:65:LYS:HG2 | 3 | 0.24 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 3 | 0.24 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 4 | 0.24 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 20 | 0.24 |
| (1,5172) | 1:B:54:LYS:HG2 | 1:B:55:ASN:H | 13 | 0.24 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 7 | 0.24 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 9 | 0.24 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 16 | 0.24 |
| (1,5138) | 1:B:39:ASN:HD21 | 1:B:46:THR:HB | 4 | 0.24 |
| (1,5117) | 1:B:36:ILE:HG12 | 1:B:37:VAL:H | 11 | 0.24 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 14 | 0.24 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 2 | 0.24 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 12 | 0.24 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 18 | 0.24 |
| (1,5058) | 1:B:26:ILE:HG12 | 1:B:29:PHE:HZ | 9 | 0.24 |
| (1,5008) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD21 | 12 | 0.24 |
| (1,5008) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD21 | 12 | 0.24 |
| (1,5000) | 1:B:15:LYS:HA | 1:B:16:ASN:HB2 | 12 | 0.24 |
| (1,5000) | 1:B:15:LYS:HA | 1:B:16:ASN:HB2 | 19 | 0.24 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 3 | 0.24 |
| (1,4952) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HB2 | 7 | 0.24 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 19 | 0.24 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 1 | 0.24 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 2 | 0.24 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 14 | 0.24 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 16 | 0.24 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB2 | 9 | 0.24 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB3 | 9 | 0.24 |
| (1,4872) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HD21 | 12 | 0.24 |
| (1,4872) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HD21 | 12 | 0.24 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 11 | 0.24 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE1 | 18 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE2 | 18 | 0.24 |
| (1,4852) | 1:A:48:ASN:HD21 | 1:A:50:MET:HE3 | 18 | 0.24 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 10 | 0.24 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 10 | 0.24 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 10 | 0.24 |
| (1,4803) | 1:A:34:ARG:HB2 | 1:A:51:ILE:H | 19 | 0.24 |
| (1,4760) | 1:A:27:SER:H | 1:A:27:SER:HB2 | 1 | 0.24 |
| (1,4760) | 1:A:27:SER:H | 1:A:27:SER:HB2 | 4 | 0.24 |
| (1,4760) | 1:A:27:SER:H | 1:A:27:SER:HB2 | 5 | 0.24 |
| (1,4760) | 1:A:27:SER:H | 1:A:27:SER:HB2 | 6 | 0.24 |
| (1,4734) | 1:A:23:THR:HG21 | 1:B:27:SER:HB2 | 2 | 0.24 |
| (1,4734) | 1:A:23:THR:HG22 | 1:B:27:SER:HB2 | 2 | 0.24 |
| (1,4734) | 1:A:23:THR:HG23 | 1:B:27:SER:HB2 | 2 | 0.24 |
| (1,4661) | 1:A:9:ARG:HD2 | 1:A:48:ASN:HD21 | 19 | 0.24 |
| (1,4661) | 1:A:9:ARG:HD3 | 1:A:48:ASN:HD21 | 19 | 0.24 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 6 | 0.24 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 6 | 0.24 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 6 | 0.24 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 1 | 0.24 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 1 | 0.24 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 1 | 0.24 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG11 | 16 | 0.24 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG12 | 16 | 0.24 |
| (1,4595) | 1:A:4:PHE:HE1 | 1:A:53:VAL:HG13 | 16 | 0.24 |
| (1,4573) | 1:A:44:ILE:HG12 | 1:A:73:PHE:HE1 | 3 | 0.24 |
| (1,4573) | 1:A:44:ILE:HG12 | 1:A:73:PHE:HE1 | 14 | 0.24 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 3 | 0.24 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 6 | 0.24 |
| (1,4477) | 1:A:19:THR:HG21 | 1:A:45:PHE:HE1 | 14 | 0.24 |
| (1,4477) | 1:A:19:THR:HG22 | 1:A:45:PHE:HE1 | 14 | 0.24 |
| (1,4477) | 1:A:19:THR:HG23 | 1:A:45:PHE:HE1 | 14 | 0.24 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG21 | 6 | 0.24 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG22 | 6 | 0.24 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG23 | 6 | 0.24 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 12 | 0.24 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 12 | 0.24 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 12 | 0.24 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE2 | 11 | 0.24 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE3 | 11 | 0.24 |
| (1,3460) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:HD11 | 4 | 0.24 |
| (1,3460) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:HD12 | 4 | 0.24 |
| (1,3460) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:HD13 | 4 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2034) | 1:B:22:ILE:HB | 1:B:45:PHE:HE1 | 6 | 0.24 |
| (1,2033) | 1:A:22:ILE:HB | 1:A:45:PHE:HE1 | 14 | 0.24 |
| (1,182) | 1:B:15:LYS:H | 1:B:18:MET:HG2 | 14 | 0.24 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 9 | 0.24 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 6 | 0.24 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 5 | 0.23 |
| (1,5246) | 1:B:76:GLU:H | 1:B:76:GLU:HB2 | 4 | 0.23 |
| (1,5218) | 1:B:64:ASP:HA | 1:B:67:ARG:HG2 | 3 | 0.23 |
| (1,5206) | 1:B:62:LEU:HA | 1:B:65:LYS:HG2 | 6 | 0.23 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 2 | 0.23 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 11 | 0.23 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 12 | 0.23 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 13 | 0.23 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 15 | 0.23 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 16 | 0.23 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 18 | 0.23 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD11 | 6 | 0.23 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD12 | 6 | 0.23 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD13 | 6 | 0.23 |
| (1,5185) | 1:B:56:THR:HG21 | 1:B:59:LEU:HB2 | 13 | 0.23 |
| (1,5185) | 1:B:56:THR:HG22 | 1:B:59:LEU:HB2 | 13 | 0.23 |
| (1,5185) | 1:B:56:THR:HG23 | 1:B:59:LEU:HB2 | 13 | 0.23 |
| (1,5175) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HD21 | 6 | 0.23 |
| (1,5175) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HD21 | 6 | 0.23 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 6 | 0.23 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 13 | 0.23 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 11 | 0.23 |
| (1,5130) | 1:B:38:LEU:HD21 | 1:B:39:ASN:HD21 | 10 | 0.23 |
| (1,5130) | 1:B:38:LEU:HD22 | 1:B:39:ASN:HD21 | 10 | 0.23 |
| (1,5130) | 1:B:38:LEU:HD23 | 1:B:39:ASN:HD21 | 10 | 0.23 |
| (1,5130) | 1:B:38:LEU:HD21 | 1:B:39:ASN:HD21 | 15 | 0.23 |
| (1,5130) | 1:B:38:LEU:HD22 | 1:B:39:ASN:HD21 | 15 | 0.23 |
| (1,5130) | 1:B:38:LEU:HD23 | 1:B:39:ASN:HD21 | 15 | 0.23 |
| (1,5116) | 1:B:36:ILE:HG21 | 1:B:48:ASN:HB2 | 12 | 0.23 |
| (1,5116) | 1:B:36:ILE:HG22 | 1:B:48:ASN:HB2 | 12 | 0.23 |
| (1,5116) | 1:B:36:ILE:HG23 | 1:B:48:ASN:HB2 | 12 | 0.23 |
| (1,5108) | 1:B:34:ARG:HB2 | 1:B:51:ILE:H | 12 | 0.23 |
| (1,5100) | 1:B:33:ILE:H | 1:B:33:ILE:HG12 | 18 | 0.23 |
| (1,5099) | 1:B:32:ASN:HD21 | 1:B:33:ILE:HB | 6 | 0.23 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 14 | 0.23 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 14 | 0.23 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 14 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 19 | 0.23 |
| (1,5081) | 1:B:29:PHE:HB2 | 1:B:51:ILE:HD11 | 6 | 0.23 |
| (1,5081) | 1:B:29:PHE:HB2 | 1:B:51:ILE:HD12 | 6 | 0.23 |
| (1,5081) | 1:B:29:PHE:HB2 | 1:B:51:ILE:HD13 | 6 | 0.23 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 20 | 0.23 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 4 | 0.23 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 9 | 0.23 |
| (1,5059) | 1:B:27:SER:H | 1:B:27:SER:HB2 | 19 | 0.23 |
| (1,5005) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HD21 | 19 | 0.23 |
| (1,5005) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HD21 | 19 | 0.23 |
| (1,5000) | 1:B:15:LYS:HA | 1:B:16:ASN:HB2 | 18 | 0.23 |
| (1,4993) | 1:B:14:ASP:HB2 | 1:B:43:GLY:H | 18 | 0.23 |
| (1,4981) | 1:B:9:ARG:H | 1:B:76:GLU:HB2 | 3 | 0.23 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 6 | 0.23 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD21 | 7 | 0.23 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD22 | 7 | 0.23 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD23 | 7 | 0.23 |
| (1,4894) | 1:A:59:LEU:HB2 | 1:A:60:THR:HG21 | 2 | 0.23 |
| (1,4894) | 1:A:59:LEU:HB2 | 1:A:60:THR:HG22 | 2 | 0.23 |
| (1,4894) | 1:A:59:LEU:HB2 | 1:A:60:THR:HG23 | 2 | 0.23 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 10 | 0.23 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 13 | 0.23 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 17 | 0.23 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 19 | 0.23 |
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD21 | 15 | 0.23 |
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD22 | 15 | 0.23 |
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD23 | 15 | 0.23 |
| (1,4872) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HD21 | 15 | 0.23 |
| (1,4872) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HD21 | 15 | 0.23 |
| (1,4866) | 1:A:54:LYS:HB2 | 1:A:54:LYS:HE2 | 15 | 0.23 |
| (1,4866) | 1:A:54:LYS:HB2 | 1:A:54:LYS:HE3 | 15 | 0.23 |
| (1,4863) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HG2 | 15 | 0.23 |
| (1,4863) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HG2 | 15 | 0.23 |
| (1,4863) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HG2 | 15 | 0.23 |
| (1,4862) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HB2 | 18 | 0.23 |
| (1,4862) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HB2 | 18 | 0.23 |
| (1,4862) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HB2 | 18 | 0.23 |
| (1,4861) | 1:A:53:VAL:HG11 | 1:A:58:LYS:HE2 | 18 | 0.23 |
| (1,4861) | 1:A:53:VAL:HG12 | 1:A:58:LYS:HE2 | 18 | 0.23 |
| (1,4861) | 1:A:53:VAL:HG13 | 1:A:58:LYS:HE2 | 18 | 0.23 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 14 | 0.23 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB2 | 15 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB3 | 15 | 0.23 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD11 | 8 | 0.23 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD12 | 8 | 0.23 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD13 | 8 | 0.23 |
| (1,4778) | 1:A:28:LYS:HG2 | 1:A:29:PHE:H | 3 | 0.23 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG21 | 18 | 0.23 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG22 | 18 | 0.23 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG23 | 18 | 0.23 |
| (1,4733) | 1:A:23:THR:HG21 | 1:A:27:SER:HB2 | 6 | 0.23 |
| (1,4733) | 1:A:23:THR:HG22 | 1:A:27:SER:HB2 | 6 | 0.23 |
| (1,4733) | 1:A:23:THR:HG23 | 1:A:27:SER:HB2 | 6 | 0.23 |
| (1,4679) | 1:A:15:LYS:HA | 1:A:16:ASN:HB2 | 10 | 0.23 |
| (1,4674) | 1:A:14:ASP:HB2 | 1:A:44:ILE:HG21 | 7 | 0.23 |
| (1,4674) | 1:A:14:ASP:HB2 | 1:A:44:ILE:HG22 | 7 | 0.23 |
| (1,4674) | 1:A:14:ASP:HB2 | 1:A:44:ILE:HG23 | 7 | 0.23 |
| (1,4671) | 1:A:14:ASP:HB2 | 1:A:43:GLY:H | 18 | 0.23 |
| (1,4573) | 1:A:44:ILE:HG12 | 1:A:73:PHE:HE1 | 2 | 0.23 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 17 | 0.23 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG21 | 18 | 0.23 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG22 | 18 | 0.23 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG23 | 18 | 0.23 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG21 | 15 | 0.23 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG22 | 15 | 0.23 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG23 | 15 | 0.23 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG21 | 16 | 0.23 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG22 | 16 | 0.23 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG23 | 16 | 0.23 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE2 | 2 | 0.23 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE3 | 2 | 0.23 |
| (1,3504) | 1:B:60:THR:HG21 | 1:B:63:MET:HE1 | 3 | 0.23 |
| (1,3504) | 1:B:60:THR:HG21 | 1:B:63:MET:HE2 | 3 | 0.23 |
| (1,3504) | 1:B:60:THR:HG21 | 1:B:63:MET:HE3 | 3 | 0.23 |
| (1,3504) | 1:B:60:THR:HG22 | 1:B:63:MET:HE1 | 3 | 0.23 |
| (1,3504) | 1:B:60:THR:HG22 | 1:B:63:MET:HE2 | 3 | 0.23 |
| (1,3504) | 1:B:60:THR:HG22 | 1:B:63:MET:HE3 | 3 | 0.23 |
| (1,3504) | 1:B:60:THR:HG23 | 1:B:63:MET:HE1 | 3 | 0.23 |
| (1,3504) | 1:B:60:THR:HG23 | 1:B:63:MET:HE2 | 3 | 0.23 |
| (1,3504) | 1:B:60:THR:HG23 | 1:B:63:MET:HE3 | 3 | 0.23 |
| (1,3095) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HZ1 | 19 | 0.23 |
| (1,3095) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HZ1 | 19 | 0.23 |
| (1,3095) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HZ1 | 19 | 0.23 |
| (1,2248) | 1:B:28:LYS:HA | 1:B:28:LYS:HG2 | 12 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1802) | 1:A:13:GLU:HB3 | 1:A:71:GLY:HA3 | 18 | 0.23 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 12 | 0.23 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 4 | 0.23 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 2 | 0.22 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 12 | 0.22 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 9 | 0.22 |
| (1,5248) | 1:B:76:GLU:HB2 | 1:B:77:ARG:H | 7 | 0.22 |
| (1,5246) | 1:B:76:GLU:H | 1:B:76:GLU:HB2 | 17 | 0.22 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 20 | 0.22 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 5 | 0.22 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD21 | 18 | 0.22 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD22 | 18 | 0.22 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD23 | 18 | 0.22 |
| (1,5185) | 1:B:56:THR:HG21 | 1:B:59:LEU:HB2 | 1 | 0.22 |
| (1,5185) | 1:B:56:THR:HG22 | 1:B:59:LEU:HB2 | 1 | 0.22 |
| (1,5185) | 1:B:56:THR:HG23 | 1:B:59:LEU:HB2 | 1 | 0.22 |
| (1,5173) | 1:B:54:LYS:HG2 | 1:B:55:ASN:HD21 | 14 | 0.22 |
| (1,5150) | 1:B:46:THR:HG21 | 1:B:48:ASN:HD21 | 15 | 0.22 |
| (1,5150) | 1:B:46:THR:HG22 | 1:B:48:ASN:HD21 | 15 | 0.22 |
| (1,5150) | 1:B:46:THR:HG23 | 1:B:48:ASN:HD21 | 15 | 0.22 |
| (1,5145) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG12 | 4 | 0.22 |
| (1,5117) | 1:B:36:ILE:HG12 | 1:B:37:VAL:H | 14 | 0.22 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 9 | 0.22 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD11 | 10 | 0.22 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD12 | 10 | 0.22 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD13 | 10 | 0.22 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 19 | 0.22 |
| (1,5073) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HE2 | 19 | 0.22 |
| (1,5073) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HE3 | 19 | 0.22 |
| (1,5051) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HD2 | 7 | 0.22 |
| (1,5051) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HD2 | 7 | 0.22 |
| (1,5051) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HD2 | 7 | 0.22 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 19 | 0.22 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 11 | 0.22 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 6 | 0.22 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD21 | 1 | 0.22 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD22 | 1 | 0.22 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD23 | 1 | 0.22 |
| (1,4910) | 1:A:64:ASP:HA | 1:A:67:ARG:HG2 | 17 | 0.22 |
| (1,4894) | 1:A:59:LEU:HB2 | 1:A:60:THR:HG21 | 14 | 0.22 |
| (1,4894) | 1:A:59:LEU:HB2 | 1:A:60:THR:HG22 | 14 | 0.22 |
| (1,4894) | 1:A:59:LEU:HB2 | 1:A:60:THR:HG23 | 14 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 4 | 0.22 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 8 | 0.22 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 9 | 0.22 |
| (1,4879) | 1:A:55:ASN:HD21 | 1:A:58:LYS:HG3 | 8 | 0.22 |
| (1,4879) | 1:A:55:ASN:HD21 | 1:A:58:LYS:HG3 | 13 | 0.22 |
| (1,4862) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HB2 | 8 | 0.22 |
| (1,4862) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HB2 | 8 | 0.22 |
| (1,4862) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HB2 | 8 | 0.22 |
| (1,4862) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HB2 | 16 | 0.22 |
| (1,4862) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HB2 | 16 | 0.22 |
| (1,4862) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HB2 | 16 | 0.22 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 14 | 0.22 |
| (1,4843) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG13 | 7 | 0.22 |
| (1,4778) | 1:A:28:LYS:HG2 | 1:A:29:PHE:H | 12 | 0.22 |
| (1,4778) | 1:A:28:LYS:HG2 | 1:A:29:PHE:H | 15 | 0.22 |
| (1,4772) | 1:A:28:LYS:HA | 1:A:28:LYS:HG2 | 20 | 0.22 |
| (1,4679) | 1:A:15:LYS:HA | 1:A:16:ASN:HB2 | 7 | 0.22 |
| (1,4672) | 1:A:14:ASP:HB2 | 1:A:43:GLY:HA2 | 7 | 0.22 |
| (1,4672) | 1:A:14:ASP:HB2 | 1:A:43:GLY:HA2 | 19 | 0.22 |
| (1,4659) | 1:A:9:ARG:HG2 | 1:A:47:CYS:H | 1 | 0.22 |
| (1,4633) | 1:A:4:PHE:H | 1:A:54:LYS:HB2 | 5 | 0.22 |
| (1,4633) | 1:A:4:PHE:H | 1:A:54:LYS:HB2 | 6 | 0.22 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 1 | 0.22 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 1 | 0.22 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 1 | 0.22 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 13 | 0.22 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 13 | 0.22 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 13 | 0.22 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG11 | 14 | 0.22 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG12 | 14 | 0.22 |
| (1,4596) | 1:B:4:PHE:HE1 | 1:B:53:VAL:HG13 | 14 | 0.22 |
| (1,4478) | 1:B:19:THR:HG21 | 1:B:45:PHE:HE1 | 15 | 0.22 |
| (1,4478) | 1:B:19:THR:HG22 | 1:B:45:PHE:HE1 | 15 | 0.22 |
| (1,4478) | 1:B:19:THR:HG23 | 1:B:45:PHE:HE1 | 15 | 0.22 |
| (1,4243) | 1:B:15:LYS:HA | 1:B:17:GLY:H | 1 | 0.22 |
| (1,3503) | 1:A:60:THR:HG21 | 1:A:63:MET:HE1 | 14 | 0.22 |
| (1,3503) | 1:A:60:THR:HG21 | 1:A:63:MET:HE2 | 14 | 0.22 |
| (1,3503) | 1:A:60:THR:HG21 | 1:A:63:MET:HE3 | 14 | 0.22 |
| (1,3503) | 1:A:60:THR:HG22 | 1:A:63:MET:HE1 | 14 | 0.22 |
| (1,3503) | 1:A:60:THR:HG22 | 1:A:63:MET:HE2 | 14 | 0.22 |
| (1,3503) | 1:A:60:THR:HG22 | 1:A:63:MET:HE3 | 14 | 0.22 |
| (1,3503) | 1:A:60:THR:HG23 | 1:A:63:MET:HE1 | 14 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3503) | 1:A:60:THR:HG23 | 1:A:63:MET:HE2 | 14 | 0.22 |
| (1,3503) | 1:A:60:THR:HG23 | 1:A:63:MET:HE3 | 14 | 0.22 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 9 | 0.22 |
| (1,3095) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HZ1 | 14 | 0.22 |
| (1,3095) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HZ1 | 14 | 0.22 |
| (1,3095) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HZ1 | 14 | 0.22 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 11 | 0.22 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 13 | 0.22 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 8 | 0.22 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 12 | 0.22 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 18 | 0.21 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 8 | 0.21 |
| (1,5246) | 1:B:76:GLU:H | 1:B:76:GLU:HB2 | 3 | 0.21 |
| (1,5245) | 1:B:69:VAL:HG11 | 1:B:70:GLN:HE21 | 20 | 0.21 |
| (1,5245) | 1:B:69:VAL:HG12 | 1:B:70:GLN:HE21 | 20 | 0.21 |
| (1,5245) | 1:B:69:VAL:HG13 | 1:B:70:GLN:HE21 | 20 | 0.21 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 1 | 0.21 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 6 | 0.21 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 10 | 0.21 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 14 | 0.21 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 17 | 0.21 |
| (1,5192) | 1:B:58:LYS:HE2 | 1:B:59:LEU:HA | 14 | 0.21 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB2 | 3 | 0.21 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB3 | 3 | 0.21 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 11 | 0.21 |
| (1,5123) | 1:B:37:VAL:HB | 1:B:48:ASN:HD21 | 13 | 0.21 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 6 | 0.21 |
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 1 | 0.21 |
| (1,4994) | 1:B:14:ASP:HB2 | 1:B:43:GLY:HA2 | 8 | 0.21 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 17 | 0.21 |
| (1,4936) | 1:A:77:ARG:H | 1:A:77:ARG:HG2 | 7 | 0.21 |
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 20 | 0.21 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 5 | 0.21 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 6 | 0.21 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 20 | 0.21 |
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD21 | 6 | 0.21 |
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD22 | 6 | 0.21 |
| (1,4892) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD23 | 6 | 0.21 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB2 | 1 | 0.21 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB3 | 1 | 0.21 |
| (1,4867) | 1:A:54:LYS:HB2 | 1:A:55:ASN:HB2 | 18 | 0.21 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 5 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 15 | 0.21 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 15 | 0.21 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 15 | 0.21 |
| (1,4843) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG13 | 11 | 0.21 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 2 | 0.21 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 6 | 0.21 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 6 | 0.21 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 6 | 0.21 |
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 4 | 0.21 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 4 | 0.21 |
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 4 | 0.21 |
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 5 | 0.21 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 5 | 0.21 |
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 5 | 0.21 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD11 | 12 | 0.21 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD12 | 12 | 0.21 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD13 | 12 | 0.21 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD11 | 12 | 0.21 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD12 | 12 | 0.21 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD13 | 12 | 0.21 |
| (1,4724) | 1:A:20:ASN:HB2 | 1:A:21:GLN:HE21 | 12 | 0.21 |
| (1,4633) | 1:A:4:PHE:H | 1:A:54:LYS:HB2 | 9 | 0.21 |
| (1,4574) | 1:B:44:ILE:HG12 | 1:B:73:PHE:HE1 | 12 | 0.21 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 18 | 0.21 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 3 | 0.21 |
| (1,4478) | 1:B:19:THR:HG21 | 1:B:45:PHE:HE1 | 3 | 0.21 |
| (1,4478) | 1:B:19:THR:HG22 | 1:B:45:PHE:HE1 | 3 | 0.21 |
| (1,4478) | 1:B:19:THR:HG23 | 1:B:45:PHE:HE1 | 3 | 0.21 |
| (1,4243) | 1:B:15:LYS:HA | 1:B:17:GLY:H | 13 | 0.21 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE2 | 5 | 0.21 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE3 | 5 | 0.21 |
| (1,3231) | 1:B:57:ASP:HB2 | 1:B:58:LYS:HG3 | 2 | 0.21 |
| (1,3231) | 1:B:57:ASP:HB3 | 1:B:58:LYS:HG3 | 2 | 0.21 |
| (1,3194) | 1:A:54:LYS:HE2 | 1:A:55:ASN:HD21 | 19 | 0.21 |
| (1,3194) | 1:A:54:LYS:HE3 | 1:A:55:ASN:HD21 | 19 | 0.21 |
| (1,3095) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HZ1 | 1 | 0.21 |
| (1,3095) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HZ1 | 1 | 0.21 |
| (1,3095) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HZ1 | 1 | 0.21 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD11 | 10 | 0.21 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD12 | 10 | 0.21 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD13 | 10 | 0.21 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD11 | 2 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD12 | 2 | 0.21 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD13 | 2 | 0.21 |
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 6 | 0.21 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 6 | 0.21 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 6 | 0.21 |
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 13 | 0.21 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 13 | 0.21 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 13 | 0.21 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 4 | 0.21 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 4 | 0.21 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 4 | 0.21 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 3 | 0.21 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 3 | 0.2 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 8 | 0.2 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 19 | 0.2 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 20 | 0.2 |
| (1,5248) | 1:B:76:GLU:HB2 | 1:B:77:ARG:H | 2 | 0.2 |
| (1,5216) | 1:B:63:MET:HE1 | 1:B:77:ARG:HB2 | 8 | 0.2 |
| (1,5216) | 1:B:63:MET:HE2 | 1:B:77:ARG:HB2 | 8 | 0.2 |
| (1,5216) | 1:B:63:MET:HE3 | 1:B:77:ARG:HB2 | 8 | 0.2 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB2 | 2 | 0.2 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB3 | 2 | 0.2 |
| (1,5175) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HD21 | 7 | 0.2 |
| (1,5175) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HD21 | 7 | 0.2 |
| (1,5165) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HB2 | 2 | 0.2 |
| (1,5165) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HB2 | 2 | 0.2 |
| (1,5165) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HB2 | 2 | 0.2 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 19 | 0.2 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB2 | 5 | 0.2 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB3 | 5 | 0.2 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 3 | 0.2 |
| (1,5073) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HE2 | 14 | 0.2 |
| (1,5073) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HE3 | 14 | 0.2 |
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 17 | 0.2 |
| (1,5065) | 1:B:27:SER:HG | 1:B:28:LYS:HD2 | 4 | 0.2 |
| (1,5051) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HD2 | 5 | 0.2 |
| (1,5051) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HD2 | 5 | 0.2 |
| (1,5051) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HD2 | 5 | 0.2 |
| (1,5034) | 1:B:23:THR:HG21 | 1:B:27:SER:HB2 | 8 | 0.2 |
| (1,5034) | 1:B:23:THR:HG22 | 1:B:27:SER:HB2 | 8 | 0.2 |
| (1,5034) | 1:B:23:THR:HG23 | 1:B:27:SER:HB2 | 8 | 0.2 |
| (1,5034) | 1:B:23:THR:HG21 | 1:B:27:SER:HB2 | 14 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5034) | 1:B:23:THR:HG22 | 1:B:27:SER:HB2 | 14 | 0.2 |
| (1,5034) | 1:B:23:THR:HG23 | 1:B:27:SER:HB2 | 14 | 0.2 |
| (1,4999) | 1:B:15:LYS:H | 1:B:18:MET:HG2 | 8 | 0.2 |
| (1,4992) | 1:B:14:ASP:HB2 | 1:B:40:ALA:HB1 | 19 | 0.2 |
| (1,4992) | 1:B:14:ASP:HB2 | 1:B:40:ALA:HB2 | 19 | 0.2 |
| (1,4992) | 1:B:14:ASP:HB2 | 1:B:40:ALA:HB3 | 19 | 0.2 |
| (1,4968) | 1:B:8:ILE:H | 1:B:8:ILE:HG12 | 16 | 0.2 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 18 | 0.2 |
| (1,4952) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HB2 | 13 | 0.2 |
| (1,4951) | 1:B:3:ASP:HB2 | 1:B:4:PHE:H | 20 | 0.2 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG11 | 18 | 0.2 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG12 | 18 | 0.2 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG13 | 18 | 0.2 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB2 | 10 | 0.2 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB3 | 10 | 0.2 |
| (1,4866) | 1:A:54:LYS:HB2 | 1:A:54:LYS:HE2 | 18 | 0.2 |
| (1,4866) | 1:A:54:LYS:HB2 | 1:A:54:LYS:HE3 | 18 | 0.2 |
| (1,4865) | 1:A:54:LYS:H | 1:A:54:LYS:HG2 | 10 | 0.2 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 8 | 0.2 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD11 | 2 | 0.2 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD12 | 2 | 0.2 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD13 | 2 | 0.2 |
| (1,4778) | 1:A:28:LYS:HG2 | 1:A:29:PHE:H | 11 | 0.2 |
| (1,4680) | 1:A:15:LYS:HA | 1:A:16:ASN:HD21 | 1 | 0.2 |
| (1,4679) | 1:A:15:LYS:HA | 1:A:16:ASN:HB2 | 5 | 0.2 |
| (1,4679) | 1:A:15:LYS:HA | 1:A:16:ASN:HB2 | 12 | 0.2 |
| (1,4672) | 1:A:14:ASP:HB2 | 1:A:43:GLY:HA2 | 20 | 0.2 |
| (1,4665) | 1:A:13:GLU:HG2 | 1:A:15:LYS:HB2 | 16 | 0.2 |
| (1,4665) | 1:A:13:GLU:HG3 | 1:A:15:LYS:HB2 | 16 | 0.2 |
| (1,4633) | 1:A:4:PHE:H | 1:A:54:LYS:HB2 | 8 | 0.2 |
| (1,4633) | 1:A:4:PHE:H | 1:A:54:LYS:HB2 | 19 | 0.2 |
| (1,4628) | 1:A:3:ASP:HB2 | 1:A:4:PHE:H | 3 | 0.2 |
| (1,4496) | 1:B:12:GLY:H | 1:B:45:PHE:HE1 | 2 | 0.2 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 16 | 0.2 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD21 | 3 | 0.2 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD22 | 3 | 0.2 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD23 | 3 | 0.2 |
| (1,3937) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HB3 | 20 | 0.2 |
| (1,3192) | 1:A:54:LYS:HA | 1:A:54:LYS:HE2 | 1 | 0.2 |
| (1,3192) | 1:A:54:LYS:HA | 1:A:54:LYS:HE3 | 1 | 0.2 |
| (1,3095) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HZ1 | 9 | 0.2 |
| (1,3095) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HZ1 | 9 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3095) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HZ1 | 9 | 0.2 |
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 3 | 0.2 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 3 | 0.2 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 3 | 0.2 |
| (1,2550) | 1:B:38:LEU:HD21 | 1:B:45:PHE:HE1 | 12 | 0.2 |
| (1,2550) | 1:B:38:LEU:HD22 | 1:B:45:PHE:HE1 | 12 | 0.2 |
| (1,2550) | 1:B:38:LEU:HD23 | 1:B:45:PHE:HE1 | 12 | 0.2 |
| (1,2033) | 1:A:22:ILE:HB | 1:A:45:PHE:HE1 | 18 | 0.2 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 19 | 0.2 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 6 | 0.2 |
| (1,5262) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HA | 14 | 0.19 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 2 | 0.19 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 9 | 0.19 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 15 | 0.19 |
| (1,5244) | 1:B:68:LYS:HD2 | 1:B:69:VAL:H | 15 | 0.19 |
| (1,5205) | 1:B:62:LEU:H | 1:B:65:LYS:HD2 | 3 | 0.19 |
| (1,5196) | 1:B:59:LEU:HB2 | 1:B:60:THR:H | 19 | 0.19 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 8 | 0.19 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 14 | 0.19 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 6 | 0.19 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 6 | 0.19 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 6 | 0.19 |
| (1,5099) | 1:B:32:ASN:HD21 | 1:B:33:ILE:HB | 11 | 0.19 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG21 | 11 | 0.19 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG22 | 11 | 0.19 |
| (1,5094) | 1:B:32:ASN:HB2 | 1:B:33:ILE:HG23 | 11 | 0.19 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 8 | 0.19 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 10 | 0.19 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 17 | 0.19 |
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 19 | 0.19 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 15 | 0.19 |
| (1,4996) | 1:B:14:ASP:HB2 | 1:B:44:ILE:HG21 | 6 | 0.19 |
| (1,4996) | 1:B:14:ASP:HB2 | 1:B:44:ILE:HG22 | 6 | 0.19 |
| (1,4996) | 1:B:14:ASP:HB2 | 1:B:44:ILE:HG23 | 6 | 0.19 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 12 | 0.19 |
| (1,4893) | 1:A:59:LEU:HB2 | 1:A:60:THR:H | 12 | 0.19 |
| (1,4862) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HB2 | 12 | 0.19 |
| (1,4862) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HB2 | 12 | 0.19 |
| (1,4862) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HB2 | 12 | 0.19 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 2 | 0.19 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 16 | 0.19 |
| (1,4778) | 1:A:28:LYS:HG2 | 1:A:29:PHE:H | 19 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4773) | 1:A:28:LYS:HA | 1:A:28:LYS:HD2 | 12 | 0.19 |
| (1,4773) | 1:A:28:LYS:HA | 1:A:28:LYS:HD2 | 16 | 0.19 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 1 | 0.19 |
| (1,4630) | 1:A:3:ASP:HB2 | 1:A:52:PHE:HD1 | 13 | 0.19 |
| (1,4630) | 1:A:3:ASP:HB2 | 1:A:52:PHE:HD2 | 13 | 0.19 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG21 | 20 | 0.19 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG22 | 20 | 0.19 |
| (1,4361) | 1:B:4:PHE:HE1 | 1:B:56:THR:HG23 | 20 | 0.19 |
| (1,3937) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HB3 | 8 | 0.19 |
| (1,3936) | 1:A:7:GLY:HA2 | 1:A:78:LEU:HB3 | 19 | 0.19 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE2 | 6 | 0.19 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE3 | 6 | 0.19 |
| (1,3621) | 1:B:41:LYS:HE2 | 1:B:44:ILE:H | 2 | 0.19 |
| (1,3621) | 1:B:41:LYS:HE3 | 1:B:44:ILE:H | 2 | 0.19 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 13 | 0.19 |
| (1,3095) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HZ1 | 4 | 0.19 |
| (1,3095) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HZ1 | 4 | 0.19 |
| (1,3095) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HZ1 | 4 | 0.19 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD11 | 1 | 0.19 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD12 | 1 | 0.19 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD13 | 1 | 0.19 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD11 | 9 | 0.19 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD12 | 9 | 0.19 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD13 | 9 | 0.19 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD11 | 5 | 0.19 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD12 | 5 | 0.19 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD13 | 5 | 0.19 |
| (1,291) | 1:A:20:ASN:H | 1:A:20:ASN:HD22 | 13 | 0.19 |
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 8 | 0.19 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 8 | 0.19 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 8 | 0.19 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD11 | 10 | 0.19 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD12 | 10 | 0.19 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD13 | 10 | 0.19 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 12 | 0.19 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 12 | 0.19 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 12 | 0.19 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 2 | 0.19 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 14 | 0.19 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 11 | 0.18 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 16 | 0.18 |
| (1,561) | 1:A:29:PHE:HD1 | 1:A:31:THR:H | 4 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,561) | 1:A:29:PHE:HD2 | 1:A:31:THR:H | 4 | 0.18 |
| (1,561) | 1:A:29:PHE:HD1 | 1:A:31:THR:H | 17 | 0.18 |
| (1,561) | 1:A:29:PHE:HD2 | 1:A:31:THR:H | 17 | 0.18 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 2 | 0.18 |
| (1,5246) | 1:B:76:GLU:H | 1:B:76:GLU:HB2 | 20 | 0.18 |
| (1,5167) | 1:B:53:VAL:HG21 | 1:B:58:LYS:HB2 | 3 | 0.18 |
| (1,5167) | 1:B:53:VAL:HG22 | 1:B:58:LYS:HB2 | 3 | 0.18 |
| (1,5167) | 1:B:53:VAL:HG23 | 1:B:58:LYS:HB2 | 3 | 0.18 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD11 | 4 | 0.18 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD12 | 4 | 0.18 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD13 | 4 | 0.18 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD11 | 13 | 0.18 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD12 | 13 | 0.18 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD13 | 13 | 0.18 |
| (1,5111) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HD1 | 10 | 0.18 |
| (1,5111) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HD2 | 10 | 0.18 |
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 15 | 0.18 |
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 15 | 0.18 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 15 | 0.18 |
| (1,5086) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HD2 | 20 | 0.18 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 5 | 0.18 |
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 11 | 0.18 |
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 14 | 0.18 |
| (1,5041) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HG2 | 17 | 0.18 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 3 | 0.18 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 7 | 0.18 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 12 | 0.18 |
| (1,5029) | 1:B:20:ASN:HB2 | 1:B:21:GLN:HE21 | 3 | 0.18 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 19 | 0.18 |
| (1,5019) | 1:B:17:GLY:HA2 | 1:B:21:GLN:HE22 | 4 | 0.18 |
| (1,4994) | 1:B:14:ASP:HB2 | 1:B:43:GLY:HA2 | 6 | 0.18 |
| (1,4994) | 1:B:14:ASP:HB2 | 1:B:43:GLY:HA2 | 9 | 0.18 |
| (1,4968) | 1:B:8:ILE:H | 1:B:8:ILE:HG12 | 8 | 0.18 |
| (1,4956) | 1:B:4:PHE:H | 1:B:54:LYS:HB2 | 2 | 0.18 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 6 | 0.18 |
| (1,4948) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HA | 20 | 0.18 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 7 | 0.18 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 8 | 0.18 |
| (1,4882) | 1:A:56:THR:HG21 | 1:A:59:LEU:HB2 | 1 | 0.18 |
| (1,4882) | 1:A:56:THR:HG22 | 1:A:59:LEU:HB2 | 1 | 0.18 |
| (1,4882) | 1:A:56:THR:HG23 | 1:A:59:LEU:HB2 | 1 | 0.18 |
| (1,4812) | 1:A:36:ILE:HG21 | 1:A:48:ASN:HB2 | 11 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4812) | 1:A:36:ILE:HG22 | 1:A:48:ASN:HB2 | 11 | 0.18 |
| (1,4812) | 1:A:36:ILE:HG23 | 1:A:48:ASN:HB2 | 11 | 0.18 |
| (1,4811) | 1:A:35:THR:HG21 | 1:B:39:ASN:HD21 | 19 | 0.18 |
| (1,4811) | 1:A:35:THR:HG22 | 1:B:39:ASN:HD21 | 19 | 0.18 |
| (1,4811) | 1:A:35:THR:HG23 | 1:B:39:ASN:HD21 | 19 | 0.18 |
| (1,4778) | 1:A:28:LYS:HG2 | 1:A:29:PHE:H | 16 | 0.18 |
| (1,4773) | 1:A:28:LYS:HA | 1:A:28:LYS:HD2 | 20 | 0.18 |
| (1,4724) | 1:A:20:ASN:HB2 | 1:A:21:GLN:HE21 | 18 | 0.18 |
| (1,4687) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HD21 | 7 | 0.18 |
| (1,4687) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HD21 | 7 | 0.18 |
| (1,4672) | 1:A:14:ASP:HB2 | 1:A:43:GLY:HA2 | 14 | 0.18 |
| (1,4628) | 1:A:3:ASP:HB2 | 1:A:4:PHE:H | 19 | 0.18 |
| (1,4495) | 1:A:12:GLY:H | 1:A:45:PHE:HE1 | 4 | 0.18 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 13 | 0.18 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 13 | 0.18 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 13 | 0.18 |
| (1,4368) | 1:A:4:PHE:HE1 | 1:A:56:THR:HA | 18 | 0.18 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 11 | 0.18 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 11 | 0.18 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 11 | 0.18 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 14 | 0.18 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 14 | 0.18 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 14 | 0.18 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG11 | 14 | 0.18 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG12 | 14 | 0.18 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG13 | 14 | 0.18 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG11 | 14 | 0.18 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG12 | 14 | 0.18 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG13 | 14 | 0.18 |
| (1,3094) | 1:A:53:VAL:HG11 | 1:A:58:LYS:HZ1 | 5 | 0.18 |
| (1,3094) | 1:A:53:VAL:HG12 | 1:A:58:LYS:HZ1 | 5 | 0.18 |
| (1,3094) | 1:A:53:VAL:HG13 | 1:A:58:LYS:HZ1 | 5 | 0.18 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD11 | 13 | 0.18 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD12 | 13 | 0.18 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD13 | 13 | 0.18 |
| (1,292) | 1:B:20:ASN:H | 1:B:20:ASN:HD22 | 7 | 0.18 |
| (1,291) | 1:A:20:ASN:H | 1:A:20:ASN:HD22 | 14 | 0.18 |
| (1,2716) | 1:B:9:ARG:HE | 1:B:46:THR:HG21 | 14 | 0.18 |
| (1,2716) | 1:B:9:ARG:HE | 1:B:46:THR:HG22 | 14 | 0.18 |
| (1,2716) | 1:B:9:ARG:HE | 1:B:46:THR:HG23 | 14 | 0.18 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD11 | 6 | 0.18 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD12 | 6 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD13 | 6 | 0.18 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD11 | 8 | 0.18 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD12 | 8 | 0.18 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD13 | 8 | 0.18 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD11 | 3 | 0.18 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD12 | 3 | 0.18 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD13 | 3 | 0.18 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD11 | 15 | 0.18 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD12 | 15 | 0.18 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD13 | 15 | 0.18 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 15 | 0.18 |
| (1,1802) | 1:A:13:GLU:HB3 | 1:A:71:GLY:HA3 | 20 | 0.18 |
| (1,1753) | 1:B:11:VAL:HG21 | 1:B:45:PHE:HE1 | 11 | 0.18 |
| (1,1753) | 1:B:11:VAL:HG22 | 1:B:45:PHE:HE1 | 11 | 0.18 |
| (1,1753) | 1:B:11:VAL:HG23 | 1:B:45:PHE:HE1 | 11 | 0.18 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 18 | 0.17 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 5 | 0.17 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 16 | 0.17 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 14 | 0.17 |
| (1,5246) | 1:B:76:GLU:H | 1:B:76:GLU:HB2 | 18 | 0.17 |
| (1,5222) | 1:B:65:LYS:H | 1:B:65:LYS:HG2 | 17 | 0.17 |
| (1,5175) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HD21 | 19 | 0.17 |
| (1,5175) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HD21 | 19 | 0.17 |
| (1,5165) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HB2 | 4 | 0.17 |
| (1,5165) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HB2 | 4 | 0.17 |
| (1,5165) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HB2 | 4 | 0.17 |
| (1,5146) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG13 | 18 | 0.17 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 10 | 0.17 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 10 | 0.17 |
| (1,5116) | 1:B:36:ILE:HG21 | 1:B:48:ASN:HB2 | 5 | 0.17 |
| (1,5116) | 1:B:36:ILE:HG22 | 1:B:48:ASN:HB2 | 5 | 0.17 |
| (1,5116) | 1:B:36:ILE:HG23 | 1:B:48:ASN:HB2 | 5 | 0.17 |
| (1,5108) | 1:B:34:ARG:HB2 | 1:B:51:ILE:H | 8 | 0.17 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 15 | 0.17 |
| (1,5067) | 1:B:28:LYS:H | 1:B:28:LYS:HG2 | 3 | 0.17 |
| (1,5054) | 1:B:26:ILE:H | 1:B:28:LYS:HG2 | 12 | 0.17 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 1 | 0.17 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 5 | 0.17 |
| (1,4999) | 1:B:15:LYS:H | 1:B:18:MET:HG2 | 13 | 0.17 |
| (1,4968) | 1:B:8:ILE:H | 1:B:8:ILE:HG12 | 13 | 0.17 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 14 | 0.17 |
| (1,4951) | 1:B:3:ASP:HB2 | 1:B:4:PHE:H | 8 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,4951) | 1:B:3:ASP:HB2 | 1:B:4:PHE:H | 18 | 0.17 |
| (1,4949) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HD2 | 3 | 0.17 |
| (1,4948) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HA | 3 | 0.17 |
| (1,4948) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HA | 8 | 0.17 |
| (1,4915) | 1:A:65:LYS:HA | 1:A:68:LYS:HD2 | 7 | 0.17 |
| (1,4910) | 1:A:64:ASP:HA | 1:A:67:ARG:HG2 | 5 | 0.17 |
| (1,4872) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HD21 | 11 | 0.17 |
| (1,4872) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HD21 | 11 | 0.17 |
| (1,4871) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HB2 | 7 | 0.17 |
| (1,4871) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HB2 | 7 | 0.17 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 4 | 0.17 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 13 | 0.17 |
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 15 | 0.17 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 19 | 0.17 |
| (1,4826) | 1:A:38:LEU:HD21 | 1:A:39:ASN:HD21 | 13 | 0.17 |
| (1,4826) | 1:A:38:LEU:HD22 | 1:A:39:ASN:HD21 | 13 | 0.17 |
| (1,4826) | 1:A:38:LEU:HD23 | 1:A:39:ASN:HD21 | 13 | 0.17 |
| (1,4803) | 1:A:34:ARG:HB2 | 1:A:51:ILE:H | 10 | 0.17 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 12 | 0.17 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 12 | 0.17 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 12 | 0.17 |
| (1,4787) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HD2 | 9 | 0.17 |
| (1,4778) | 1:A:28:LYS:HG2 | 1:A:29:PHE:H | 1 | 0.17 |
| (1,4776) | 1:A:28:LYS:HB2 | 1:A:29:PHE:H | 20 | 0.17 |
| (1,4769) | 1:A:28:LYS:H | 1:A:28:LYS:HG2 | 18 | 0.17 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD11 | 6 | 0.17 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD12 | 6 | 0.17 |
| (1,4763) | 1:A:27:SER:HB2 | 1:A:33:ILE:HD13 | 6 | 0.17 |
| (1,4752) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HD2 | 3 | 0.17 |
| (1,4752) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HD2 | 3 | 0.17 |
| (1,4752) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HD2 | 3 | 0.17 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 14 | 0.17 |
| (1,4733) | 1:A:23:THR:HG21 | 1:A:27:SER:HB2 | 12 | 0.17 |
| (1,4733) | 1:A:23:THR:HG22 | 1:A:27:SER:HB2 | 12 | 0.17 |
| (1,4733) | 1:A:23:THR:HG23 | 1:A:27:SER:HB2 | 12 | 0.17 |
| (1,4726) | 1:A:20:ASN:HB2 | 1:B:33:ILE:HD11 | 1 | 0.17 |
| (1,4726) | 1:A:20:ASN:HB2 | 1:B:33:ILE:HD12 | 1 | 0.17 |
| (1,4726) | 1:A:20:ASN:HB2 | 1:B:33:ILE:HD13 | 1 | 0.17 |
| (1,4724) | 1:A:20:ASN:HB2 | 1:A:21:GLN:HE21 | 3 | 0.17 |
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 1 | 0.17 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 19 | 0.17 |
| (1,4496) | 1:B:12:GLY:H | 1:B:45:PHE:HE1 | 9 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 18 | 0.17 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 18 | 0.17 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 18 | 0.17 |
| (1,4368) | 1:A:4:PHE:HE1 | 1:A:56:THR:HA | 15 | 0.17 |
| (1,4363) | 1:B:29:PHE:HE1 | 1:B:66:LEU:HG | 2 | 0.17 |
| (1,4363) | 1:B:29:PHE:HE1 | 1:B:66:LEU:HG | 19 | 0.17 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 11 | 0.17 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 11 | 0.17 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 11 | 0.17 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 7 | 0.17 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 20 | 0.17 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG21 | 2 | 0.17 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG22 | 2 | 0.17 |
| (1,3393) | 1:B:58:LYS:HZ1 | 1:B:61:THR:HG23 | 2 | 0.17 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG21 | 6 | 0.17 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG22 | 6 | 0.17 |
| (1,3392) | 1:A:58:LYS:HZ1 | 1:A:61:THR:HG23 | 6 | 0.17 |
| (1,3094) | 1:A:53:VAL:HG11 | 1:A:58:LYS:HZ1 | 9 | 0.17 |
| (1,3094) | 1:A:53:VAL:HG12 | 1:A:58:LYS:HZ1 | 9 | 0.17 |
| (1,3094) | 1:A:53:VAL:HG13 | 1:A:58:LYS:HZ1 | 9 | 0.17 |
| (1,2716) | 1:B:9:ARG:HE | 1:B:46:THR:HG21 | 6 | 0.17 |
| (1,2716) | 1:B:9:ARG:HE | 1:B:46:THR:HG22 | 6 | 0.17 |
| (1,2716) | 1:B:9:ARG:HE | 1:B:46:THR:HG23 | 6 | 0.17 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 19 | 0.17 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD11 | 7 | 0.17 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD12 | 7 | 0.17 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD13 | 7 | 0.17 |
| (1,1881) | 1:B:68:LYS:HE2 | 1:B:69:VAL:HG21 | 17 | 0.17 |
| (1,1881) | 1:B:68:LYS:HE2 | 1:B:69:VAL:HG22 | 17 | 0.17 |
| (1,1881) | 1:B:68:LYS:HE2 | 1:B:69:VAL:HG23 | 17 | 0.17 |
| (1,1881) | 1:B:68:LYS:HE3 | 1:B:69:VAL:HG21 | 17 | 0.17 |
| (1,1881) | 1:B:68:LYS:HE3 | 1:B:69:VAL:HG22 | 17 | 0.17 |
| (1,1881) | 1:B:68:LYS:HE3 | 1:B:69:VAL:HG23 | 17 | 0.17 |
| (1,1873) | 1:B:15:LYS:HD2 | 1:B:71:GLY:HA3 | 15 | 0.17 |
| (1,1873) | 1:B:15:LYS:HD3 | 1:B:71:GLY:HA3 | 15 | 0.17 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 7 | 0.16 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 2 | 0.16 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 12 | 0.16 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 13 | 0.16 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 5 | 0.16 |
| (1,5192) | 1:B:58:LYS:HE2 | 1:B:59:LEU:HA | 6 | 0.16 |
| (1,5182) | 1:B:55:ASN:HD21 | 1:B:58:LYS:HG3 | 15 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,5145) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG12 | 15 | 0.16 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 1 | 0.16 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE2 | 4 | 0.16 |
| (1,5137) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HE3 | 4 | 0.16 |
| (1,5116) | 1:B:36:ILE:HG21 | 1:B:48:ASN:HB2 | 9 | 0.16 |
| (1,5116) | 1:B:36:ILE:HG22 | 1:B:48:ASN:HB2 | 9 | 0.16 |
| (1,5116) | 1:B:36:ILE:HG23 | 1:B:48:ASN:HB2 | 9 | 0.16 |
| (1,5116) | 1:B:36:ILE:HG21 | 1:B:48:ASN:HB2 | 19 | 0.16 |
| (1,5116) | 1:B:36:ILE:HG22 | 1:B:48:ASN:HB2 | 19 | 0.16 |
| (1,5116) | 1:B:36:ILE:HG23 | 1:B:48:ASN:HB2 | 19 | 0.16 |
| (1,5111) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HD1 | 15 | 0.16 |
| (1,5111) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HD2 | 15 | 0.16 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD11 | 15 | 0.16 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD12 | 15 | 0.16 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD13 | 15 | 0.16 |
| (1,5051) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HD2 | 18 | 0.16 |
| (1,5051) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HD2 | 18 | 0.16 |
| (1,5051) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HD2 | 18 | 0.16 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 9 | 0.16 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 15 | 0.16 |
| (1,5019) | 1:B:17:GLY:HA2 | 1:B:21:GLN:HE22 | 7 | 0.16 |
| (1,5000) | 1:B:15:LYS:HA | 1:B:16:ASN:HB2 | 1 | 0.16 |
| (1,5000) | 1:B:15:LYS:HA | 1:B:16:ASN:HB2 | 16 | 0.16 |
| (1,4953) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HD1 | 2 | 0.16 |
| (1,4953) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HD2 | 2 | 0.16 |
| (1,4952) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HB2 | 2 | 0.16 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 10 | 0.16 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 10 | 0.16 |
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 8 | 0.16 |
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 9 | 0.16 |
| (1,4902) | 1:A:62:LEU:H | 1:A:65:LYS:HD2 | 17 | 0.16 |
| (1,4888) | 1:A:58:LYS:HG2 | 1:A:58:LYS:HE2 | 16 | 0.16 |
| (1,4882) | 1:A:56:THR:HG21 | 1:A:59:LEU:HB2 | 8 | 0.16 |
| (1,4882) | 1:A:56:THR:HG22 | 1:A:59:LEU:HB2 | 8 | 0.16 |
| (1,4882) | 1:A:56:THR:HG23 | 1:A:59:LEU:HB2 | 8 | 0.16 |
| (1,4861) | 1:A:53:VAL:HG11 | 1:A:58:LYS:HE2 | 14 | 0.16 |
| (1,4861) | 1:A:53:VAL:HG12 | 1:A:58:LYS:HE2 | 14 | 0.16 |
| (1,4861) | 1:A:53:VAL:HG13 | 1:A:58:LYS:HE2 | 14 | 0.16 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 3 | 0.16 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 10 | 0.16 |
| (1,4806) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HD1 | 7 | 0.16 |
| (1,4806) | 1:A:34:ARG:HG2 | 1:A:52:PHE:HD2 | 7 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4773) | 1:A:28:LYS:HA | 1:A:28:LYS:HD2 | 6 | 0.16 |
| (1,4773) | 1:A:28:LYS:HA | 1:A:28:LYS:HD2 | 15 | 0.16 |
| (1,4766) | 1:A:27:SER:HB2 | 1:B:24:GLY:H | 7 | 0.16 |
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 14 | 0.16 |
| (1,4690) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD21 | 19 | 0.16 |
| (1,4690) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD21 | 19 | 0.16 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 6 | 0.16 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 8 | 0.16 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 4 | 0.16 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 9 | 0.16 |
| (1,4628) | 1:A:3:ASP:HB2 | 1:A:4:PHE:H | 2 | 0.16 |
| (1,3937) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HB3 | 4 | 0.16 |
| (1,3937) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HB3 | 14 | 0.16 |
| (1,3936) | 1:A:7:GLY:HA2 | 1:A:78:LEU:HB3 | 2 | 0.16 |
| (1,3503) | 1:A:60:THR:HG21 | 1:A:63:MET:HE1 | 2 | 0.16 |
| (1,3503) | 1:A:60:THR:HG21 | 1:A:63:MET:HE2 | 2 | 0.16 |
| (1,3503) | 1:A:60:THR:HG21 | 1:A:63:MET:HE3 | 2 | 0.16 |
| (1,3503) | 1:A:60:THR:HG22 | 1:A:63:MET:HE1 | 2 | 0.16 |
| (1,3503) | 1:A:60:THR:HG22 | 1:A:63:MET:HE2 | 2 | 0.16 |
| (1,3503) | 1:A:60:THR:HG22 | 1:A:63:MET:HE3 | 2 | 0.16 |
| (1,3503) | 1:A:60:THR:HG23 | 1:A:63:MET:HE1 | 2 | 0.16 |
| (1,3503) | 1:A:60:THR:HG23 | 1:A:63:MET:HE2 | 2 | 0.16 |
| (1,3503) | 1:A:60:THR:HG23 | 1:A:63:MET:HE3 | 2 | 0.16 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 19 | 0.16 |
| (1,3197) | 1:B:54:LYS:H | 1:B:54:LYS:HE2 | 12 | 0.16 |
| (1,3197) | 1:B:54:LYS:H | 1:B:54:LYS:HE3 | 12 | 0.16 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD11 | 18 | 0.16 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD12 | 18 | 0.16 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD13 | 18 | 0.16 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD11 | 17 | 0.16 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD12 | 17 | 0.16 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD13 | 17 | 0.16 |
| (1,292) | 1:B:20:ASN:H | 1:B:20:ASN:HD22 | 12 | 0.16 |
| (1,2715) | 1:A:9:ARG:HE | 1:A:46:THR:HG21 | 5 | 0.16 |
| (1,2715) | 1:A:9:ARG:HE | 1:A:46:THR:HG22 | 5 | 0.16 |
| (1,2715) | 1:A:9:ARG:HE | 1:A:46:THR:HG23 | 5 | 0.16 |
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 9 | 0.16 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 9 | 0.16 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 9 | 0.16 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 7 | 0.16 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 7 | 0.16 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 7 | 0.16 |

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wwPDB NMR Structure Validation Summary Report

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 9 | 0.16 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD11 | 1 | 0.16 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD12 | 1 | 0.16 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD13 | 1 | 0.16 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD11 | 18 | 0.16 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD12 | 18 | 0.16 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD13 | 18 | 0.16 |
| (1,2264) | 1:B:28:LYS:HA | 1:B:28:LYS:HE2 | 12 | 0.16 |
| (1,2264) | 1:B:28:LYS:HA | 1:B:28:LYS:HE3 | 12 | 0.16 |
| (1,2253) | 1:A:27:SER:HG | 1:A:28:LYS:HG3 | 20 | 0.16 |
| (1,2033) | 1:A:22:ILE:HB | 1:A:45:PHE:HE1 | 12 | 0.16 |
| (1,1880) | 1:A:68:LYS:HE2 | 1:A:69:VAL:HG21 | 1 | 0.16 |
| (1,1880) | 1:A:68:LYS:HE2 | 1:A:69:VAL:HG22 | 1 | 0.16 |
| (1,1880) | 1:A:68:LYS:HE2 | 1:A:69:VAL:HG23 | 1 | 0.16 |
| (1,1880) | 1:A:68:LYS:HE3 | 1:A:69:VAL:HG21 | 1 | 0.16 |
| (1,1880) | 1:A:68:LYS:HE3 | 1:A:69:VAL:HG22 | 1 | 0.16 |
| (1,1880) | 1:A:68:LYS:HE3 | 1:A:69:VAL:HG23 | 1 | 0.16 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 4 | 0.16 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 4 | 0.16 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 4 | 0.16 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 4 | 0.16 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 4 | 0.16 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 4 | 0.16 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 4 | 0.16 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 4 | 0.16 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 4 | 0.16 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 2 | 0.16 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 16 | 0.16 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 17 | 0.16 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 18 | 0.16 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 13 | 0.15 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 12 | 0.15 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 14 | 0.15 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 20 | 0.15 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 5 | 0.15 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 19 | 0.15 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 3 | 0.15 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 4 | 0.15 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 17 | 0.15 |
| (1,5248) | 1:B:76:GLU:HB2 | 1:B:77:ARG:H | 14 | 0.15 |
| (1,5222) | 1:B:65:LYS:H | 1:B:65:LYS:HG2 | 10 | 0.15 |
| (1,5191) | 1:B:58:LYS:HG2 | 1:B:58:LYS:HE2 | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5185) | 1:B:56:THR:HG21 | 1:B:59:LEU:HB2 | 15 | 0.15 |
| (1,5185) | 1:B:56:THR:HG22 | 1:B:59:LEU:HB2 | 15 | 0.15 |
| (1,5185) | 1:B:56:THR:HG23 | 1:B:59:LEU:HB2 | 15 | 0.15 |
| (1,5185) | 1:B:56:THR:HG21 | 1:B:59:LEU:HB2 | 19 | 0.15 |
| (1,5185) | 1:B:56:THR:HG22 | 1:B:59:LEU:HB2 | 19 | 0.15 |
| (1,5185) | 1:B:56:THR:HG23 | 1:B:59:LEU:HB2 | 19 | 0.15 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 2 | 0.15 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD11 | 14 | 0.15 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD12 | 14 | 0.15 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD13 | 14 | 0.15 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 7 | 0.15 |
| (1,5123) | 1:B:37:VAL:HB | 1:B:48:ASN:HD21 | 17 | 0.15 |
| (1,5116) | 1:B:36:ILE:HG21 | 1:B:48:ASN:HB2 | 13 | 0.15 |
| (1,5116) | 1:B:36:ILE:HG22 | 1:B:48:ASN:HB2 | 13 | 0.15 |
| (1,5116) | 1:B:36:ILE:HG23 | 1:B:48:ASN:HB2 | 13 | 0.15 |
| (1,5111) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HD1 | 3 | 0.15 |
| (1,5111) | 1:B:34:ARG:HG2 | 1:B:52:PHE:HD2 | 3 | 0.15 |
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 9 | 0.15 |
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 9 | 0.15 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 9 | 0.15 |
| (1,5086) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HD2 | 12 | 0.15 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 12 | 0.15 |
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 8 | 0.15 |
| (1,5067) | 1:B:28:LYS:H | 1:B:28:LYS:HG2 | 14 | 0.15 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 13 | 0.15 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 16 | 0.15 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 18 | 0.15 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 17 | 0.15 |
| (1,5009) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD21 | 2 | 0.15 |
| (1,5009) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD21 | 2 | 0.15 |
| (1,5009) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD21 | 10 | 0.15 |
| (1,5009) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD21 | 10 | 0.15 |
| (1,5005) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HD21 | 20 | 0.15 |
| (1,5005) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HD21 | 20 | 0.15 |
| (1,5000) | 1:B:15:LYS:HA | 1:B:16:ASN:HB2 | 2 | 0.15 |
| (1,5000) | 1:B:15:LYS:HA | 1:B:16:ASN:HB2 | 6 | 0.15 |
| (1,4964) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HG2 | 18 | 0.15 |
| (1,4964) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HG2 | 18 | 0.15 |
| (1,4964) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HG2 | 18 | 0.15 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 13 | 0.15 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 16 | 0.15 |
| (1,4904) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HD2 | 12 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4904) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HD2 | 12 | 0.15 |
| (1,4904) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HD2 | 12 | 0.15 |
| (1,4882) | 1:A:56:THR:HG21 | 1:A:59:LEU:HB2 | 14 | 0.15 |
| (1,4882) | 1:A:56:THR:HG22 | 1:A:59:LEU:HB2 | 14 | 0.15 |
| (1,4882) | 1:A:56:THR:HG23 | 1:A:59:LEU:HB2 | 14 | 0.15 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 20 | 0.15 |
| (1,4812) | 1:A:36:ILE:HG21 | 1:A:48:ASN:HB2 | 17 | 0.15 |
| (1,4812) | 1:A:36:ILE:HG22 | 1:A:48:ASN:HB2 | 17 | 0.15 |
| (1,4812) | 1:A:36:ILE:HG23 | 1:A:48:ASN:HB2 | 17 | 0.15 |
| (1,4812) | 1:A:36:ILE:HG21 | 1:A:48:ASN:HB2 | 18 | 0.15 |
| (1,4812) | 1:A:36:ILE:HG22 | 1:A:48:ASN:HB2 | 18 | 0.15 |
| (1,4812) | 1:A:36:ILE:HG23 | 1:A:48:ASN:HB2 | 18 | 0.15 |
| (1,4795) | 1:A:32:ASN:HB2 | 1:B:20:ASN:H | 10 | 0.15 |
| (1,4787) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HD2 | 12 | 0.15 |
| (1,4773) | 1:A:28:LYS:HA | 1:A:28:LYS:HD2 | 11 | 0.15 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 2 | 0.15 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 3 | 0.15 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 4 | 0.15 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 9 | 0.15 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 10 | 0.15 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 17 | 0.15 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 20 | 0.15 |
| (1,4733) | 1:A:23:THR:HG21 | 1:A:27:SER:HB2 | 1 | 0.15 |
| (1,4733) | 1:A:23:THR:HG22 | 1:A:27:SER:HB2 | 1 | 0.15 |
| (1,4733) | 1:A:23:THR:HG23 | 1:A:27:SER:HB2 | 1 | 0.15 |
| (1,4733) | 1:A:23:THR:HG21 | 1:A:27:SER:HB2 | 3 | 0.15 |
| (1,4733) | 1:A:23:THR:HG22 | 1:A:27:SER:HB2 | 3 | 0.15 |
| (1,4733) | 1:A:23:THR:HG23 | 1:A:27:SER:HB2 | 3 | 0.15 |
| (1,4733) | 1:A:23:THR:HG21 | 1:A:27:SER:HB2 | 13 | 0.15 |
| (1,4733) | 1:A:23:THR:HG22 | 1:A:27:SER:HB2 | 13 | 0.15 |
| (1,4733) | 1:A:23:THR:HG23 | 1:A:27:SER:HB2 | 13 | 0.15 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 12 | 0.15 |
| (1,4693) | 1:A:16:ASN:HA | 1:B:32:ASN:HD21 | 13 | 0.15 |
| (1,4687) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HD21 | 20 | 0.15 |
| (1,4687) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HD21 | 20 | 0.15 |
| (1,4665) | 1:A:13:GLU:HG2 | 1:A:15:LYS:HB2 | 14 | 0.15 |
| (1,4665) | 1:A:13:GLU:HG3 | 1:A:15:LYS:HB2 | 14 | 0.15 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 16 | 0.15 |
| (1,4627) | 1:A:3:ASP:HA | 1:A:54:LYS:HB2 | 9 | 0.15 |
| (1,4627) | 1:A:3:ASP:HA | 1:A:54:LYS:HB2 | 13 | 0.15 |
| (1,4620) | 1:B:82:GLU:HA | 1:B:83:HIS:HD2 | 5 | 0.15 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 11 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 11 | 0.15 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 11 | 0.15 |
| (1,4475) | 1:A:22:ILE:HD11 | 1:A:45:PHE:HE1 | 6 | 0.15 |
| (1,4475) | 1:A:22:ILE:HD12 | 1:A:45:PHE:HE1 | 6 | 0.15 |
| (1,4475) | 1:A:22:ILE:HD13 | 1:A:45:PHE:HE1 | 6 | 0.15 |
| (1,4475) | 1:A:22:ILE:HD11 | 1:A:45:PHE:HE1 | 16 | 0.15 |
| (1,4475) | 1:A:22:ILE:HD12 | 1:A:45:PHE:HE1 | 16 | 0.15 |
| (1,4475) | 1:A:22:ILE:HD13 | 1:A:45:PHE:HE1 | 16 | 0.15 |
| (1,4377) | 1:B:4:PHE:H | 1:B:4:PHE:HE1 | 7 | 0.15 |
| (1,4363) | 1:B:29:PHE:HE1 | 1:B:66:LEU:HG | 1 | 0.15 |
| (1,4243) | 1:B:15:LYS:HA | 1:B:17:GLY:H | 17 | 0.15 |
| (1,4198) | 1:A:82:GLU:H | 1:A:83:HIS:HB3 | 2 | 0.15 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 14 | 0.15 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 14 | 0.15 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 14 | 0.15 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 12 | 0.15 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 12 | 0.15 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 12 | 0.15 |
| (1,4082) | 1:A:82:GLU:HA | 1:A:82:GLU:HG3 | 2 | 0.15 |
| (1,4082) | 1:A:82:GLU:HA | 1:A:82:GLU:HG3 | 18 | 0.15 |
| (1,4079) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 11 | 0.15 |
| (1,4079) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 13 | 0.15 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 1 | 0.15 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 1 | 0.15 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 1 | 0.15 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG11 | 19 | 0.15 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG12 | 19 | 0.15 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG13 | 19 | 0.15 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG11 | 19 | 0.15 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG12 | 19 | 0.15 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG13 | 19 | 0.15 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB2 | 1 | 0.15 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB3 | 1 | 0.15 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 12 | 0.15 |
| (1,3194) | 1:A:54:LYS:HE2 | 1:A:55:ASN:HD21 | 20 | 0.15 |
| (1,3194) | 1:A:54:LYS:HE3 | 1:A:55:ASN:HD21 | 20 | 0.15 |
| (1,3190) | 1:A:54:LYS:H | 1:A:54:LYS:HD2 | 15 | 0.15 |
| (1,3190) | 1:A:54:LYS:H | 1:A:54:LYS:HD3 | 15 | 0.15 |
| (1,3095) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HZ1 | 18 | 0.15 |
| (1,3095) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HZ1 | 18 | 0.15 |
| (1,3095) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HZ1 | 18 | 0.15 |
| (1,292) | 1:B:20:ASN:H | 1:B:20:ASN:HD22 | 14 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 10 | 0.15 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 10 | 0.15 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 10 | 0.15 |
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 18 | 0.15 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 18 | 0.15 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 18 | 0.15 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 4 | 0.15 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 4 | 0.15 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 4 | 0.15 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 11 | 0.15 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 11 | 0.15 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 11 | 0.15 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 2 | 0.15 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 3 | 0.15 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 17 | 0.15 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 17 | 0.15 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD11 | 3 | 0.15 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD12 | 3 | 0.15 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD13 | 3 | 0.15 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD11 | 14 | 0.15 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD12 | 14 | 0.15 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD13 | 14 | 0.15 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 14 | 0.15 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 14 | 0.15 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 14 | 0.15 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 15 | 0.15 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 15 | 0.15 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 15 | 0.15 |
| (1,1802) | 1:A:13:GLU:HB3 | 1:A:71:GLY:HA3 | 1 | 0.15 |
| (1,1420) | 1:B:40:ALA:H | 1:B:41:LYS:HD2 | 13 | 0.15 |
| (1,1420) | 1:B:40:ALA:H | 1:B:41:LYS:HD3 | 13 | 0.15 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 20 | 0.15 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 17 | 0.14 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 19 | 0.14 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 8 | 0.14 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 9 | 0.14 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 18 | 0.14 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 20 | 0.14 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 10 | 0.14 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 14 | 0.14 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 17 | 0.14 |
| (1,5246) | 1:B:76:GLU:H | 1:B:76:GLU:HB2 | 15 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD11 | 13 | 0.14 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD12 | 13 | 0.14 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD13 | 13 | 0.14 |
| (1,5192) | 1:B:58:LYS:HE2 | 1:B:59:LEU:HA | 13 | 0.14 |
| (1,5182) | 1:B:55:ASN:HD21 | 1:B:58:LYS:HG3 | 12 | 0.14 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB2 | 14 | 0.14 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB3 | 14 | 0.14 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 12 | 0.14 |
| (1,5123) | 1:B:37:VAL:HB | 1:B:48:ASN:HD21 | 10 | 0.14 |
| (1,5087) | 1:B:29:PHE:HZ | 1:B:65:LYS:HG2 | 12 | 0.14 |
| (1,5086) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HD2 | 17 | 0.14 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD11 | 3 | 0.14 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD12 | 3 | 0.14 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD13 | 3 | 0.14 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD11 | 11 | 0.14 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD12 | 11 | 0.14 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD13 | 11 | 0.14 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 18 | 0.14 |
| (1,5071) | 1:B:28:LYS:HA | 1:B:28:LYS:HD2 | 3 | 0.14 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 4 | 0.14 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 20 | 0.14 |
| (1,5034) | 1:B:23:THR:HG21 | 1:B:27:SER:HB2 | 16 | 0.14 |
| (1,5034) | 1:B:23:THR:HG22 | 1:B:27:SER:HB2 | 16 | 0.14 |
| (1,5034) | 1:B:23:THR:HG23 | 1:B:27:SER:HB2 | 16 | 0.14 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 16 | 0.14 |
| (1,4868) | 1:A:54:LYS:HB2 | 1:A:55:ASN:HD21 | 20 | 0.14 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD11 | 12 | 0.14 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD12 | 12 | 0.14 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD13 | 12 | 0.14 |
| (1,4847) | 1:A:46:THR:HG21 | 1:A:48:ASN:HD21 | 1 | 0.14 |
| (1,4847) | 1:A:46:THR:HG22 | 1:A:48:ASN:HD21 | 1 | 0.14 |
| (1,4847) | 1:A:46:THR:HG23 | 1:A:48:ASN:HD21 | 1 | 0.14 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG21 | 10 | 0.14 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG22 | 10 | 0.14 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG23 | 10 | 0.14 |
| (1,4812) | 1:A:36:ILE:HG21 | 1:A:48:ASN:HB2 | 9 | 0.14 |
| (1,4812) | 1:A:36:ILE:HG22 | 1:A:48:ASN:HB2 | 9 | 0.14 |
| (1,4812) | 1:A:36:ILE:HG23 | 1:A:48:ASN:HB2 | 9 | 0.14 |
| (1,4803) | 1:A:34:ARG:HB2 | 1:A:51:ILE:H | 6 | 0.14 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 1 | 0.14 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 11 | 0.14 |
| (1,4728) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HG12 | 2 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4696) | 1:A:16:ASN:HB2 | 1:A:18:MET:H | 1 | 0.14 |
| (1,4691) | 1:A:15:LYS:HE2 | 1:A:16:ASN:HD21 | 8 | 0.14 |
| (1,4691) | 1:A:15:LYS:HE3 | 1:A:16:ASN:HD21 | 8 | 0.14 |
| (1,4671) | 1:A:14:ASP:HB2 | 1:A:43:GLY:H | 16 | 0.14 |
| (1,4661) | 1:A:9:ARG:HD2 | 1:A:48:ASN:HD21 | 6 | 0.14 |
| (1,4661) | 1:A:9:ARG:HD3 | 1:A:48:ASN:HD21 | 6 | 0.14 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 3 | 0.14 |
| (1,4633) | 1:A:4:PHE:H | 1:A:54:LYS:HB2 | 10 | 0.14 |
| (1,4495) | 1:A:12:GLY:H | 1:A:45:PHE:HE1 | 12 | 0.14 |
| (1,4475) | 1:A:22:ILE:HD11 | 1:A:45:PHE:HE1 | 10 | 0.14 |
| (1,4475) | 1:A:22:ILE:HD12 | 1:A:45:PHE:HE1 | 10 | 0.14 |
| (1,4475) | 1:A:22:ILE:HD13 | 1:A:45:PHE:HE1 | 10 | 0.14 |
| (1,4243) | 1:B:15:LYS:HA | 1:B:17:GLY:H | 6 | 0.14 |
| (1,4199) | 1:B:82:GLU:H | 1:B:83:HIS:HB3 | 14 | 0.14 |
| (1,4193) | 1:B:5:LEU:HB2 | 1:B:83:HIS:HB3 | 18 | 0.14 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 20 | 0.14 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 20 | 0.14 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 20 | 0.14 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 3 | 0.14 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 3 | 0.14 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 3 | 0.14 |
| (1,4106) | 1:B:15:LYS:HB3 | 1:B:18:MET:HB3 | 14 | 0.14 |
| (1,4079) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 6 | 0.14 |
| (1,4079) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 10 | 0.14 |
| (1,4078) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 5 | 0.14 |
| (1,4078) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 15 | 0.14 |
| (1,3937) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HB3 | 11 | 0.14 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 14 | 0.14 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 14 | 0.14 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 14 | 0.14 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 16 | 0.14 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 16 | 0.14 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 16 | 0.14 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 17 | 0.14 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 17 | 0.14 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 17 | 0.14 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 10 | 0.14 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 10 | 0.14 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 10 | 0.14 |
| (1,3755) | 1:A:69:VAL:H | 1:A:70:GLN:HB2 | 9 | 0.14 |
| (1,3755) | 1:A:69:VAL:H | 1:A:70:GLN:HB3 | 9 | 0.14 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 15 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 15 | 0.14 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 15 | 0.14 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE2 | 12 | 0.14 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE3 | 12 | 0.14 |
| (1,3617) | 1:B:65:LYS:HA | 1:B:65:LYS:HE2 | 15 | 0.14 |
| (1,3617) | 1:B:65:LYS:HA | 1:B:65:LYS:HE3 | 15 | 0.14 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE1 | 2 | 0.14 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE2 | 2 | 0.14 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE3 | 2 | 0.14 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE1 | 1 | 0.14 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE2 | 1 | 0.14 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE3 | 1 | 0.14 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE1 | 12 | 0.14 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE2 | 12 | 0.14 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE3 | 12 | 0.14 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 20 | 0.14 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 7 | 0.14 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 18 | 0.14 |
| (1,3191) | 1:B:54:LYS:H | 1:B:54:LYS:HD2 | 4 | 0.14 |
| (1,3191) | 1:B:54:LYS:H | 1:B:54:LYS:HD3 | 4 | 0.14 |
| (1,308) | 1:A:33:ILE:HG13 | 1:B:20:ASN:HD22 | 15 | 0.14 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD11 | 4 | 0.14 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD12 | 4 | 0.14 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD13 | 4 | 0.14 |
| (1,292) | 1:B:20:ASN:H | 1:B:20:ASN:HD22 | 11 | 0.14 |
| (1,291) | 1:A:20:ASN:H | 1:A:20:ASN:HD22 | 16 | 0.14 |
| (1,2765) | 1:A:9:ARG:HG2 | 1:A:48:ASN:HA | 9 | 0.14 |
| (1,2716) | 1:B:9:ARG:HE | 1:B:46:THR:HG21 | 19 | 0.14 |
| (1,2716) | 1:B:9:ARG:HE | 1:B:46:THR:HG22 | 19 | 0.14 |
| (1,2716) | 1:B:9:ARG:HE | 1:B:46:THR:HG23 | 19 | 0.14 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 3 | 0.14 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 3 | 0.14 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 3 | 0.14 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 13 | 0.14 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 13 | 0.14 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 13 | 0.14 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 17 | 0.14 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 17 | 0.14 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 17 | 0.14 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 18 | 0.14 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 18 | 0.14 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 18 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 20 | 0.14 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 5 | 0.14 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 8 | 0.14 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 8 | 0.14 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 8 | 0.14 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD11 | 7 | 0.14 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD12 | 7 | 0.14 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD13 | 7 | 0.14 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD11 | 2 | 0.14 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD12 | 2 | 0.14 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD13 | 2 | 0.14 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD11 | 12 | 0.14 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD12 | 12 | 0.14 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD13 | 12 | 0.14 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 13 | 0.14 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 13 | 0.14 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 13 | 0.14 |
| (1,2260) | 1:B:68:LYS:HA | 1:B:68:LYS:HD2 | 15 | 0.14 |
| (1,2034) | 1:B:22:ILE:HB | 1:B:45:PHE:HE1 | 9 | 0.14 |
| (1,2033) | 1:A:22:ILE:HB | 1:A:45:PHE:HE1 | 4 | 0.14 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 9 | 0.14 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 18 | 0.14 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 14 | 0.14 |
| (1,1875) | 1:B:11:VAL:HG21 | 1:B:41:LYS:HE2 | 15 | 0.14 |
| (1,1875) | 1:B:11:VAL:HG21 | 1:B:41:LYS:HE3 | 15 | 0.14 |
| (1,1875) | 1:B:11:VAL:HG22 | 1:B:41:LYS:HE2 | 15 | 0.14 |
| (1,1875) | 1:B:11:VAL:HG22 | 1:B:41:LYS:HE3 | 15 | 0.14 |
| (1,1875) | 1:B:11:VAL:HG23 | 1:B:41:LYS:HE2 | 15 | 0.14 |
| (1,1875) | 1:B:11:VAL:HG23 | 1:B:41:LYS:HE3 | 15 | 0.14 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG11 | 4 | 0.14 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG12 | 4 | 0.14 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG13 | 4 | 0.14 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG11 | 4 | 0.14 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG12 | 4 | 0.14 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG13 | 4 | 0.14 |
| (1,181) | 1:A:15:LYS:H | 1:A:18:MET:HG2 | 2 | 0.14 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 19 | 0.14 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 19 | 0.14 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 19 | 0.14 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 19 | 0.14 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 19 | 0.14 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 19 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 19 | 0.14 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 19 | 0.14 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 19 | 0.14 |
| (1,1419) | 1:A:40:ALA:H | 1:A:41:LYS:HD2 | 1 | 0.14 |
| (1,1419) | 1:A:40:ALA:H | 1:A:41:LYS:HD3 | 1 | 0.14 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 1 | 0.14 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 18 | 0.14 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 16 | 0.13 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 15 | 0.13 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 1 | 0.13 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 20 | 0.13 |
| (1,561) | 1:A:29:PHE:HD1 | 1:A:31:THR:H | 20 | 0.13 |
| (1,561) | 1:A:29:PHE:HD2 | 1:A:31:THR:H | 20 | 0.13 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 3 | 0.13 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 18 | 0.13 |
| (1,5246) | 1:B:76:GLU:H | 1:B:76:GLU:HB2 | 1 | 0.13 |
| (1,5222) | 1:B:65:LYS:H | 1:B:65:LYS:HG2 | 11 | 0.13 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD11 | 15 | 0.13 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD12 | 15 | 0.13 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD13 | 15 | 0.13 |
| (1,5123) | 1:B:37:VAL:HB | 1:B:48:ASN:HD21 | 19 | 0.13 |
| (1,5099) | 1:B:32:ASN:HD21 | 1:B:33:ILE:HB | 18 | 0.13 |
| (1,5086) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HD2 | 14 | 0.13 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 13 | 0.13 |
| (1,5067) | 1:B:28:LYS:H | 1:B:28:LYS:HG2 | 7 | 0.13 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE2 | 12 | 0.13 |
| (1,5042) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HE3 | 12 | 0.13 |
| (1,4968) | 1:B:8:ILE:H | 1:B:8:ILE:HG12 | 11 | 0.13 |
| (1,4968) | 1:B:8:ILE:H | 1:B:8:ILE:HG12 | 12 | 0.13 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 2 | 0.13 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG11 | 9 | 0.13 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG12 | 9 | 0.13 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG13 | 9 | 0.13 |
| (1,4910) | 1:A:64:ASP:HA | 1:A:67:ARG:HG2 | 3 | 0.13 |
| (1,4910) | 1:A:64:ASP:HA | 1:A:67:ARG:HG2 | 4 | 0.13 |
| (1,4902) | 1:A:62:LEU:H | 1:A:65:LYS:HD2 | 4 | 0.13 |
| (1,4882) | 1:A:56:THR:HG21 | 1:A:59:LEU:HB2 | 12 | 0.13 |
| (1,4882) | 1:A:56:THR:HG22 | 1:A:59:LEU:HB2 | 12 | 0.13 |
| (1,4882) | 1:A:56:THR:HG23 | 1:A:59:LEU:HB2 | 12 | 0.13 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 5 | 0.13 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 12 | 0.13 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 16 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4838) | 1:A:41:LYS:H | 1:A:45:PHE:HB2 | 5 | 0.13 |
| (1,4819) | 1:A:37:VAL:HB | 1:A:48:ASN:HD21 | 13 | 0.13 |
| (1,4812) | 1:A:36:ILE:HG21 | 1:A:48:ASN:HB2 | 8 | 0.13 |
| (1,4812) | 1:A:36:ILE:HG22 | 1:A:48:ASN:HB2 | 8 | 0.13 |
| (1,4812) | 1:A:36:ILE:HG23 | 1:A:48:ASN:HB2 | 8 | 0.13 |
| (1,4801) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG2 | 10 | 0.13 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 15 | 0.13 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 15 | 0.13 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 15 | 0.13 |
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 7 | 0.13 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 7 | 0.13 |
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 7 | 0.13 |
| (1,4777) | 1:A:28:LYS:HG2 | 1:A:28:LYS:HE2 | 20 | 0.13 |
| (1,4777) | 1:A:28:LYS:HG2 | 1:A:28:LYS:HE3 | 20 | 0.13 |
| (1,4773) | 1:A:28:LYS:HA | 1:A:28:LYS:HD2 | 10 | 0.13 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 7 | 0.13 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 8 | 0.13 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 15 | 0.13 |
| (1,4734) | 1:A:23:THR:HG21 | 1:B:27:SER:HB2 | 16 | 0.13 |
| (1,4734) | 1:A:23:THR:HG22 | 1:B:27:SER:HB2 | 16 | 0.13 |
| (1,4734) | 1:A:23:THR:HG23 | 1:B:27:SER:HB2 | 16 | 0.13 |
| (1,4726) | 1:A:20:ASN:HB2 | 1:B:33:ILE:HD11 | 19 | 0.13 |
| (1,4726) | 1:A:20:ASN:HB2 | 1:B:33:ILE:HD12 | 19 | 0.13 |
| (1,4726) | 1:A:20:ASN:HB2 | 1:B:33:ILE:HD13 | 19 | 0.13 |
| (1,4720) | 1:A:20:ASN:H | 1:B:32:ASN:HB2 | 10 | 0.13 |
| (1,4703) | 1:A:17:GLY:HA2 | 1:A:21:GLN:HE22 | 10 | 0.13 |
| (1,4633) | 1:A:4:PHE:H | 1:A:54:LYS:HB2 | 1 | 0.13 |
| (1,4629) | 1:A:3:ASP:HB2 | 1:A:52:PHE:HB2 | 18 | 0.13 |
| (1,4627) | 1:A:3:ASP:HA | 1:A:54:LYS:HB2 | 1 | 0.13 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 17 | 0.13 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 17 | 0.13 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 17 | 0.13 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 2 | 0.13 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 2 | 0.13 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 2 | 0.13 |
| (1,4574) | 1:B:44:ILE:HG12 | 1:B:73:PHE:HE1 | 8 | 0.13 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 16 | 0.13 |
| (1,4496) | 1:B:12:GLY:H | 1:B:45:PHE:HE1 | 6 | 0.13 |
| (1,4478) | 1:B:19:THR:HG21 | 1:B:45:PHE:HE1 | 13 | 0.13 |
| (1,4478) | 1:B:19:THR:HG22 | 1:B:45:PHE:HE1 | 13 | 0.13 |
| (1,4478) | 1:B:19:THR:HG23 | 1:B:45:PHE:HE1 | 13 | 0.13 |
| (1,4478) | 1:B:19:THR:HG21 | 1:B:45:PHE:HE1 | 14 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4478) | 1:B:19:THR:HG22 | 1:B:45:PHE:HE1 | 14 | 0.13 |
| (1,4478) | 1:B:19:THR:HG23 | 1:B:45:PHE:HE1 | 14 | 0.13 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 15 | 0.13 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 15 | 0.13 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 15 | 0.13 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 4 | 0.13 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 4 | 0.13 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 4 | 0.13 |
| (1,4259) | 1:B:41:LYS:HG2 | 1:B:42:ASP:HA | 14 | 0.13 |
| (1,4259) | 1:B:41:LYS:HG3 | 1:B:42:ASP:HA | 14 | 0.13 |
| (1,4199) | 1:B:82:GLU:H | 1:B:83:HIS:HB3 | 18 | 0.13 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 1 | 0.13 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 1 | 0.13 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 1 | 0.13 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 2 | 0.13 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 2 | 0.13 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 2 | 0.13 |
| (1,4078) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 4 | 0.13 |
| (1,4078) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 9 | 0.13 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD21 | 6 | 0.13 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD22 | 6 | 0.13 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD23 | 6 | 0.13 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 10 | 0.13 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 10 | 0.13 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 10 | 0.13 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 5 | 0.13 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 5 | 0.13 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 5 | 0.13 |
| (1,3768) | 1:B:69:VAL:HA | 1:B:70:GLN:HG2 | 13 | 0.13 |
| (1,3768) | 1:B:69:VAL:HA | 1:B:70:GLN:HG3 | 13 | 0.13 |
| (1,3767) | 1:A:69:VAL:HA | 1:A:70:GLN:HG2 | 7 | 0.13 |
| (1,3767) | 1:A:69:VAL:HA | 1:A:70:GLN:HG3 | 7 | 0.13 |
| (1,3748) | 1:B:69:VAL:HG11 | 1:B:70:GLN:HB2 | 14 | 0.13 |
| (1,3748) | 1:B:69:VAL:HG11 | 1:B:70:GLN:HB3 | 14 | 0.13 |
| (1,3748) | 1:B:69:VAL:HG12 | 1:B:70:GLN:HB2 | 14 | 0.13 |
| (1,3748) | 1:B:69:VAL:HG12 | 1:B:70:GLN:HB3 | 14 | 0.13 |
| (1,3748) | 1:B:69:VAL:HG13 | 1:B:70:GLN:HB2 | 14 | 0.13 |
| (1,3748) | 1:B:69:VAL:HG13 | 1:B:70:GLN:HB3 | 14 | 0.13 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG21 | 6 | 0.13 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG22 | 6 | 0.13 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG23 | 6 | 0.13 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG11 | 17 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG12 | 17 | 0.13 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG13 | 17 | 0.13 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG11 | 17 | 0.13 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG12 | 17 | 0.13 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG13 | 17 | 0.13 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG11 | 20 | 0.13 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG12 | 20 | 0.13 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG13 | 20 | 0.13 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG11 | 20 | 0.13 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG12 | 20 | 0.13 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG13 | 20 | 0.13 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 7 | 0.13 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 7 | 0.13 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 7 | 0.13 |
| (1,3517) | 1:A:63:MET:HE1 | 1:A:77:ARG:HA | 4 | 0.13 |
| (1,3517) | 1:A:63:MET:HE2 | 1:A:77:ARG:HA | 4 | 0.13 |
| (1,3517) | 1:A:63:MET:HE3 | 1:A:77:ARG:HA | 4 | 0.13 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE1 | 10 | 0.13 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE2 | 10 | 0.13 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE3 | 10 | 0.13 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 14 | 0.13 |
| (1,3095) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HZ1 | 10 | 0.13 |
| (1,3095) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HZ1 | 10 | 0.13 |
| (1,3095) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HZ1 | 10 | 0.13 |
| (1,291) | 1:A:20:ASN:H | 1:A:20:ASN:HD22 | 7 | 0.13 |
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 20 | 0.13 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 20 | 0.13 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 20 | 0.13 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 5 | 0.13 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 7 | 0.13 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 9 | 0.13 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 11 | 0.13 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 12 | 0.13 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 13 | 0.13 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 15 | 0.13 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 4 | 0.13 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD11 | 20 | 0.13 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD12 | 20 | 0.13 |
| (1,2398) | 1:B:35:THR:HB | 1:B:36:ILE:HD13 | 20 | 0.13 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD11 | 10 | 0.13 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD12 | 10 | 0.13 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD13 | 10 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD11 | 20 | 0.13 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD12 | 20 | 0.13 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD13 | 20 | 0.13 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 7 | 0.13 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 7 | 0.13 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 7 | 0.13 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 15 | 0.13 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 15 | 0.13 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 15 | 0.13 |
| (1,2259) | 1:A:68:LYS:HA | 1:A:68:LYS:HD2 | 10 | 0.13 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 17 | 0.13 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 17 | 0.13 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 17 | 0.13 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 14 | 0.13 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 8 | 0.13 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 8 | 0.13 |
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 8 | 0.13 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 11 | 0.13 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 11 | 0.13 |
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 11 | 0.13 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 13 | 0.13 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 16 | 0.13 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 19 | 0.13 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 8 | 0.13 |
| (1,1881) | 1:B:68:LYS:HE2 | 1:B:69:VAL:HG21 | 1 | 0.13 |
| (1,1881) | 1:B:68:LYS:HE2 | 1:B:69:VAL:HG22 | 1 | 0.13 |
| (1,1881) | 1:B:68:LYS:HE2 | 1:B:69:VAL:HG23 | 1 | 0.13 |
| (1,1881) | 1:B:68:LYS:HE3 | 1:B:69:VAL:HG21 | 1 | 0.13 |
| (1,1881) | 1:B:68:LYS:HE3 | 1:B:69:VAL:HG22 | 1 | 0.13 |
| (1,1881) | 1:B:68:LYS:HE3 | 1:B:69:VAL:HG23 | 1 | 0.13 |
| (1,1778) | 1:A:11:VAL:HG11 | 1:A:73:PHE:HE1 | 4 | 0.13 |
| (1,1778) | 1:A:11:VAL:HG12 | 1:A:73:PHE:HE1 | 4 | 0.13 |
| (1,1778) | 1:A:11:VAL:HG13 | 1:A:73:PHE:HE1 | 4 | 0.13 |
| (1,1753) | 1:B:11:VAL:HG21 | 1:B:45:PHE:HE1 | 18 | 0.13 |
| (1,1753) | 1:B:11:VAL:HG22 | 1:B:45:PHE:HE1 | 18 | 0.13 |
| (1,1753) | 1:B:11:VAL:HG23 | 1:B:45:PHE:HE1 | 18 | 0.13 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 5 | 0.13 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 5 | 0.13 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 5 | 0.13 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 13 | 0.13 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 13 | 0.13 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 13 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 13 | 0.13 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 13 | 0.13 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 13 | 0.13 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 1 | 0.12 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 20 | 0.12 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 7 | 0.12 |
| (1,84) | 1:A:9:ARG:HE | 1:A:11:VAL:HG21 | 10 | 0.12 |
| (1,84) | 1:A:9:ARG:HE | 1:A:11:VAL:HG22 | 10 | 0.12 |
| (1,84) | 1:A:9:ARG:HE | 1:A:11:VAL:HG23 | 10 | 0.12 |
| (1,743) | 1:B:41:LYS:HB2 | 1:B:42:ASP:H | 13 | 0.12 |
| (1,743) | 1:B:41:LYS:HB3 | 1:B:42:ASP:H | 13 | 0.12 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 17 | 0.12 |
| (1,579) | 1:A:32:ASN:HD21 | 1:A:33:ILE:HB | 15 | 0.12 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 18 | 0.12 |
| (1,5226) | 1:B:65:LYS:HA | 1:B:68:LYS:HD2 | 20 | 0.12 |
| (1,5206) | 1:B:62:LEU:HA | 1:B:65:LYS:HG2 | 8 | 0.12 |
| (1,5201) | 1:B:59:LEU:HD21 | 1:B:77:ARG:HG2 | 16 | 0.12 |
| (1,5201) | 1:B:59:LEU:HD22 | 1:B:77:ARG:HG2 | 16 | 0.12 |
| (1,5201) | 1:B:59:LEU:HD23 | 1:B:77:ARG:HG2 | 16 | 0.12 |
| (1,5185) | 1:B:56:THR:HG21 | 1:B:59:LEU:HB2 | 10 | 0.12 |
| (1,5185) | 1:B:56:THR:HG22 | 1:B:59:LEU:HB2 | 10 | 0.12 |
| (1,5185) | 1:B:56:THR:HG23 | 1:B:59:LEU:HB2 | 10 | 0.12 |
| (1,5185) | 1:B:56:THR:HG21 | 1:B:59:LEU:HB2 | 12 | 0.12 |
| (1,5185) | 1:B:56:THR:HG22 | 1:B:59:LEU:HB2 | 12 | 0.12 |
| (1,5185) | 1:B:56:THR:HG23 | 1:B:59:LEU:HB2 | 12 | 0.12 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB2 | 13 | 0.12 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB3 | 13 | 0.12 |
| (1,5175) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HD21 | 17 | 0.12 |
| (1,5175) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HD21 | 17 | 0.12 |
| (1,5161) | 1:B:52:PHE:HB2 | 1:B:53:VAL:H | 4 | 0.12 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD11 | 5 | 0.12 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD12 | 5 | 0.12 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD13 | 5 | 0.12 |
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 10 | 0.12 |
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 14 | 0.12 |
| (1,5146) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG13 | 10 | 0.12 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB2 | 17 | 0.12 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB3 | 17 | 0.12 |
| (1,5067) | 1:B:28:LYS:H | 1:B:28:LYS:HG2 | 6 | 0.12 |
| (1,5056) | 1:B:26:ILE:HG12 | 1:B:27:SER:H | 6 | 0.12 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 8 | 0.12 |
| (1,5034) | 1:B:23:THR:HG21 | 1:B:27:SER:HB2 | 5 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5034) | 1:B:23:THR:HG22 | 1:B:27:SER:HB2 | 5 | 0.12 |
| (1,5034) | 1:B:23:THR:HG23 | 1:B:27:SER:HB2 | 5 | 0.12 |
| (1,5034) | 1:B:23:THR:HG21 | 1:B:27:SER:HB2 | 17 | 0.12 |
| (1,5034) | 1:B:23:THR:HG22 | 1:B:27:SER:HB2 | 17 | 0.12 |
| (1,5034) | 1:B:23:THR:HG23 | 1:B:27:SER:HB2 | 17 | 0.12 |
| (1,5029) | 1:B:20:ASN:HB2 | 1:B:21:GLN:HE21 | 9 | 0.12 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 9 | 0.12 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 17 | 0.12 |
| (1,5013) | 1:B:16:ASN:HB2 | 1:B:18:MET:H | 9 | 0.12 |
| (1,5009) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD21 | 4 | 0.12 |
| (1,5009) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD21 | 4 | 0.12 |
| (1,5008) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD21 | 16 | 0.12 |
| (1,5008) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD21 | 16 | 0.12 |
| (1,4968) | 1:B:8:ILE:H | 1:B:8:ILE:HG12 | 2 | 0.12 |
| (1,4968) | 1:B:8:ILE:H | 1:B:8:ILE:HG12 | 18 | 0.12 |
| (1,4948) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HA | 10 | 0.12 |
| (1,4948) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HA | 16 | 0.12 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 18 | 0.12 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 8 | 0.12 |
| (1,4934) | 1:A:76:GLU:HA | 1:A:77:ARG:HB2 | 10 | 0.12 |
| (1,4910) | 1:A:64:ASP:HA | 1:A:67:ARG:HG2 | 14 | 0.12 |
| (1,4910) | 1:A:64:ASP:HA | 1:A:67:ARG:HG2 | 20 | 0.12 |
| (1,4882) | 1:A:56:THR:HG21 | 1:A:59:LEU:HB2 | 5 | 0.12 |
| (1,4882) | 1:A:56:THR:HG22 | 1:A:59:LEU:HB2 | 5 | 0.12 |
| (1,4882) | 1:A:56:THR:HG23 | 1:A:59:LEU:HB2 | 5 | 0.12 |
| (1,4843) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG13 | 1 | 0.12 |
| (1,4812) | 1:A:36:ILE:HG21 | 1:A:48:ASN:HB2 | 6 | 0.12 |
| (1,4812) | 1:A:36:ILE:HG22 | 1:A:48:ASN:HB2 | 6 | 0.12 |
| (1,4812) | 1:A:36:ILE:HG23 | 1:A:48:ASN:HB2 | 6 | 0.12 |
| (1,4778) | 1:A:28:LYS:HG2 | 1:A:29:PHE:H | 4 | 0.12 |
| (1,4778) | 1:A:28:LYS:HG2 | 1:A:29:PHE:H | 5 | 0.12 |
| (1,4777) | 1:A:28:LYS:HG2 | 1:A:28:LYS:HE2 | 2 | 0.12 |
| (1,4777) | 1:A:28:LYS:HG2 | 1:A:28:LYS:HE3 | 2 | 0.12 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG21 | 5 | 0.12 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG22 | 5 | 0.12 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG23 | 5 | 0.12 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 5 | 0.12 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 6 | 0.12 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 12 | 0.12 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 16 | 0.12 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 18 | 0.12 |
| (1,4705) | 1:A:18:MET:H | 1:B:32:ASN:HD21 | 2 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4687) | 1:A:15:LYS:HG2 | 1:A:16:ASN:HD21 | 14 | 0.12 |
| (1,4687) | 1:A:15:LYS:HG3 | 1:A:16:ASN:HD21 | 14 | 0.12 |
| (1,4679) | 1:A:15:LYS:HA | 1:A:16:ASN:HB2 | 1 | 0.12 |
| (1,4671) | 1:A:14:ASP:HB2 | 1:A:43:GLY:H | 20 | 0.12 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 19 | 0.12 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 20 | 0.12 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 15 | 0.12 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 15 | 0.12 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 15 | 0.12 |
| (1,4574) | 1:B:44:ILE:HG12 | 1:B:73:PHE:HE1 | 5 | 0.12 |
| (1,4574) | 1:B:44:ILE:HG12 | 1:B:73:PHE:HE1 | 19 | 0.12 |
| (1,4562) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HE2 | 6 | 0.12 |
| (1,4562) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HE3 | 6 | 0.12 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 20 | 0.12 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 20 | 0.12 |
| (1,4495) | 1:A:12:GLY:H | 1:A:45:PHE:HE1 | 20 | 0.12 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 15 | 0.12 |
| (1,4477) | 1:A:19:THR:HG21 | 1:A:45:PHE:HE1 | 7 | 0.12 |
| (1,4477) | 1:A:19:THR:HG22 | 1:A:45:PHE:HE1 | 7 | 0.12 |
| (1,4477) | 1:A:19:THR:HG23 | 1:A:45:PHE:HE1 | 7 | 0.12 |
| (1,4477) | 1:A:19:THR:HG21 | 1:A:45:PHE:HE1 | 10 | 0.12 |
| (1,4477) | 1:A:19:THR:HG22 | 1:A:45:PHE:HE1 | 10 | 0.12 |
| (1,4477) | 1:A:19:THR:HG23 | 1:A:45:PHE:HE1 | 10 | 0.12 |
| (1,4475) | 1:A:22:ILE:HD11 | 1:A:45:PHE:HE1 | 8 | 0.12 |
| (1,4475) | 1:A:22:ILE:HD12 | 1:A:45:PHE:HE1 | 8 | 0.12 |
| (1,4475) | 1:A:22:ILE:HD13 | 1:A:45:PHE:HE1 | 8 | 0.12 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 1 | 0.12 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 1 | 0.12 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 1 | 0.12 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 11 | 0.12 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 11 | 0.12 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 11 | 0.12 |
| (1,4366) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HA | 1 | 0.12 |
| (1,4363) | 1:B:29:PHE:HE1 | 1:B:66:LEU:HG | 9 | 0.12 |
| (1,4333) | 1:B:83:HIS:HA | 1:B:83:HIS:HB3 | 5 | 0.12 |
| (1,4199) | 1:B:82:GLU:H | 1:B:83:HIS:HB3 | 20 | 0.12 |
| (1,4198) | 1:A:82:GLU:H | 1:A:83:HIS:HB3 | 17 | 0.12 |
| (1,4193) | 1:B:5:LEU:HB2 | 1:B:83:HIS:HB3 | 16 | 0.12 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 11 | 0.12 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 11 | 0.12 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 11 | 0.12 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 4 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 4 | 0.12 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 4 | 0.12 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 7 | 0.12 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 7 | 0.12 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 7 | 0.12 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 11 | 0.12 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 11 | 0.12 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 11 | 0.12 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 14 | 0.12 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 14 | 0.12 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 14 | 0.12 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 9 | 0.12 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 9 | 0.12 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 9 | 0.12 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 11 | 0.12 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 11 | 0.12 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 11 | 0.12 |
| (1,4083) | 1:B:82:GLU:HA | 1:B:82:GLU:HG3 | 7 | 0.12 |
| (1,4082) | 1:A:82:GLU:HA | 1:A:82:GLU:HG3 | 14 | 0.12 |
| (1,3936) | 1:A:7:GLY:HA2 | 1:A:78:LEU:HB3 | 20 | 0.12 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 6 | 0.12 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 6 | 0.12 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 6 | 0.12 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 7 | 0.12 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 7 | 0.12 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 7 | 0.12 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 9 | 0.12 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 9 | 0.12 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 9 | 0.12 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 18 | 0.12 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 18 | 0.12 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 18 | 0.12 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 12 | 0.12 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 12 | 0.12 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 12 | 0.12 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 20 | 0.12 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 20 | 0.12 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 20 | 0.12 |
| (1,3755) | 1:A:69:VAL:H | 1:A:70:GLN:HB2 | 11 | 0.12 |
| (1,3755) | 1:A:69:VAL:H | 1:A:70:GLN:HB3 | 11 | 0.12 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG11 | 4 | 0.12 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG12 | 4 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG13 | 4 | 0.12 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG11 | 4 | 0.12 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG12 | 4 | 0.12 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG13 | 4 | 0.12 |
| (1,3700) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD21 | 6 | 0.12 |
| (1,3700) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD21 | 6 | 0.12 |
| (1,3699) | 1:A:15:LYS:HE2 | 1:A:16:ASN:HD21 | 7 | 0.12 |
| (1,3699) | 1:A:15:LYS:HE3 | 1:A:16:ASN:HD21 | 7 | 0.12 |
| (1,3621) | 1:B:41:LYS:HE2 | 1:B:44:ILE:H | 9 | 0.12 |
| (1,3621) | 1:B:41:LYS:HE3 | 1:B:44:ILE:H | 9 | 0.12 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 17 | 0.12 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 17 | 0.12 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 17 | 0.12 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 4 | 0.12 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 4 | 0.12 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 4 | 0.12 |
| (1,3546) | 1:B:61:THR:HA | 1:B:64:ASP:HB3 | 3 | 0.12 |
| (1,3544) | 1:B:64:ASP:HB3 | 1:B:65:LYS:HB2 | 20 | 0.12 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE1 | 15 | 0.12 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE2 | 15 | 0.12 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE3 | 15 | 0.12 |
| (1,3220) | 1:A:4:PHE:HD1 | 1:A:56:THR:HG21 | 2 | 0.12 |
| (1,3220) | 1:A:4:PHE:HD1 | 1:A:56:THR:HG22 | 2 | 0.12 |
| (1,3220) | 1:A:4:PHE:HD1 | 1:A:56:THR:HG23 | 2 | 0.12 |
| (1,3220) | 1:A:4:PHE:HD2 | 1:A:56:THR:HG21 | 2 | 0.12 |
| (1,3220) | 1:A:4:PHE:HD2 | 1:A:56:THR:HG22 | 2 | 0.12 |
| (1,3220) | 1:A:4:PHE:HD2 | 1:A:56:THR:HG23 | 2 | 0.12 |
| (1,3189) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD21 | 13 | 0.12 |
| (1,3189) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD21 | 13 | 0.12 |
| (1,292) | 1:B:20:ASN:H | 1:B:20:ASN:HD22 | 4 | 0.12 |
| (1,292) | 1:B:20:ASN:H | 1:B:20:ASN:HD22 | 18 | 0.12 |
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 17 | 0.12 |
| (1,2715) | 1:A:9:ARG:HE | 1:A:46:THR:HG21 | 12 | 0.12 |
| (1,2715) | 1:A:9:ARG:HE | 1:A:46:THR:HG22 | 12 | 0.12 |
| (1,2715) | 1:A:9:ARG:HE | 1:A:46:THR:HG23 | 12 | 0.12 |
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 4 | 0.12 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 4 | 0.12 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 4 | 0.12 |
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 19 | 0.12 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 19 | 0.12 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 19 | 0.12 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 10 | 0.12 |

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wwPDB NMR Structure Validation Summary Report

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 15 | 0.12 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 19 | 0.12 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD11 | 4 | 0.12 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD12 | 4 | 0.12 |
| (1,2397) | 1:A:35:THR:HB | 1:A:36:ILE:HD13 | 4 | 0.12 |
| (1,2389) | 1:A:36:ILE:HG21 | 1:A:48:ASN:H | 18 | 0.12 |
| (1,2389) | 1:A:36:ILE:HG22 | 1:A:48:ASN:H | 18 | 0.12 |
| (1,2389) | 1:A:36:ILE:HG23 | 1:A:48:ASN:H | 18 | 0.12 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 10 | 0.12 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 10 | 0.12 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 10 | 0.12 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 5 | 0.12 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 5 | 0.12 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 5 | 0.12 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 7 | 0.12 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 7 | 0.12 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 7 | 0.12 |
| (1,2250) | 1:B:27:SER:HG | 1:B:28:LYS:HG2 | 5 | 0.12 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 3 | 0.12 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 18 | 0.12 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 19 | 0.12 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 4 | 0.12 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 20 | 0.12 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 4 | 0.12 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 4 | 0.12 |
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 4 | 0.12 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 9 | 0.12 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 9 | 0.12 |
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 9 | 0.12 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 1 | 0.12 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 5 | 0.12 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 15 | 0.12 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 9 | 0.12 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 13 | 0.12 |
| (1,1879) | 1:B:25:VAL:HG21 | 1:B:65:LYS:HE2 | 15 | 0.12 |
| (1,1879) | 1:B:25:VAL:HG21 | 1:B:65:LYS:HE3 | 15 | 0.12 |
| (1,1879) | 1:B:25:VAL:HG22 | 1:B:65:LYS:HE2 | 15 | 0.12 |
| (1,1879) | 1:B:25:VAL:HG22 | 1:B:65:LYS:HE3 | 15 | 0.12 |
| (1,1879) | 1:B:25:VAL:HG23 | 1:B:65:LYS:HE2 | 15 | 0.12 |
| (1,1879) | 1:B:25:VAL:HG23 | 1:B:65:LYS:HE3 | 15 | 0.12 |
| (1,1874) | 1:A:11:VAL:HG21 | 1:A:41:LYS:HE2 | 11 | 0.12 |
| (1,1874) | 1:A:11:VAL:HG21 | 1:A:41:LYS:HE3 | 11 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1874) | 1:A:11:VAL:HG22 | 1:A:41:LYS:HE2 | 11 | 0.12 |
| (1,1874) | 1:A:11:VAL:HG22 | 1:A:41:LYS:HE3 | 11 | 0.12 |
| (1,1874) | 1:A:11:VAL:HG23 | 1:A:41:LYS:HE2 | 11 | 0.12 |
| (1,1874) | 1:A:11:VAL:HG23 | 1:A:41:LYS:HE3 | 11 | 0.12 |
| (1,1803) | 1:B:13:GLU:HB3 | 1:B:71:GLY:HA3 | 2 | 0.12 |
| (1,1803) | 1:B:13:GLU:HB3 | 1:B:71:GLY:HA3 | 18 | 0.12 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 2 | 0.12 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 2 | 0.12 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 2 | 0.12 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 3 | 0.12 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 3 | 0.12 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 3 | 0.12 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 18 | 0.12 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 18 | 0.12 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 18 | 0.12 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 18 | 0.12 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 18 | 0.12 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 18 | 0.12 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 18 | 0.12 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 18 | 0.12 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 18 | 0.12 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 10 | 0.12 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 10 | 0.12 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 10 | 0.12 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 10 | 0.12 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 10 | 0.12 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 10 | 0.12 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 10 | 0.12 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 10 | 0.12 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 10 | 0.12 |
| (1,1474) | 1:B:5:LEU:HG | 1:B:52:PHE:HE1 | 12 | 0.12 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 8 | 0.12 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 14 | 0.12 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 8 | 0.11 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 1 | 0.11 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 5 | 0.11 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 13 | 0.11 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 3 | 0.11 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 4 | 0.11 |
| (1,734) | 1:A:41:LYS:H | 1:A:46:THR:H | 11 | 0.11 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 8 | 0.11 |
| (1,561) | 1:A:29:PHE:HD1 | 1:A:31:THR:H | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,561) | 1:A:29:PHE:HD2 | 1:A:31:THR:H | 3 | 0.11 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 16 | 0.11 |
| (1,5248) | 1:B:76:GLU:HB2 | 1:B:77:ARG:H | 8 | 0.11 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 7 | 0.11 |
| (1,5218) | 1:B:64:ASP:HA | 1:B:67:ARG:HG2 | 4 | 0.11 |
| (1,5171) | 1:B:54:LYS:HB2 | 1:B:55:ASN:HD21 | 11 | 0.11 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE1 | 4 | 0.11 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE2 | 4 | 0.11 |
| (1,5155) | 1:B:48:ASN:HD21 | 1:B:50:MET:HE3 | 4 | 0.11 |
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 11 | 0.11 |
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 18 | 0.11 |
| (1,5145) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG12 | 11 | 0.11 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB2 | 19 | 0.11 |
| (1,5135) | 1:B:39:ASN:HD21 | 1:B:41:LYS:HB3 | 19 | 0.11 |
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 8 | 0.11 |
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 8 | 0.11 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 8 | 0.11 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD11 | 8 | 0.11 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD12 | 8 | 0.11 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD13 | 8 | 0.11 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 1 | 0.11 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 1 | 0.11 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 1 | 0.11 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 6 | 0.11 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 10 | 0.11 |
| (1,5034) | 1:B:23:THR:HG21 | 1:B:27:SER:HB2 | 7 | 0.11 |
| (1,5034) | 1:B:23:THR:HG22 | 1:B:27:SER:HB2 | 7 | 0.11 |
| (1,5034) | 1:B:23:THR:HG23 | 1:B:27:SER:HB2 | 7 | 0.11 |
| (1,5006) | 1:B:15:LYS:HG2 | 1:B:18:MET:HG2 | 9 | 0.11 |
| (1,5006) | 1:B:15:LYS:HG3 | 1:B:18:MET:HG2 | 9 | 0.11 |
| (1,4996) | 1:B:14:ASP:HB2 | 1:B:44:ILE:HG21 | 17 | 0.11 |
| (1,4996) | 1:B:14:ASP:HB2 | 1:B:44:ILE:HG22 | 17 | 0.11 |
| (1,4996) | 1:B:14:ASP:HB2 | 1:B:44:ILE:HG23 | 17 | 0.11 |
| (1,4968) | 1:B:8:ILE:H | 1:B:8:ILE:HG12 | 10 | 0.11 |
| (1,4954) | 1:B:3:ASP:HB2 | 1:B:54:LYS:HA | 4 | 0.11 |
| (1,4912) | 1:A:65:LYS:H | 1:A:65:LYS:HD2 | 10 | 0.11 |
| (1,4898) | 1:A:59:LEU:HD21 | 1:A:77:ARG:HG2 | 1 | 0.11 |
| (1,4898) | 1:A:59:LEU:HD22 | 1:A:77:ARG:HG2 | 1 | 0.11 |
| (1,4898) | 1:A:59:LEU:HD23 | 1:A:77:ARG:HG2 | 1 | 0.11 |
| (1,4889) | 1:A:58:LYS:HE2 | 1:A:59:LEU:HA | 10 | 0.11 |
| (1,4888) | 1:A:58:LYS:HG2 | 1:A:58:LYS:HE2 | 1 | 0.11 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 1 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 2 | 0.11 |
| (1,4819) | 1:A:37:VAL:HB | 1:A:48:ASN:HD21 | 12 | 0.11 |
| (1,4778) | 1:A:28:LYS:HG2 | 1:A:29:PHE:H | 6 | 0.11 |
| (1,4778) | 1:A:28:LYS:HG2 | 1:A:29:PHE:H | 8 | 0.11 |
| (1,4746) | 1:A:25:VAL:H | 1:A:28:LYS:HD2 | 2 | 0.11 |
| (1,4727) | 1:A:20:ASN:HD21 | 1:B:33:ILE:HG12 | 8 | 0.11 |
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 18 | 0.11 |
| (1,4695) | 1:A:16:ASN:HB2 | 1:A:17:GLY:H | 11 | 0.11 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 12 | 0.11 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 20 | 0.11 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 20 | 0.11 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 20 | 0.11 |
| (1,4614) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HD2 | 6 | 0.11 |
| (1,4613) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HD2 | 15 | 0.11 |
| (1,4573) | 1:A:44:ILE:HG12 | 1:A:73:PHE:HE1 | 8 | 0.11 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 1 | 0.11 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 1 | 0.11 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 13 | 0.11 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 13 | 0.11 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 15 | 0.11 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 15 | 0.11 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 17 | 0.11 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 17 | 0.11 |
| (1,4417) | 1:B:29:PHE:HA | 1:B:29:PHE:HD1 | 4 | 0.11 |
| (1,4417) | 1:B:29:PHE:HA | 1:B:29:PHE:HD2 | 4 | 0.11 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 10 | 0.11 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 10 | 0.11 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 10 | 0.11 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 11 | 0.11 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 11 | 0.11 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 11 | 0.11 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 12 | 0.11 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 12 | 0.11 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 12 | 0.11 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 15 | 0.11 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 15 | 0.11 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 15 | 0.11 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 19 | 0.11 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 19 | 0.11 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 19 | 0.11 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 15 | 0.11 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 15 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 15 | 0.11 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 17 | 0.11 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 17 | 0.11 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 17 | 0.11 |
| (1,4363) | 1:B:29:PHE:HE1 | 1:B:66:LEU:HG | 10 | 0.11 |
| (1,4363) | 1:B:29:PHE:HE1 | 1:B:66:LEU:HG | 14 | 0.11 |
| (1,4279) | 1:B:60:THR:HB | 1:B:61:THR:H | 3 | 0.11 |
| (1,4259) | 1:B:41:LYS:HG2 | 1:B:42:ASP:HA | 1 | 0.11 |
| (1,4259) | 1:B:41:LYS:HG3 | 1:B:42:ASP:HA | 1 | 0.11 |
| (1,4243) | 1:B:15:LYS:HA | 1:B:17:GLY:H | 4 | 0.11 |
| (1,4243) | 1:B:15:LYS:HA | 1:B:17:GLY:H | 10 | 0.11 |
| (1,4242) | 1:A:15:LYS:HA | 1:A:17:GLY:H | 12 | 0.11 |
| (1,4217) | 1:B:8:ILE:HA | 1:B:78:LEU:HB2 | 8 | 0.11 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 10 | 0.11 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 10 | 0.11 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 10 | 0.11 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 20 | 0.11 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 20 | 0.11 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 20 | 0.11 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 6 | 0.11 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 6 | 0.11 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 6 | 0.11 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD21 | 15 | 0.11 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD22 | 15 | 0.11 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD23 | 15 | 0.11 |
| (1,3936) | 1:A:7:GLY:HA2 | 1:A:78:LEU:HB3 | 6 | 0.11 |
| (1,3936) | 1:A:7:GLY:HA2 | 1:A:78:LEU:HB3 | 18 | 0.11 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 20 | 0.11 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 20 | 0.11 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 20 | 0.11 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 2 | 0.11 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 2 | 0.11 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 2 | 0.11 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 15 | 0.11 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 15 | 0.11 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 15 | 0.11 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 19 | 0.11 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 19 | 0.11 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 19 | 0.11 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 1 | 0.11 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 1 | 0.11 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 1 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 2 | 0.11 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 2 | 0.11 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 2 | 0.11 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 3 | 0.11 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 3 | 0.11 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 3 | 0.11 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 8 | 0.11 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 8 | 0.11 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 8 | 0.11 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 18 | 0.11 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 18 | 0.11 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 18 | 0.11 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE2 | 15 | 0.11 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE3 | 15 | 0.11 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE2 | 7 | 0.11 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE3 | 7 | 0.11 |
| (1,3620) | 1:A:41:LYS:HE2 | 1:A:44:ILE:H | 1 | 0.11 |
| (1,3620) | 1:A:41:LYS:HE3 | 1:A:44:ILE:H | 1 | 0.11 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 20 | 0.11 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 20 | 0.11 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 20 | 0.11 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 15 | 0.11 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 15 | 0.11 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 15 | 0.11 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE1 | 19 | 0.11 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE2 | 19 | 0.11 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE3 | 19 | 0.11 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE1 | 16 | 0.11 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE2 | 16 | 0.11 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE3 | 16 | 0.11 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 6 | 0.11 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 17 | 0.11 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 19 | 0.11 |
| (1,3240) | 1:A:55:ASN:H | 1:A:58:LYS:HB2 | 6 | 0.11 |
| (1,3194) | 1:A:54:LYS:HE2 | 1:A:55:ASN:HD21 | 1 | 0.11 |
| (1,3194) | 1:A:54:LYS:HE3 | 1:A:55:ASN:HD21 | 1 | 0.11 |
| (1,3192) | 1:A:54:LYS:HA | 1:A:54:LYS:HE2 | 17 | 0.11 |
| (1,3192) | 1:A:54:LYS:HA | 1:A:54:LYS:HE3 | 17 | 0.11 |
| (1,3190) | 1:A:54:LYS:H | 1:A:54:LYS:HD2 | 18 | 0.11 |
| (1,3190) | 1:A:54:LYS:H | 1:A:54:LYS:HD3 | 18 | 0.11 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 15 | 0.11 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 15 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 15 | 0.11 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 15 | 0.11 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 15 | 0.11 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 15 | 0.11 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD11 | 12 | 0.11 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD12 | 12 | 0.11 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD13 | 12 | 0.11 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD11 | 1 | 0.11 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD12 | 1 | 0.11 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD13 | 1 | 0.11 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD11 | 15 | 0.11 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD12 | 15 | 0.11 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD13 | 15 | 0.11 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD11 | 16 | 0.11 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD12 | 16 | 0.11 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD13 | 16 | 0.11 |
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 1 | 0.11 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 1 | 0.11 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 1 | 0.11 |
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 15 | 0.11 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 15 | 0.11 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 15 | 0.11 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 8 | 0.11 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 8 | 0.11 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 8 | 0.11 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 12 | 0.11 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 12 | 0.11 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 12 | 0.11 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 4 | 0.11 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 18 | 0.11 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 3 | 0.11 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 6 | 0.11 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 16 | 0.11 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 18 | 0.11 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 7 | 0.11 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 7 | 0.11 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 7 | 0.11 |
| (1,2390) | 1:B:36:ILE:HG21 | 1:B:48:ASN:H | 4 | 0.11 |
| (1,2390) | 1:B:36:ILE:HG22 | 1:B:48:ASN:H | 4 | 0.11 |
| (1,2390) | 1:B:36:ILE:HG23 | 1:B:48:ASN:H | 4 | 0.11 |
| (1,2390) | 1:B:36:ILE:HG21 | 1:B:48:ASN:H | 5 | 0.11 |
| (1,2390) | 1:B:36:ILE:HG22 | 1:B:48:ASN:H | 5 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2390) | 1:B:36:ILE:HG23 | 1:B:48:ASN:H | 5 | 0.11 |
| (1,2390) | 1:B:36:ILE:HG21 | 1:B:48:ASN:H | 9 | 0.11 |
| (1,2390) | 1:B:36:ILE:HG22 | 1:B:48:ASN:H | 9 | 0.11 |
| (1,2390) | 1:B:36:ILE:HG23 | 1:B:48:ASN:H | 9 | 0.11 |
| (1,2390) | 1:B:36:ILE:HG21 | 1:B:48:ASN:H | 15 | 0.11 |
| (1,2390) | 1:B:36:ILE:HG22 | 1:B:48:ASN:H | 15 | 0.11 |
| (1,2390) | 1:B:36:ILE:HG23 | 1:B:48:ASN:H | 15 | 0.11 |
| (1,2390) | 1:B:36:ILE:HG21 | 1:B:48:ASN:H | 16 | 0.11 |
| (1,2390) | 1:B:36:ILE:HG22 | 1:B:48:ASN:H | 16 | 0.11 |
| (1,2390) | 1:B:36:ILE:HG23 | 1:B:48:ASN:H | 16 | 0.11 |
| (1,2389) | 1:A:36:ILE:HG21 | 1:A:48:ASN:H | 8 | 0.11 |
| (1,2389) | 1:A:36:ILE:HG22 | 1:A:48:ASN:H | 8 | 0.11 |
| (1,2389) | 1:A:36:ILE:HG23 | 1:A:48:ASN:H | 8 | 0.11 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 12 | 0.11 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 12 | 0.11 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 12 | 0.11 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 18 | 0.11 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 18 | 0.11 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 18 | 0.11 |
| (1,2370) | 1:A:36:ILE:HG21 | 1:B:39:ASN:HB2 | 10 | 0.11 |
| (1,2370) | 1:A:36:ILE:HG21 | 1:B:39:ASN:HB3 | 10 | 0.11 |
| (1,2370) | 1:A:36:ILE:HG22 | 1:B:39:ASN:HB2 | 10 | 0.11 |
| (1,2370) | 1:A:36:ILE:HG22 | 1:B:39:ASN:HB3 | 10 | 0.11 |
| (1,2370) | 1:A:36:ILE:HG23 | 1:B:39:ASN:HB2 | 10 | 0.11 |
| (1,2370) | 1:A:36:ILE:HG23 | 1:B:39:ASN:HB3 | 10 | 0.11 |
| (1,2259) | 1:A:68:LYS:HA | 1:A:68:LYS:HD2 | 6 | 0.11 |
| (1,2034) | 1:B:22:ILE:HB | 1:B:45:PHE:HE1 | 4 | 0.11 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 4 | 0.11 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 10 | 0.11 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 11 | 0.11 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 17 | 0.11 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 20 | 0.11 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 3 | 0.11 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 8 | 0.11 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 9 | 0.11 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 16 | 0.11 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 19 | 0.11 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 11 | 0.11 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 11 | 0.11 |
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 11 | 0.11 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 15 | 0.11 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 15 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 15 | 0.11 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 17 | 0.11 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 17 | 0.11 |
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 17 | 0.11 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 19 | 0.11 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 19 | 0.11 |
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 19 | 0.11 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 4 | 0.11 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 4 | 0.11 |
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 4 | 0.11 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 12 | 0.11 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 12 | 0.11 |
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 12 | 0.11 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 13 | 0.11 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 13 | 0.11 |
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 13 | 0.11 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 15 | 0.11 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 15 | 0.11 |
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 15 | 0.11 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 19 | 0.11 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 19 | 0.11 |
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 19 | 0.11 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 8 | 0.11 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 12 | 0.11 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 1 | 0.11 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 5 | 0.11 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 7 | 0.11 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 12 | 0.11 |
| (1,1881) | 1:B:68:LYS:HE2 | 1:B:69:VAL:HG21 | 20 | 0.11 |
| (1,1881) | 1:B:68:LYS:HE2 | 1:B:69:VAL:HG22 | 20 | 0.11 |
| (1,1881) | 1:B:68:LYS:HE2 | 1:B:69:VAL:HG23 | 20 | 0.11 |
| (1,1881) | 1:B:68:LYS:HE3 | 1:B:69:VAL:HG21 | 20 | 0.11 |
| (1,1881) | 1:B:68:LYS:HE3 | 1:B:69:VAL:HG22 | 20 | 0.11 |
| (1,1881) | 1:B:68:LYS:HE3 | 1:B:69:VAL:HG23 | 20 | 0.11 |
| (1,1859) | 1:B:14:ASP:HA | 1:B:15:LYS:HB3 | 8 | 0.11 |
| (1,181) | 1:A:15:LYS:H | 1:A:18:MET:HG2 | 15 | 0.11 |
| (1,1803) | 1:B:13:GLU:HB3 | 1:B:71:GLY:HA3 | 6 | 0.11 |
| (1,1778) | 1:A:11:VAL:HG11 | 1:A:73:PHE:HE1 | 13 | 0.11 |
| (1,1778) | 1:A:11:VAL:HG12 | 1:A:73:PHE:HE1 | 13 | 0.11 |
| (1,1778) | 1:A:11:VAL:HG13 | 1:A:73:PHE:HE1 | 13 | 0.11 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 7 | 0.11 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 7 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 7 | 0.11 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 10 | 0.11 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 10 | 0.11 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 10 | 0.11 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 1 | 0.11 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 1 | 0.11 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 1 | 0.11 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 8 | 0.11 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 8 | 0.11 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 8 | 0.11 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 18 | 0.11 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 18 | 0.11 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 18 | 0.11 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 15 | 0.11 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 15 | 0.11 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 15 | 0.11 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 15 | 0.11 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 15 | 0.11 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 15 | 0.11 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 15 | 0.11 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 15 | 0.11 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 15 | 0.11 |
| (1,1455) | 1:A:3:ASP:HB2 | 1:A:53:VAL:H | 1 | 0.11 |
| (1,1356) | 1:B:77:ARG:HG2 | 1:B:78:LEU:H | 8 | 0.11 |
| (1,1038) | 1:A:58:LYS:HZ1 | 1:A:61:THR:H | 12 | 0.11 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 10 | 0.1 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 12 | 0.1 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 9 | 0.1 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 16 | 0.1 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 19 | 0.1 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 1 | 0.1 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD1 | 18 | 0.1 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD2 | 18 | 0.1 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 6 | 0.1 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 11 | 0.1 |
| (1,562) | 1:B:29:PHE:HD1 | 1:B:31:THR:H | 15 | 0.1 |
| (1,562) | 1:B:29:PHE:HD2 | 1:B:31:THR:H | 15 | 0.1 |
| (1,5185) | 1:B:56:THR:HG21 | 1:B:59:LEU:HB2 | 9 | 0.1 |
| (1,5185) | 1:B:56:THR:HG22 | 1:B:59:LEU:HB2 | 9 | 0.1 |
| (1,5185) | 1:B:56:THR:HG23 | 1:B:59:LEU:HB2 | 9 | 0.1 |
| (1,5182) | 1:B:55:ASN:HD21 | 1:B:58:LYS:HG3 | 13 | 0.1 |
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 2 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 5 | 0.1 |
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 20 | 0.1 |
| (1,5140) | 1:B:39:ASN:HD21 | 1:B:48:ASN:HD21 | 11 | 0.1 |
| (1,5099) | 1:B:32:ASN:HD21 | 1:B:33:ILE:HB | 7 | 0.1 |
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 12 | 0.1 |
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 12 | 0.1 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 12 | 0.1 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 16 | 0.1 |
| (1,5075) | 1:B:28:LYS:HG2 | 1:B:28:LYS:HE2 | 9 | 0.1 |
| (1,5075) | 1:B:28:LYS:HG2 | 1:B:28:LYS:HE3 | 9 | 0.1 |
| (1,5061) | 1:B:27:SER:H | 1:B:33:ILE:HG12 | 10 | 0.1 |
| (1,5051) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HD2 | 15 | 0.1 |
| (1,5051) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HD2 | 15 | 0.1 |
| (1,5051) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HD2 | 15 | 0.1 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 19 | 0.1 |
| (1,5029) | 1:B:20:ASN:HB2 | 1:B:21:GLN:HE21 | 6 | 0.1 |
| (1,5029) | 1:B:20:ASN:HB2 | 1:B:21:GLN:HE21 | 10 | 0.1 |
| (1,5028) | 1:B:20:ASN:HB2 | 1:B:21:GLN:H | 13 | 0.1 |
| (1,5009) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD21 | 7 | 0.1 |
| (1,5009) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD21 | 7 | 0.1 |
| (1,4968) | 1:B:8:ILE:H | 1:B:8:ILE:HG12 | 14 | 0.1 |
| (1,4950) | 1:B:3:ASP:HA | 1:B:54:LYS:HB2 | 9 | 0.1 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 1 | 0.1 |
| (1,4946) | 1:A:82:GLU:H | 1:A:82:GLU:HG2 | 4 | 0.1 |
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 16 | 0.1 |
| (1,4898) | 1:A:59:LEU:HD21 | 1:A:77:ARG:HG2 | 7 | 0.1 |
| (1,4898) | 1:A:59:LEU:HD22 | 1:A:77:ARG:HG2 | 7 | 0.1 |
| (1,4898) | 1:A:59:LEU:HD23 | 1:A:77:ARG:HG2 | 7 | 0.1 |
| (1,4871) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HB2 | 12 | 0.1 |
| (1,4871) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HB2 | 12 | 0.1 |
| (1,4862) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HB2 | 4 | 0.1 |
| (1,4862) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HB2 | 4 | 0.1 |
| (1,4862) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HB2 | 4 | 0.1 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 13 | 0.1 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 15 | 0.1 |
| (1,4834) | 1:A:39:ASN:HD21 | 1:A:46:THR:HB | 2 | 0.1 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD2 | 10 | 0.1 |
| (1,4832) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HD3 | 10 | 0.1 |
| (1,4802) | 1:A:34:ARG:HB2 | 1:A:50:MET:HG3 | 6 | 0.1 |
| (1,4797) | 1:A:33:ILE:HD11 | 1:B:20:ASN:HB2 | 20 | 0.1 |
| (1,4797) | 1:A:33:ILE:HD12 | 1:B:20:ASN:HB2 | 20 | 0.1 |
| (1,4797) | 1:A:33:ILE:HD13 | 1:B:20:ASN:HB2 | 20 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4795) | 1:A:32:ASN:HB2 | 1:B:20:ASN:H | 8 | 0.1 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 5 | 0.1 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 5 | 0.1 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD11 | 1 | 0.1 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD12 | 1 | 0.1 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD13 | 1 | 0.1 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD11 | 9 | 0.1 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD12 | 9 | 0.1 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD13 | 9 | 0.1 |
| (1,4778) | 1:A:28:LYS:HG2 | 1:A:29:PHE:H | 7 | 0.1 |
| (1,4778) | 1:A:28:LYS:HG2 | 1:A:29:PHE:H | 9 | 0.1 |
| (1,4733) | 1:A:23:THR:HG21 | 1:A:27:SER:HB2 | 18 | 0.1 |
| (1,4733) | 1:A:23:THR:HG22 | 1:A:27:SER:HB2 | 18 | 0.1 |
| (1,4733) | 1:A:23:THR:HG23 | 1:A:27:SER:HB2 | 18 | 0.1 |
| (1,4724) | 1:A:20:ASN:HB2 | 1:A:21:GLN:HE21 | 6 | 0.1 |
| (1,4710) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG12 | 8 | 0.1 |
| (1,4703) | 1:A:17:GLY:HA2 | 1:A:21:GLN:HE22 | 1 | 0.1 |
| (1,4702) | 1:A:17:GLY:HA2 | 1:A:21:GLN:HE21 | 2 | 0.1 |
| (1,4695) | 1:A:16:ASN:HB2 | 1:A:17:GLY:H | 2 | 0.1 |
| (1,4690) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD21 | 12 | 0.1 |
| (1,4690) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD21 | 12 | 0.1 |
| (1,4678) | 1:A:15:LYS:H | 1:A:18:MET:HG2 | 7 | 0.1 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 4 | 0.1 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 5 | 0.1 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 11 | 0.1 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 17 | 0.1 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 5 | 0.1 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 5 | 0.1 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 5 | 0.1 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 11 | 0.1 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 11 | 0.1 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 11 | 0.1 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 14 | 0.1 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 14 | 0.1 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 14 | 0.1 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 18 | 0.1 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 18 | 0.1 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 18 | 0.1 |
| (1,4613) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HD2 | 5 | 0.1 |
| (1,4612) | 1:B:50:MET:HE1 | 1:B:83:HIS:HD2 | 17 | 0.1 |
| (1,4612) | 1:B:50:MET:HE2 | 1:B:83:HIS:HD2 | 17 | 0.1 |
| (1,4612) | 1:B:50:MET:HE3 | 1:B:83:HIS:HD2 | 17 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4574) | 1:B:44:ILE:HG12 | 1:B:73:PHE:HE1 | 20 | 0.1 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 8 | 0.1 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 4 | 0.1 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 4 | 0.1 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 6 | 0.1 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 6 | 0.1 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 8 | 0.1 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 8 | 0.1 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 10 | 0.1 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 10 | 0.1 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 2 | 0.1 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 2 | 0.1 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 3 | 0.1 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 3 | 0.1 |
| (1,4496) | 1:B:12:GLY:H | 1:B:45:PHE:HE1 | 11 | 0.1 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 12 | 0.1 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 12 | 0.1 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 12 | 0.1 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 14 | 0.1 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 14 | 0.1 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 14 | 0.1 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 19 | 0.1 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 19 | 0.1 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 19 | 0.1 |
| (1,4413) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 4 | 0.1 |
| (1,4413) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 4 | 0.1 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 1 | 0.1 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 1 | 0.1 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 1 | 0.1 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 4 | 0.1 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 4 | 0.1 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 4 | 0.1 |
| (1,4362) | 1:A:29:PHE:HE1 | 1:A:66:LEU:HG | 8 | 0.1 |
| (1,4324) | 1:A:80:ASN:HA | 1:A:81:LEU:HG | 3 | 0.1 |
| (1,4278) | 1:A:60:THR:HB | 1:A:61:THR:H | 2 | 0.1 |
| (1,4259) | 1:B:41:LYS:HG2 | 1:B:42:ASP:HA | 18 | 0.1 |
| (1,4259) | 1:B:41:LYS:HG3 | 1:B:42:ASP:HA | 18 | 0.1 |
| (1,4258) | 1:A:41:LYS:HG2 | 1:A:42:ASP:HA | 9 | 0.1 |
| (1,4258) | 1:A:41:LYS:HG3 | 1:A:42:ASP:HA | 9 | 0.1 |
| (1,4243) | 1:B:15:LYS:HA | 1:B:17:GLY:H | 7 | 0.1 |
| (1,4243) | 1:B:15:LYS:HA | 1:B:17:GLY:H | 14 | 0.1 |
| (1,4198) | 1:A:82:GLU:H | 1:A:83:HIS:HB3 | 14 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4193) | 1:B:5:LEU:HB2 | 1:B:83:HIS:HB3 | 8 | 0.1 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 6 | 0.1 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 6 | 0.1 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 6 | 0.1 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 7 | 0.1 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 7 | 0.1 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 7 | 0.1 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 9 | 0.1 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 9 | 0.1 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 9 | 0.1 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 16 | 0.1 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 16 | 0.1 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 16 | 0.1 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 3 | 0.1 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 3 | 0.1 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 3 | 0.1 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 13 | 0.1 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 13 | 0.1 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 13 | 0.1 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 6 | 0.1 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 6 | 0.1 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 6 | 0.1 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 8 | 0.1 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 8 | 0.1 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 8 | 0.1 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 15 | 0.1 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 15 | 0.1 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 15 | 0.1 |
| (1,4106) | 1:B:15:LYS:HB3 | 1:B:18:MET:HB3 | 7 | 0.1 |
| (1,4074) | 1:A:82:GLU:HA | 1:A:83:HIS:HB2 | 14 | 0.1 |
| (1,4016) | 1:A:78:LEU:H | 1:A:79:SER:HB2 | 7 | 0.1 |
| (1,4016) | 1:A:78:LEU:H | 1:A:79:SER:HB3 | 7 | 0.1 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD11 | 3 | 0.1 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD12 | 3 | 0.1 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD13 | 3 | 0.1 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 7 | 0.1 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 7 | 0.1 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 7 | 0.1 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 11 | 0.1 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 11 | 0.1 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 11 | 0.1 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 19 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 19 | 0.1 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 19 | 0.1 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 4 | 0.1 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 4 | 0.1 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 4 | 0.1 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 19 | 0.1 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 19 | 0.1 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 19 | 0.1 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 20 | 0.1 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 20 | 0.1 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 20 | 0.1 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 13 | 0.1 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 13 | 0.1 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 13 | 0.1 |
| (1,3768) | 1:B:69:VAL:HA | 1:B:70:GLN:HG2 | 10 | 0.1 |
| (1,3768) | 1:B:69:VAL:HA | 1:B:70:GLN:HG3 | 10 | 0.1 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG21 | 3 | 0.1 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG22 | 3 | 0.1 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG23 | 3 | 0.1 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 2 | 0.1 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 2 | 0.1 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 2 | 0.1 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 5 | 0.1 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 5 | 0.1 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 5 | 0.1 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 8 | 0.1 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 8 | 0.1 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 8 | 0.1 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 17 | 0.1 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 17 | 0.1 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 17 | 0.1 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 19 | 0.1 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 19 | 0.1 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 19 | 0.1 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB2 | 6 | 0.1 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB3 | 6 | 0.1 |
| (1,3537) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HB2 | 1 | 0.1 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE1 | 13 | 0.1 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE2 | 13 | 0.1 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE3 | 13 | 0.1 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE1 | 5 | 0.1 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE2 | 5 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE3 | 5 | 0.1 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE1 | 20 | 0.1 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE2 | 20 | 0.1 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE3 | 20 | 0.1 |
| (1,3282) | 1:A:58:LYS:HD2 | 1:A:62:LEU:H | 7 | 0.1 |
| (1,3282) | 1:A:58:LYS:HD3 | 1:A:62:LEU:H | 7 | 0.1 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 16 | 0.1 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 19 | 0.1 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 5 | 0.1 |
| (1,3192) | 1:A:54:LYS:HA | 1:A:54:LYS:HE2 | 7 | 0.1 |
| (1,3192) | 1:A:54:LYS:HA | 1:A:54:LYS:HE3 | 7 | 0.1 |
| (1,3188) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD21 | 16 | 0.1 |
| (1,3188) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD21 | 16 | 0.1 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 9 | 0.1 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 9 | 0.1 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 9 | 0.1 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 9 | 0.1 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 9 | 0.1 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 9 | 0.1 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD11 | 13 | 0.1 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD12 | 13 | 0.1 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD13 | 13 | 0.1 |
| (1,2990) | 1:A:20:ASN:HD22 | 1:B:51:ILE:HG21 | 13 | 0.1 |
| (1,2990) | 1:A:20:ASN:HD22 | 1:B:51:ILE:HG22 | 13 | 0.1 |
| (1,2990) | 1:A:20:ASN:HD22 | 1:B:51:ILE:HG23 | 13 | 0.1 |
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 16 | 0.1 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 16 | 0.1 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 16 | 0.1 |
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 17 | 0.1 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 17 | 0.1 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 17 | 0.1 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 1 | 0.1 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 1 | 0.1 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 1 | 0.1 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 9 | 0.1 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 9 | 0.1 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 9 | 0.1 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 6 | 0.1 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 10 | 0.1 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 14 | 0.1 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 2 | 0.1 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 11 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 14 | 0.1 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 20 | 0.1 |
| (1,2606) | 1:B:14:ASP:HB2 | 1:B:43:GLY:HA3 | 8 | 0.1 |
| (1,2550) | 1:B:38:LEU:HD21 | 1:B:45:PHE:HE1 | 7 | 0.1 |
| (1,2550) | 1:B:38:LEU:HD22 | 1:B:45:PHE:HE1 | 7 | 0.1 |
| (1,2550) | 1:B:38:LEU:HD23 | 1:B:45:PHE:HE1 | 7 | 0.1 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 6 | 0.1 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 6 | 0.1 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 6 | 0.1 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 12 | 0.1 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 12 | 0.1 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 12 | 0.1 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 14 | 0.1 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 14 | 0.1 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 14 | 0.1 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 9 | 0.1 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 9 | 0.1 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 9 | 0.1 |
| (1,2390) | 1:B:36:ILE:HG21 | 1:B:48:ASN:H | 2 | 0.1 |
| (1,2390) | 1:B:36:ILE:HG22 | 1:B:48:ASN:H | 2 | 0.1 |
| (1,2390) | 1:B:36:ILE:HG23 | 1:B:48:ASN:H | 2 | 0.1 |
| (1,2390) | 1:B:36:ILE:HG21 | 1:B:48:ASN:H | 12 | 0.1 |
| (1,2390) | 1:B:36:ILE:HG22 | 1:B:48:ASN:H | 12 | 0.1 |
| (1,2390) | 1:B:36:ILE:HG23 | 1:B:48:ASN:H | 12 | 0.1 |
| (1,2390) | 1:B:36:ILE:HG21 | 1:B:48:ASN:H | 19 | 0.1 |
| (1,2390) | 1:B:36:ILE:HG22 | 1:B:48:ASN:H | 19 | 0.1 |
| (1,2390) | 1:B:36:ILE:HG23 | 1:B:48:ASN:H | 19 | 0.1 |
| (1,2389) | 1:A:36:ILE:HG21 | 1:A:48:ASN:H | 9 | 0.1 |
| (1,2389) | 1:A:36:ILE:HG22 | 1:A:48:ASN:H | 9 | 0.1 |
| (1,2389) | 1:A:36:ILE:HG23 | 1:A:48:ASN:H | 9 | 0.1 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 16 | 0.1 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 16 | 0.1 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 16 | 0.1 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 20 | 0.1 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 20 | 0.1 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 20 | 0.1 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 3 | 0.1 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 3 | 0.1 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 3 | 0.1 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 11 | 0.1 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 11 | 0.1 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 11 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2250) | 1:B:27:SER:HG | 1:B:28:LYS:HG2 | 13 | 0.1 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 4 | 0.1 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 4 | 0.1 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 4 | 0.1 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 16 | 0.1 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 16 | 0.1 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 16 | 0.1 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 6 | 0.1 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 6 | 0.1 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 6 | 0.1 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 5 | 0.1 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 15 | 0.1 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 16 | 0.1 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 7 | 0.1 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 10 | 0.1 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 11 | 0.1 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 14 | 0.1 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 17 | 0.1 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 18 | 0.1 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 10 | 0.1 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 10 | 0.1 |
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 10 | 0.1 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 12 | 0.1 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 12 | 0.1 |
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 12 | 0.1 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 3 | 0.1 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 3 | 0.1 |
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 3 | 0.1 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 16 | 0.1 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 16 | 0.1 |
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 16 | 0.1 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 2 | 0.1 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 6 | 0.1 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 10 | 0.1 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 11 | 0.1 |
| (1,1879) | 1:B:25:VAL:HG21 | 1:B:65:LYS:HE2 | 6 | 0.1 |
| (1,1879) | 1:B:25:VAL:HG21 | 1:B:65:LYS:HE3 | 6 | 0.1 |
| (1,1879) | 1:B:25:VAL:HG22 | 1:B:65:LYS:HE2 | 6 | 0.1 |
| (1,1879) | 1:B:25:VAL:HG22 | 1:B:65:LYS:HE3 | 6 | 0.1 |
| (1,1879) | 1:B:25:VAL:HG23 | 1:B:65:LYS:HE2 | 6 | 0.1 |
| (1,1879) | 1:B:25:VAL:HG23 | 1:B:65:LYS:HE3 | 6 | 0.1 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG11 | 9 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG12 | 9 | 0.1 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG13 | 9 | 0.1 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG11 | 9 | 0.1 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG12 | 9 | 0.1 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG13 | 9 | 0.1 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG11 | 13 | 0.1 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG12 | 13 | 0.1 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG13 | 13 | 0.1 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG11 | 13 | 0.1 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG12 | 13 | 0.1 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG13 | 13 | 0.1 |
| (1,1803) | 1:B:13:GLU:HB3 | 1:B:71:GLY:HA3 | 3 | 0.1 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 8 | 0.1 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 8 | 0.1 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 8 | 0.1 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 14 | 0.1 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 14 | 0.1 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 14 | 0.1 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 20 | 0.1 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 20 | 0.1 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 20 | 0.1 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 4 | 0.1 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 4 | 0.1 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 4 | 0.1 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 9 | 0.1 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 9 | 0.1 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 9 | 0.1 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 10 | 0.1 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 10 | 0.1 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 10 | 0.1 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 12 | 0.1 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 12 | 0.1 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 12 | 0.1 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 13 | 0.1 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 13 | 0.1 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 13 | 0.1 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG21 | 5 | 0.1 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG22 | 5 | 0.1 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG23 | 5 | 0.1 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG21 | 5 | 0.1 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG22 | 5 | 0.1 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG23 | 5 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG21 | 5 | 0.1 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG22 | 5 | 0.1 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG23 | 5 | 0.1 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG21 | 16 | 0.1 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG22 | 16 | 0.1 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG23 | 16 | 0.1 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG21 | 16 | 0.1 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG22 | 16 | 0.1 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG23 | 16 | 0.1 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG21 | 16 | 0.1 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG22 | 16 | 0.1 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG23 | 16 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 4 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 4 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 4 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 4 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 4 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 4 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 4 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 4 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 4 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 11 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 11 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 11 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 11 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 11 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 11 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 11 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 11 | 0.1 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 11 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 11 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 11 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 11 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 11 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 11 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 11 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 11 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 11 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 11 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 17 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 17 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 17 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 17 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 17 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 17 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 17 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 17 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 17 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 20 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 20 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 20 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 20 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 20 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 20 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 20 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 20 | 0.1 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 20 | 0.1 |
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 15 | 0.1 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 15 | 0.1 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 15 | 0.1 |
| (1,1370) | 1:B:78:LEU:HD21 | 1:B:79:SER:H | 3 | 0.1 |
| (1,1370) | 1:B:78:LEU:HD22 | 1:B:79:SER:H | 3 | 0.1 |
| (1,1370) | 1:B:78:LEU:HD23 | 1:B:79:SER:H | 3 | 0.1 |
| (1,1222) | 1:B:69:VAL:H | 1:B:72:VAL:H | 8 | 0.1 |
| (1,1182) | 1:B:67:ARG:HE | 1:B:75:VAL:H | 6 | 0.1 |
| (1,1120) | 1:B:65:LYS:H | 1:B:68:LYS:HE2 | 16 | 0.1 |
| (1,1120) | 1:B:65:LYS:H | 1:B:68:LYS:HE3 | 16 | 0.1 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 2 | 0.09 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 4 | 0.09 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 5 | 0.09 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 17 | 0.09 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 13 | 0.09 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 9 | 0.09 |
| (1,713) | 1:B:41:LYS:H | 1:B:41:LYS:HG2 | 13 | 0.09 |
| (1,713) | 1:B:41:LYS:H | 1:B:41:LYS:HG3 | 13 | 0.09 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 19 | 0.09 |
| (1,579) | 1:A:32:ASN:HD21 | 1:A:33:ILE:HB | 14 | 0.09 |
| (1,5262) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HA | 18 | 0.09 |
| (1,5248) | 1:B:76:GLU:HB2 | 1:B:77:ARG:H | 10 | 0.09 |
| (1,5245) | 1:B:69:VAL:HG11 | 1:B:70:GLN:HE21 | 13 | 0.09 |
| (1,5245) | 1:B:69:VAL:HG12 | 1:B:70:GLN:HE21 | 13 | 0.09 |
| (1,5245) | 1:B:69:VAL:HG13 | 1:B:70:GLN:HE21 | 13 | 0.09 |
| (1,5206) | 1:B:62:LEU:HA | 1:B:65:LYS:HG2 | 9 | 0.09 |
| (1,5206) | 1:B:62:LEU:HA | 1:B:65:LYS:HG2 | 13 | 0.09 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,5174) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HB2 | 7 | 0.09 |
| (1,5174) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HB2 | 7 | 0.09 |
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 6 | 0.09 |
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 7 | 0.09 |
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 8 | 0.09 |
| (1,5126) | 1:B:37:VAL:HG11 | 1:B:48:ASN:HD21 | 9 | 0.09 |
| (1,5126) | 1:B:37:VAL:HG12 | 1:B:48:ASN:HD21 | 9 | 0.09 |
| (1,5126) | 1:B:37:VAL:HG13 | 1:B:48:ASN:HD21 | 9 | 0.09 |
| (1,5089) | 1:B:31:THR:HG21 | 1:B:58:LYS:HE2 | 10 | 0.09 |
| (1,5089) | 1:B:31:THR:HG22 | 1:B:58:LYS:HE2 | 10 | 0.09 |
| (1,5089) | 1:B:31:THR:HG23 | 1:B:58:LYS:HE2 | 10 | 0.09 |
| (1,5086) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HD2 | 10 | 0.09 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 2 | 0.09 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 2 | 0.09 |
| (1,4983) | 1:B:9:ARG:HG2 | 1:B:47:CYS:H | 19 | 0.09 |
| (1,4950) | 1:B:3:ASP:HA | 1:B:54:LYS:HB2 | 5 | 0.09 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD21 | 8 | 0.09 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD22 | 8 | 0.09 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD23 | 8 | 0.09 |
| (1,4915) | 1:A:65:LYS:HA | 1:A:68:LYS:HD2 | 1 | 0.09 |
| (1,4898) | 1:A:59:LEU:HD21 | 1:A:77:ARG:HG2 | 4 | 0.09 |
| (1,4898) | 1:A:59:LEU:HD22 | 1:A:77:ARG:HG2 | 4 | 0.09 |
| (1,4898) | 1:A:59:LEU:HD23 | 1:A:77:ARG:HG2 | 4 | 0.09 |
| (1,4869) | 1:A:54:LYS:HG2 | 1:A:55:ASN:H | 6 | 0.09 |
| (1,4862) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HB2 | 17 | 0.09 |
| (1,4862) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HB2 | 17 | 0.09 |
| (1,4862) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HB2 | 17 | 0.09 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 3 | 0.09 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 4 | 0.09 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 19 | 0.09 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 20 | 0.09 |
| (1,4795) | 1:A:32:ASN:HB2 | 1:B:20:ASN:H | 18 | 0.09 |
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 13 | 0.09 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 13 | 0.09 |
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 13 | 0.09 |
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 19 | 0.09 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 19 | 0.09 |
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 19 | 0.09 |
| (1,4775) | 1:A:28:LYS:HB2 | 1:A:28:LYS:HE2 | 15 | 0.09 |
| (1,4775) | 1:A:28:LYS:HB2 | 1:A:28:LYS:HE3 | 15 | 0.09 |
| (1,4769) | 1:A:28:LYS:H | 1:A:28:LYS:HG2 | 10 | 0.09 |
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 19 | 0.09 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4723) | 1:A:20:ASN:HB2 | 1:A:21:GLN:H | 16 | 0.09 |
| (1,4715) | 1:A:18:MET:HG2 | 1:A:45:PHE:HE1 | 12 | 0.09 |
| (1,4695) | 1:A:16:ASN:HB2 | 1:A:17:GLY:H | 17 | 0.09 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 15 | 0.09 |
| (1,4627) | 1:A:3:ASP:HA | 1:A:54:LYS:HB2 | 11 | 0.09 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 20 | 0.09 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 20 | 0.09 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 20 | 0.09 |
| (1,4613) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HD2 | 4 | 0.09 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 16 | 0.09 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 2 | 0.09 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 2 | 0.09 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 14 | 0.09 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 14 | 0.09 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 16 | 0.09 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 16 | 0.09 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 17 | 0.09 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 17 | 0.09 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 18 | 0.09 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 18 | 0.09 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 20 | 0.09 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 20 | 0.09 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 4 | 0.09 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 4 | 0.09 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 6 | 0.09 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 6 | 0.09 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 11 | 0.09 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 11 | 0.09 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 16 | 0.09 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 16 | 0.09 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 19 | 0.09 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 19 | 0.09 |
| (1,4496) | 1:B:12:GLY:H | 1:B:45:PHE:HE1 | 16 | 0.09 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 1 | 0.09 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 1 | 0.09 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 1 | 0.09 |
| (1,4413) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 1 | 0.09 |
| (1,4413) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 1 | 0.09 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 2 | 0.09 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 2 | 0.09 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 2 | 0.09 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 5 | 0.09 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 5 | 0.09 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 5 | 0.09 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 6 | 0.09 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 6 | 0.09 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 6 | 0.09 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 8 | 0.09 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 8 | 0.09 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 8 | 0.09 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 16 | 0.09 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 16 | 0.09 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 16 | 0.09 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 3 | 0.09 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 3 | 0.09 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 3 | 0.09 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 6 | 0.09 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 6 | 0.09 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 6 | 0.09 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 10 | 0.09 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 10 | 0.09 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 10 | 0.09 |
| (1,4362) | 1:A:29:PHE:HE1 | 1:A:66:LEU:HG | 2 | 0.09 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG21 | 2 | 0.09 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG22 | 2 | 0.09 |
| (1,4360) | 1:A:4:PHE:HE1 | 1:A:56:THR:HG23 | 2 | 0.09 |
| (1,4278) | 1:A:60:THR:HB | 1:A:61:THR:H | 14 | 0.09 |
| (1,4199) | 1:B:82:GLU:H | 1:B:83:HIS:HB3 | 13 | 0.09 |
| (1,4198) | 1:A:82:GLU:H | 1:A:83:HIS:HB3 | 6 | 0.09 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 13 | 0.09 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 13 | 0.09 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 13 | 0.09 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 18 | 0.09 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 18 | 0.09 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 18 | 0.09 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 6 | 0.09 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 6 | 0.09 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 6 | 0.09 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 10 | 0.09 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 10 | 0.09 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 10 | 0.09 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 16 | 0.09 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 16 | 0.09 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 16 | 0.09 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 18 | 0.09 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 18 | 0.09 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 18 | 0.09 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 3 | 0.09 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 3 | 0.09 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 3 | 0.09 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 5 | 0.09 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 5 | 0.09 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 5 | 0.09 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 10 | 0.09 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 10 | 0.09 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 10 | 0.09 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 11 | 0.09 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 11 | 0.09 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 11 | 0.09 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 8 | 0.09 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 8 | 0.09 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 8 | 0.09 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 17 | 0.09 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 17 | 0.09 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 17 | 0.09 |
| (1,4106) | 1:B:15:LYS:HB3 | 1:B:18:MET:HB3 | 3 | 0.09 |
| (1,4106) | 1:B:15:LYS:HB3 | 1:B:18:MET:HB3 | 18 | 0.09 |
| (1,4075) | 1:B:82:GLU:HA | 1:B:83:HIS:HB2 | 7 | 0.09 |
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD11 | 19 | 0.09 |
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD12 | 19 | 0.09 |
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD13 | 19 | 0.09 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD11 | 19 | 0.09 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD12 | 19 | 0.09 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD13 | 19 | 0.09 |
| (1,3937) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HB3 | 12 | 0.09 |
| (1,3936) | 1:A:7:GLY:HA2 | 1:A:78:LEU:HB3 | 12 | 0.09 |
| (1,3897) | 1:B:74:THR:HA | 1:B:76:GLU:HG2 | 17 | 0.09 |
| (1,3897) | 1:B:74:THR:HA | 1:B:76:GLU:HG3 | 17 | 0.09 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 9 | 0.09 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 9 | 0.09 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 9 | 0.09 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 13 | 0.09 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 13 | 0.09 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 13 | 0.09 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 15 | 0.09 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 15 | 0.09 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 15 | 0.09 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 1 | 0.09 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 1 | 0.09 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 1 | 0.09 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 4 | 0.09 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 4 | 0.09 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 4 | 0.09 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 11 | 0.09 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 11 | 0.09 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 11 | 0.09 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 4 | 0.09 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 4 | 0.09 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 4 | 0.09 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 6 | 0.09 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 6 | 0.09 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 6 | 0.09 |
| (1,3734) | 1:B:20:ASN:HA | 1:B:22:ILE:HB | 8 | 0.09 |
| (1,3734) | 1:B:20:ASN:HA | 1:B:22:ILE:HB | 9 | 0.09 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG11 | 15 | 0.09 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG12 | 15 | 0.09 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG13 | 15 | 0.09 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG11 | 15 | 0.09 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG12 | 15 | 0.09 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG13 | 15 | 0.09 |
| (1,3699) | 1:A:15:LYS:HE2 | 1:A:16:ASN:HD21 | 1 | 0.09 |
| (1,3699) | 1:A:15:LYS:HE3 | 1:A:16:ASN:HD21 | 1 | 0.09 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 10 | 0.09 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 10 | 0.09 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 10 | 0.09 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 11 | 0.09 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 11 | 0.09 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 11 | 0.09 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 13 | 0.09 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 13 | 0.09 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 13 | 0.09 |
| (1,3544) | 1:B:64:ASP:HB3 | 1:B:65:LYS:HB2 | 3 | 0.09 |
| (1,3537) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HB2 | 19 | 0.09 |
| (1,3536) | 1:A:64:ASP:HB2 | 1:A:65:LYS:HB2 | 12 | 0.09 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE1 | 5 | 0.09 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE2 | 5 | 0.09 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE3 | 5 | 0.09 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE1 | 9 | 0.09 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE2 | 9 | 0.09 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE3 | 9 | 0.09 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 5 | 0.09 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 8 | 0.09 |
| (1,3275) | 1:B:30:ASP:HB2 | 1:B:58:LYS:HD2 | 16 | 0.09 |
| (1,3275) | 1:B:30:ASP:HB2 | 1:B:58:LYS:HD3 | 16 | 0.09 |
| (1,3275) | 1:B:30:ASP:HB3 | 1:B:58:LYS:HD2 | 16 | 0.09 |
| (1,3275) | 1:B:30:ASP:HB3 | 1:B:58:LYS:HD3 | 16 | 0.09 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 5 | 0.09 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 13 | 0.09 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 13 | 0.09 |
| (1,3195) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD21 | 12 | 0.09 |
| (1,3195) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD21 | 12 | 0.09 |
| (1,3189) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD21 | 20 | 0.09 |
| (1,3189) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD21 | 20 | 0.09 |
| (1,3184) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD22 | 8 | 0.09 |
| (1,3184) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD22 | 8 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 13 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 13 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 13 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 13 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 13 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 13 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 16 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 16 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 16 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 16 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 16 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 16 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 20 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 20 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 20 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 20 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 20 | 0.09 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 20 | 0.09 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 14 | 0.09 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 14 | 0.09 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 14 | 0.09 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 14 | 0.09 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 14 | 0.09 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 14 | 0.09 |
| (1,292) | 1:B:20:ASN:H | 1:B:20:ASN:HD22 | 15 | 0.09 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 15 | 0.09 |
| (1,2766) | 1:B:9:ARG:HG2 | 1:B:48:ASN:HA | 8 | 0.09 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 8 | 0.09 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 12 | 0.09 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 13 | 0.09 |
| (1,2605) | 1:A:14:ASP:HB2 | 1:A:43:GLY:HA3 | 7 | 0.09 |
| (1,244) | 1:A:15:LYS:HG2 | 1:A:19:THR:H | 18 | 0.09 |
| (1,244) | 1:A:15:LYS:HG3 | 1:A:19:THR:H | 18 | 0.09 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 1 | 0.09 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 1 | 0.09 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 1 | 0.09 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 2 | 0.09 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 2 | 0.09 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 2 | 0.09 |
| (1,2390) | 1:B:36:ILE:HG21 | 1:B:48:ASN:H | 17 | 0.09 |
| (1,2390) | 1:B:36:ILE:HG22 | 1:B:48:ASN:H | 17 | 0.09 |
| (1,2390) | 1:B:36:ILE:HG23 | 1:B:48:ASN:H | 17 | 0.09 |
| (1,2389) | 1:A:36:ILE:HG21 | 1:A:48:ASN:H | 11 | 0.09 |
| (1,2389) | 1:A:36:ILE:HG22 | 1:A:48:ASN:H | 11 | 0.09 |
| (1,2389) | 1:A:36:ILE:HG23 | 1:A:48:ASN:H | 11 | 0.09 |
| (1,2389) | 1:A:36:ILE:HG21 | 1:A:48:ASN:H | 13 | 0.09 |
| (1,2389) | 1:A:36:ILE:HG22 | 1:A:48:ASN:H | 13 | 0.09 |
| (1,2389) | 1:A:36:ILE:HG23 | 1:A:48:ASN:H | 13 | 0.09 |
| (1,2389) | 1:A:36:ILE:HG21 | 1:A:48:ASN:H | 16 | 0.09 |
| (1,2389) | 1:A:36:ILE:HG22 | 1:A:48:ASN:H | 16 | 0.09 |
| (1,2389) | 1:A:36:ILE:HG23 | 1:A:48:ASN:H | 16 | 0.09 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 1 | 0.09 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 1 | 0.09 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 1 | 0.09 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 4 | 0.09 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 4 | 0.09 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 4 | 0.09 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 9 | 0.09 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 9 | 0.09 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 9 | 0.09 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 11 | 0.09 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 11 | 0.09 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 11 | 0.09 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 10 | 0.09 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 10 | 0.09 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 10 | 0.09 |
| (1,2267) | 1:A:29:PHE:HD1 | 1:A:31:THR:HB | 14 | 0.09 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2267) | 1:A:29:PHE:HD2 | 1:A:31:THR:HB | 14 | 0.09 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 3 | 0.09 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 3 | 0.09 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 3 | 0.09 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 5 | 0.09 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 5 | 0.09 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 5 | 0.09 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 8 | 0.09 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 8 | 0.09 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 8 | 0.09 |
| (1,2175) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HE2 | 13 | 0.09 |
| (1,2175) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HE3 | 13 | 0.09 |
| (1,2175) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HE2 | 13 | 0.09 |
| (1,2175) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HE3 | 13 | 0.09 |
| (1,2175) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HE2 | 13 | 0.09 |
| (1,2175) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HE3 | 13 | 0.09 |
| (1,2136) | 1:B:67:ARG:HE | 1:B:75:VAL:HG11 | 19 | 0.09 |
| (1,2136) | 1:B:67:ARG:HE | 1:B:75:VAL:HG12 | 19 | 0.09 |
| (1,2136) | 1:B:67:ARG:HE | 1:B:75:VAL:HG13 | 19 | 0.09 |
| (1,2135) | 1:A:67:ARG:HE | 1:A:75:VAL:HG11 | 1 | 0.09 |
| (1,2135) | 1:A:67:ARG:HE | 1:A:75:VAL:HG12 | 1 | 0.09 |
| (1,2135) | 1:A:67:ARG:HE | 1:A:75:VAL:HG13 | 1 | 0.09 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 15 | 0.09 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 15 | 0.09 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 15 | 0.09 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 18 | 0.09 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 18 | 0.09 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 18 | 0.09 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 9 | 0.09 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 9 | 0.09 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 9 | 0.09 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 3 | 0.09 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 3 | 0.09 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 3 | 0.09 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 1 | 0.09 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 2 | 0.09 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 7 | 0.09 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 8 | 0.09 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 9 | 0.09 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 1 | 0.09 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 5 | 0.09 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 6 | 0.09 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 12 | 0.09 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 18 | 0.09 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 18 | 0.09 |
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 18 | 0.09 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 20 | 0.09 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 3 | 0.09 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 16 | 0.09 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG11 | 4 | 0.09 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG12 | 4 | 0.09 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG13 | 4 | 0.09 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG11 | 4 | 0.09 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG12 | 4 | 0.09 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG13 | 4 | 0.09 |
| (1,1803) | 1:B:13:GLU:HB3 | 1:B:71:GLY:HA3 | 12 | 0.09 |
| (1,1803) | 1:B:13:GLU:HB3 | 1:B:71:GLY:HA3 | 20 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 1 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 1 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 1 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 3 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 3 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 3 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 11 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 11 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 11 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 13 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 13 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 13 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 17 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 17 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 17 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 18 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 18 | 0.09 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 18 | 0.09 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 6 | 0.09 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 6 | 0.09 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 6 | 0.09 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 7 | 0.09 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 7 | 0.09 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 7 | 0.09 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG21 | 2 | 0.09 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG22 | 2 | 0.09 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG23 | 2 | 0.09 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG21 | 2 | 0.09 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG22 | 2 | 0.09 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG23 | 2 | 0.09 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG21 | 2 | 0.09 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG22 | 2 | 0.09 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG23 | 2 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 9 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 9 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 9 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 9 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 9 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 9 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 9 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 9 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 9 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 12 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 12 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 12 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 12 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 12 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 12 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 12 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 12 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 12 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 20 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 20 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 20 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 20 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 20 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 20 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 20 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 20 | 0.09 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 20 | 0.09 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 7 | 0.09 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 7 | 0.09 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 7 | 0.09 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 7 | 0.09 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 7 | 0.09 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 7 | 0.09 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 7 | 0.09 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 7 | 0.09 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 7 | 0.09 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 16 | 0.09 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 16 | 0.09 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 16 | 0.09 |
| (1,1455) | 1:A:3:ASP:HB2 | 1:A:53:VAL:H | 13 | 0.09 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 7 | 0.09 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 20 | 0.09 |
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 10 | 0.09 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 2 | 0.08 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 3 | 0.08 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 11 | 0.08 |
| (1,946) | 1:A:55:ASN:H | 1:A:56:THR:HG21 | 2 | 0.08 |
| (1,946) | 1:A:55:ASN:H | 1:A:56:THR:HG22 | 2 | 0.08 |
| (1,946) | 1:A:55:ASN:H | 1:A:56:THR:HG23 | 2 | 0.08 |
| (1,85) | 1:B:9:ARG:HE | 1:B:11:VAL:HG21 | 18 | 0.08 |
| (1,85) | 1:B:9:ARG:HE | 1:B:11:VAL:HG22 | 18 | 0.08 |
| (1,85) | 1:B:9:ARG:HE | 1:B:11:VAL:HG23 | 18 | 0.08 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 20 | 0.08 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 10 | 0.08 |
| (1,751) | 1:B:40:ALA:HB1 | 1:B:43:GLY:H | 4 | 0.08 |
| (1,751) | 1:B:40:ALA:HB2 | 1:B:43:GLY:H | 4 | 0.08 |
| (1,751) | 1:B:40:ALA:HB3 | 1:B:43:GLY:H | 4 | 0.08 |
| (1,735) | 1:B:41:LYS:H | 1:B:46:THR:H | 3 | 0.08 |
| (1,735) | 1:B:41:LYS:H | 1:B:46:THR:H | 13 | 0.08 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD1 | 6 | 0.08 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD2 | 6 | 0.08 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 7 | 0.08 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 14 | 0.08 |
| (1,5262) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HA | 20 | 0.08 |
| (1,5248) | 1:B:76:GLU:HB2 | 1:B:77:ARG:H | 16 | 0.08 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 11 | 0.08 |
| (1,5223) | 1:B:65:LYS:H | 1:B:65:LYS:HD2 | 13 | 0.08 |
| (1,5206) | 1:B:62:LEU:HA | 1:B:65:LYS:HG2 | 18 | 0.08 |
| (1,5185) | 1:B:56:THR:HG21 | 1:B:59:LEU:HB2 | 3 | 0.08 |
| (1,5185) | 1:B:56:THR:HG22 | 1:B:59:LEU:HB2 | 3 | 0.08 |
| (1,5185) | 1:B:56:THR:HG23 | 1:B:59:LEU:HB2 | 3 | 0.08 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD11 | 1 | 0.08 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD12 | 1 | 0.08 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD13 | 1 | 0.08 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD11 | 8 | 0.08 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD12 | 8 | 0.08 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD13 | 8 | 0.08 |
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 9 | 0.08 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 12 | 0.08 |
| (1,5126) | 1:B:37:VAL:HG11 | 1:B:48:ASN:HD21 | 12 | 0.08 |
| (1,5126) | 1:B:37:VAL:HG12 | 1:B:48:ASN:HD21 | 12 | 0.08 |
| (1,5126) | 1:B:37:VAL:HG13 | 1:B:48:ASN:HD21 | 12 | 0.08 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 11 | 0.08 |
| (1,5056) | 1:B:26:ILE:HG12 | 1:B:27:SER:H | 17 | 0.08 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 11 | 0.08 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 17 | 0.08 |
| (1,5034) | 1:B:23:THR:HG21 | 1:B:27:SER:HB2 | 3 | 0.08 |
| (1,5034) | 1:B:23:THR:HG22 | 1:B:27:SER:HB2 | 3 | 0.08 |
| (1,5034) | 1:B:23:THR:HG23 | 1:B:27:SER:HB2 | 3 | 0.08 |
| (1,5034) | 1:B:23:THR:HG21 | 1:B:27:SER:HB2 | 4 | 0.08 |
| (1,5034) | 1:B:23:THR:HG22 | 1:B:27:SER:HB2 | 4 | 0.08 |
| (1,5034) | 1:B:23:THR:HG23 | 1:B:27:SER:HB2 | 4 | 0.08 |
| (1,5028) | 1:B:20:ASN:HB2 | 1:B:21:GLN:H | 11 | 0.08 |
| (1,5028) | 1:B:20:ASN:HB2 | 1:B:21:GLN:H | 12 | 0.08 |
| (1,5019) | 1:B:17:GLY:HA2 | 1:B:21:GLN:HE22 | 16 | 0.08 |
| (1,5007) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HB2 | 6 | 0.08 |
| (1,5007) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HB2 | 6 | 0.08 |
| (1,4968) | 1:B:8:ILE:H | 1:B:8:ILE:HG12 | 1 | 0.08 |
| (1,4968) | 1:B:8:ILE:H | 1:B:8:ILE:HG12 | 5 | 0.08 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 1 | 0.08 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD21 | 15 | 0.08 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD22 | 15 | 0.08 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD23 | 15 | 0.08 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD21 | 16 | 0.08 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD22 | 16 | 0.08 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD23 | 16 | 0.08 |
| (1,4933) | 1:A:69:VAL:HG11 | 1:A:70:GLN:HE21 | 12 | 0.08 |
| (1,4933) | 1:A:69:VAL:HG12 | 1:A:70:GLN:HE21 | 12 | 0.08 |
| (1,4933) | 1:A:69:VAL:HG13 | 1:A:70:GLN:HE21 | 12 | 0.08 |
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 3 | 0.08 |
| (1,4912) | 1:A:65:LYS:H | 1:A:65:LYS:HD2 | 1 | 0.08 |
| (1,4888) | 1:A:58:LYS:HG2 | 1:A:58:LYS:HE2 | 14 | 0.08 |
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 9 | 0.08 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 7 | 0.08 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 18 | 0.08 |
| (1,4813) | 1:A:36:ILE:HG12 | 1:A:37:VAL:H | 5 | 0.08 |
| (1,4812) | 1:A:36:ILE:HG21 | 1:A:48:ASN:HB2 | 13 | 0.08 |
| (1,4812) | 1:A:36:ILE:HG22 | 1:A:48:ASN:HB2 | 13 | 0.08 |
| (1,4812) | 1:A:36:ILE:HG23 | 1:A:48:ASN:HB2 | 13 | 0.08 |
| (1,4795) | 1:A:32:ASN:HB2 | 1:B:20:ASN:H | 16 | 0.08 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 6 | 0.08 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 6 | 0.08 |
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 6 | 0.08 |
| (1,4787) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HD2 | 7 | 0.08 |
| (1,4733) | 1:A:23:THR:HG21 | 1:A:27:SER:HB2 | 20 | 0.08 |
| (1,4733) | 1:A:23:THR:HG22 | 1:A:27:SER:HB2 | 20 | 0.08 |
| (1,4733) | 1:A:23:THR:HG23 | 1:A:27:SER:HB2 | 20 | 0.08 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 9 | 0.08 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 14 | 0.08 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 11 | 0.08 |
| (1,4632) | 1:A:4:PHE:H | 1:A:52:PHE:HB2 | 14 | 0.08 |
| (1,4627) | 1:A:3:ASP:HA | 1:A:54:LYS:HB2 | 10 | 0.08 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 1 | 0.08 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 1 | 0.08 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 1 | 0.08 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 2 | 0.08 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 2 | 0.08 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 2 | 0.08 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 4 | 0.08 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 4 | 0.08 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 4 | 0.08 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 10 | 0.08 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 10 | 0.08 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 10 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 1 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 1 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 1 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 7 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 7 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 7 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 8 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 8 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 8 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 12 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 12 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 12 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 13 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 13 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 13 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 18 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 18 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 18 | 0.08 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 19 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 19 | 0.08 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 19 | 0.08 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 8 | 0.08 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 2 | 0.08 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 3 | 0.08 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 9 | 0.08 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG21 | 6 | 0.08 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG22 | 6 | 0.08 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG23 | 6 | 0.08 |
| (1,4571) | 1:A:44:ILE:HG13 | 1:A:73:PHE:HE1 | 8 | 0.08 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 3 | 0.08 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 3 | 0.08 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 5 | 0.08 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 5 | 0.08 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 7 | 0.08 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 7 | 0.08 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 9 | 0.08 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 9 | 0.08 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 13 | 0.08 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 13 | 0.08 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 1 | 0.08 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 1 | 0.08 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 10 | 0.08 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 10 | 0.08 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 14 | 0.08 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 14 | 0.08 |
| (1,4495) | 1:A:12:GLY:H | 1:A:45:PHE:HE1 | 2 | 0.08 |
| (1,4475) | 1:A:22:ILE:HD11 | 1:A:45:PHE:HE1 | 5 | 0.08 |
| (1,4475) | 1:A:22:ILE:HD12 | 1:A:45:PHE:HE1 | 5 | 0.08 |
| (1,4475) | 1:A:22:ILE:HD13 | 1:A:45:PHE:HE1 | 5 | 0.08 |
| (1,4417) | 1:B:29:PHE:HA | 1:B:29:PHE:HD1 | 6 | 0.08 |
| (1,4417) | 1:B:29:PHE:HA | 1:B:29:PHE:HD2 | 6 | 0.08 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 14 | 0.08 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 14 | 0.08 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 14 | 0.08 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 18 | 0.08 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 18 | 0.08 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 18 | 0.08 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 20 | 0.08 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 20 | 0.08 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 20 | 0.08 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 5 | 0.08 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 5 | 0.08 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 5 | 0.08 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 14 | 0.08 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 14 | 0.08 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 14 | 0.08 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 18 | 0.08 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 18 | 0.08 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 18 | 0.08 |
| (1,4367) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HA | 11 | 0.08 |
| (1,4259) | 1:B:41:LYS:HG2 | 1:B:42:ASP:HA | 8 | 0.08 |
| (1,4259) | 1:B:41:LYS:HG3 | 1:B:42:ASP:HA | 8 | 0.08 |
| (1,4259) | 1:B:41:LYS:HG2 | 1:B:42:ASP:HA | 10 | 0.08 |
| (1,4259) | 1:B:41:LYS:HG3 | 1:B:42:ASP:HA | 10 | 0.08 |
| (1,4259) | 1:B:41:LYS:HG2 | 1:B:42:ASP:HA | 12 | 0.08 |
| (1,4259) | 1:B:41:LYS:HG3 | 1:B:42:ASP:HA | 12 | 0.08 |
| (1,4258) | 1:A:41:LYS:HG2 | 1:A:42:ASP:HA | 6 | 0.08 |
| (1,4258) | 1:A:41:LYS:HG3 | 1:A:42:ASP:HA | 6 | 0.08 |
| (1,4256) | 1:A:41:LYS:HA | 1:A:42:ASP:H | 15 | 0.08 |
| (1,4199) | 1:B:82:GLU:H | 1:B:83:HIS:HB3 | 3 | 0.08 |
| (1,4199) | 1:B:82:GLU:H | 1:B:83:HIS:HB3 | 16 | 0.08 |
| (1,4198) | 1:A:82:GLU:H | 1:A:83:HIS:HB3 | 7 | 0.08 |
| (1,4198) | 1:A:82:GLU:H | 1:A:83:HIS:HB3 | 18 | 0.08 |
| (1,4198) | 1:A:82:GLU:H | 1:A:83:HIS:HB3 | 20 | 0.08 |
| (1,4193) | 1:B:5:LEU:HB2 | 1:B:83:HIS:HB3 | 1 | 0.08 |
| (1,4193) | 1:B:5:LEU:HB2 | 1:B:83:HIS:HB3 | 5 | 0.08 |
| (1,4191) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HB3 | 5 | 0.08 |
| (1,4191) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HB3 | 5 | 0.08 |
| (1,4191) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HB3 | 5 | 0.08 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 8 | 0.08 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 8 | 0.08 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 8 | 0.08 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 8 | 0.08 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 8 | 0.08 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 8 | 0.08 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 9 | 0.08 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 9 | 0.08 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 9 | 0.08 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 1 | 0.08 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 1 | 0.08 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 1 | 0.08 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 13 | 0.08 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 13 | 0.08 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 13 | 0.08 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 14 | 0.08 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 14 | 0.08 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 14 | 0.08 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 5 | 0.08 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 5 | 0.08 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 5 | 0.08 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 7 | 0.08 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 7 | 0.08 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 7 | 0.08 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 10 | 0.08 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 10 | 0.08 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 10 | 0.08 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 14 | 0.08 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 14 | 0.08 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 14 | 0.08 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 18 | 0.08 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 18 | 0.08 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 18 | 0.08 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD11 | 14 | 0.08 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD12 | 14 | 0.08 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD13 | 14 | 0.08 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 9 | 0.08 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 20 | 0.08 |
| (1,4115) | 1:A:18:MET:HA | 1:A:21:GLN:HB2 | 5 | 0.08 |
| (1,4115) | 1:A:18:MET:HA | 1:A:21:GLN:HB2 | 9 | 0.08 |
| (1,4106) | 1:B:15:LYS:HB3 | 1:B:18:MET:HB3 | 8 | 0.08 |
| (1,4023) | 1:B:80:ASN:HB3 | 1:B:81:LEU:HD21 | 8 | 0.08 |
| (1,4023) | 1:B:80:ASN:HB3 | 1:B:81:LEU:HD22 | 8 | 0.08 |
| (1,4023) | 1:B:80:ASN:HB3 | 1:B:81:LEU:HD23 | 8 | 0.08 |
| (1,4016) | 1:A:78:LEU:H | 1:A:79:SER:HB2 | 11 | 0.08 |
| (1,4016) | 1:A:78:LEU:H | 1:A:79:SER:HB3 | 11 | 0.08 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD11 | 10 | 0.08 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD12 | 10 | 0.08 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD13 | 10 | 0.08 |
| (1,3921) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HD2 | 16 | 0.08 |
| (1,3921) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HD3 | 16 | 0.08 |
| (1,3921) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HD2 | 16 | 0.08 |
| (1,3921) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HD3 | 16 | 0.08 |
| (1,3921) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HD2 | 16 | 0.08 |
| (1,3921) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HD3 | 16 | 0.08 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 2 | 0.08 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 2 | 0.08 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 2 | 0.08 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 18 | 0.08 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 18 | 0.08 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 18 | 0.08 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 1 | 0.08 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 1 | 0.08 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 1 | 0.08 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 6 | 0.08 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 6 | 0.08 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 6 | 0.08 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 7 | 0.08 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 7 | 0.08 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 7 | 0.08 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 10 | 0.08 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 10 | 0.08 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 10 | 0.08 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 5 | 0.08 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 5 | 0.08 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 5 | 0.08 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 6 | 0.08 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 6 | 0.08 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 6 | 0.08 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 15 | 0.08 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 15 | 0.08 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 15 | 0.08 |
| (1,3734) | 1:B:20:ASN:HA | 1:B:22:ILE:HB | 4 | 0.08 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG11 | 18 | 0.08 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG12 | 18 | 0.08 |
| (1,3711) | 1:A:15:LYS:HD2 | 1:A:69:VAL:HG13 | 18 | 0.08 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG11 | 18 | 0.08 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG12 | 18 | 0.08 |
| (1,3711) | 1:A:15:LYS:HD3 | 1:A:69:VAL:HG13 | 18 | 0.08 |
| (1,3701) | 1:A:15:LYS:HE2 | 1:A:18:MET:H | 11 | 0.08 |
| (1,3701) | 1:A:15:LYS:HE3 | 1:A:18:MET:H | 11 | 0.08 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE2 | 5 | 0.08 |
| (1,3697) | 1:A:15:LYS:H | 1:A:15:LYS:HE3 | 5 | 0.08 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 3 | 0.08 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 3 | 0.08 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 3 | 0.08 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 4 | 0.08 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 4 | 0.08 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 4 | 0.08 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 20 | 0.08 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 20 | 0.08 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 20 | 0.08 |
| (1,3537) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HB2 | 9 | 0.08 |
| (1,3536) | 1:A:64:ASP:HB2 | 1:A:65:LYS:HB2 | 14 | 0.08 |
| (1,3536) | 1:A:64:ASP:HB2 | 1:A:65:LYS:HB2 | 18 | 0.08 |
| (1,3530) | 1:B:9:ARG:H | 1:B:63:MET:HE1 | 4 | 0.08 |
| (1,3530) | 1:B:9:ARG:H | 1:B:63:MET:HE2 | 4 | 0.08 |
| (1,3530) | 1:B:9:ARG:H | 1:B:63:MET:HE3 | 4 | 0.08 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 18 | 0.08 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 18 | 0.08 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 18 | 0.08 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 19 | 0.08 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 19 | 0.08 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 19 | 0.08 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE1 | 6 | 0.08 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE2 | 6 | 0.08 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE3 | 6 | 0.08 |
| (1,3465) | 1:A:30:ASP:H | 1:A:62:LEU:HD11 | 17 | 0.08 |
| (1,3465) | 1:A:30:ASP:H | 1:A:62:LEU:HD12 | 17 | 0.08 |
| (1,3465) | 1:A:30:ASP:H | 1:A:62:LEU:HD13 | 17 | 0.08 |
| (1,3275) | 1:B:30:ASP:HB2 | 1:B:58:LYS:HD2 | 15 | 0.08 |
| (1,3275) | 1:B:30:ASP:HB2 | 1:B:58:LYS:HD3 | 15 | 0.08 |
| (1,3275) | 1:B:30:ASP:HB3 | 1:B:58:LYS:HD2 | 15 | 0.08 |
| (1,3275) | 1:B:30:ASP:HB3 | 1:B:58:LYS:HD3 | 15 | 0.08 |
| (1,3274) | 1:A:30:ASP:HB2 | 1:A:58:LYS:HD2 | 8 | 0.08 |
| (1,3274) | 1:A:30:ASP:HB2 | 1:A:58:LYS:HD3 | 8 | 0.08 |
| (1,3274) | 1:A:30:ASP:HB3 | 1:A:58:LYS:HD2 | 8 | 0.08 |
| (1,3274) | 1:A:30:ASP:HB3 | 1:A:58:LYS:HD3 | 8 | 0.08 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 2 | 0.08 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 14 | 0.08 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 15 | 0.08 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 18 | 0.08 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 1 | 0.08 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 4 | 0.08 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 16 | 0.08 |
| (1,3195) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD21 | 8 | 0.08 |
| (1,3195) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD21 | 8 | 0.08 |
| (1,3193) | 1:B:54:LYS:HA | 1:B:54:LYS:HE2 | 17 | 0.08 |
| (1,3193) | 1:B:54:LYS:HA | 1:B:54:LYS:HE3 | 17 | 0.08 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3094) | 1:A:53:VAL:HG11 | 1:A:58:LYS:HZ1 | 17 | 0.08 |
| (1,3094) | 1:A:53:VAL:HG12 | 1:A:58:LYS:HZ1 | 17 | 0.08 |
| (1,3094) | 1:A:53:VAL:HG13 | 1:A:58:LYS:HZ1 | 17 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 5 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 5 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 5 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 5 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 5 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 5 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 6 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 6 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 6 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 6 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 6 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 6 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 10 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 10 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 10 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 10 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 10 | 0.08 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 10 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 2 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 2 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 2 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 2 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 2 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 2 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 8 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 8 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 8 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 8 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 8 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 8 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 18 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 18 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 18 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 18 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 18 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 18 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 19 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 19 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 19 | 0.08 |

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wwPDB NMR Structure Validation Summary Report

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 19 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 19 | 0.08 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 19 | 0.08 |
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD11 | 4 | 0.08 |
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD12 | 4 | 0.08 |
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD13 | 4 | 0.08 |
| (1,303) | 1:A:33:ILE:HG13 | 1:B:20:ASN:HD21 | 6 | 0.08 |
| (1,3) | 1:A:2:THR:HG21 | 1:A:4:PHE:H | 16 | 0.08 |
| (1,3) | 1:A:2:THR:HG22 | 1:A:4:PHE:H | 16 | 0.08 |
| (1,3) | 1:A:2:THR:HG23 | 1:A:4:PHE:H | 16 | 0.08 |
| (1,2960) | 1:A:15:LYS:HG2 | 1:A:16:ASN:H | 20 | 0.08 |
| (1,2960) | 1:A:15:LYS:HG3 | 1:A:16:ASN:H | 20 | 0.08 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 10 | 0.08 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 10 | 0.08 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 10 | 0.08 |
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 3 | 0.08 |
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 11 | 0.08 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 11 | 0.08 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 11 | 0.08 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 15 | 0.08 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 15 | 0.08 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 15 | 0.08 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 1 | 0.08 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 16 | 0.08 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 1 | 0.08 |
| (1,2606) | 1:B:14:ASP:HB2 | 1:B:43:GLY:HA3 | 6 | 0.08 |
| (1,2588) | 1:B:15:LYS:H | 1:B:40:ALA:HB1 | 19 | 0.08 |
| (1,2588) | 1:B:15:LYS:H | 1:B:40:ALA:HB2 | 19 | 0.08 |
| (1,2588) | 1:B:15:LYS:H | 1:B:40:ALA:HB3 | 19 | 0.08 |
| (1,2571) | 1:A:40:ALA:HA | 1:A:45:PHE:HA | 10 | 0.08 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 7 | 0.08 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 7 | 0.08 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 7 | 0.08 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 3 | 0.08 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 3 | 0.08 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 3 | 0.08 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 11 | 0.08 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 11 | 0.08 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 11 | 0.08 |
| (1,2389) | 1:A:36:ILE:HG21 | 1:A:48:ASN:H | 1 | 0.08 |
| (1,2389) | 1:A:36:ILE:HG22 | 1:A:48:ASN:H | 1 | 0.08 |
| (1,2389) | 1:A:36:ILE:HG23 | 1:A:48:ASN:H | 1 | 0.08 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 8 | 0.08 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 8 | 0.08 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 8 | 0.08 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 14 | 0.08 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 14 | 0.08 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 14 | 0.08 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 2 | 0.08 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 2 | 0.08 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 2 | 0.08 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 17 | 0.08 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 17 | 0.08 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 17 | 0.08 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 19 | 0.08 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 19 | 0.08 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 19 | 0.08 |
| (1,2370) | 1:A:36:ILE:HG21 | 1:B:39:ASN:HB2 | 4 | 0.08 |
| (1,2370) | 1:A:36:ILE:HG21 | 1:B:39:ASN:HB3 | 4 | 0.08 |
| (1,2370) | 1:A:36:ILE:HG22 | 1:B:39:ASN:HB2 | 4 | 0.08 |
| (1,2370) | 1:A:36:ILE:HG22 | 1:B:39:ASN:HB3 | 4 | 0.08 |
| (1,2370) | 1:A:36:ILE:HG23 | 1:B:39:ASN:HB2 | 4 | 0.08 |
| (1,2370) | 1:A:36:ILE:HG23 | 1:B:39:ASN:HB3 | 4 | 0.08 |
| (1,2268) | 1:B:29:PHE:HD1 | 1:B:31:THR:HB | 1 | 0.08 |
| (1,2268) | 1:B:29:PHE:HD2 | 1:B:31:THR:HB | 1 | 0.08 |
| (1,2268) | 1:B:29:PHE:HD1 | 1:B:31:THR:HB | 14 | 0.08 |
| (1,2268) | 1:B:29:PHE:HD2 | 1:B:31:THR:HB | 14 | 0.08 |
| (1,2267) | 1:A:29:PHE:HD1 | 1:A:31:THR:HB | 6 | 0.08 |
| (1,2267) | 1:A:29:PHE:HD2 | 1:A:31:THR:HB | 6 | 0.08 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 19 | 0.08 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 19 | 0.08 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 19 | 0.08 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 2 | 0.08 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 2 | 0.08 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 2 | 0.08 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 12 | 0.08 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 12 | 0.08 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 12 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 1 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 1 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 1 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 2 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 2 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 2 | 0.08 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 4 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 4 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 4 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 5 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 5 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 5 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 12 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 12 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 12 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 18 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 18 | 0.08 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 18 | 0.08 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 2 | 0.08 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 2 | 0.08 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 2 | 0.08 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 20 | 0.08 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 20 | 0.08 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 20 | 0.08 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 11 | 0.08 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 11 | 0.08 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 11 | 0.08 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 14 | 0.08 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 14 | 0.08 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 14 | 0.08 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 12 | 0.08 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 13 | 0.08 |
| (1,1986) | 1:A:20:ASN:H | 1:A:21:GLN:HB2 | 13 | 0.08 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 6 | 0.08 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 6 | 0.08 |
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 6 | 0.08 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 7 | 0.08 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 7 | 0.08 |
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 7 | 0.08 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 4 | 0.08 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 7 | 0.08 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 18 | 0.08 |
| (1,1898) | 1:B:16:ASN:HB3 | 1:B:17:GLY:H | 18 | 0.08 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG11 | 1 | 0.08 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG12 | 1 | 0.08 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG13 | 1 | 0.08 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG11 | 1 | 0.08 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG12 | 1 | 0.08 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG13 | 1 | 0.08 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG11 | 16 | 0.08 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG12 | 16 | 0.08 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG13 | 16 | 0.08 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG11 | 16 | 0.08 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG12 | 16 | 0.08 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG13 | 16 | 0.08 |
| (1,1806) | 1:A:13:GLU:HB2 | 1:A:15:LYS:HD2 | 8 | 0.08 |
| (1,1806) | 1:A:13:GLU:HB2 | 1:A:15:LYS:HD3 | 8 | 0.08 |
| (1,1803) | 1:B:13:GLU:HB3 | 1:B:71:GLY:HA3 | 9 | 0.08 |
| (1,1803) | 1:B:13:GLU:HB3 | 1:B:71:GLY:HA3 | 13 | 0.08 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 9 | 0.08 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 9 | 0.08 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 9 | 0.08 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 14 | 0.08 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 14 | 0.08 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 14 | 0.08 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 16 | 0.08 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 16 | 0.08 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 16 | 0.08 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 17 | 0.08 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 17 | 0.08 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 17 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG21 | 4 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG22 | 4 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG23 | 4 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG21 | 4 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG22 | 4 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG23 | 4 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG21 | 4 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG22 | 4 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG23 | 4 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG21 | 10 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG22 | 10 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG23 | 10 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG21 | 10 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG22 | 10 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG23 | 10 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG21 | 10 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG22 | 10 | 0.08 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG23 | 10 | 0.08 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 19 | 0.08 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 19 | 0.08 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 19 | 0.08 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 19 | 0.08 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 19 | 0.08 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 19 | 0.08 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 19 | 0.08 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 19 | 0.08 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 19 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 2 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 2 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 2 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 2 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 2 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 2 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 2 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 2 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 2 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 6 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 6 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 6 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 6 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 6 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 6 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 6 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 6 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 6 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 8 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 8 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 8 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 8 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 8 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 8 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 8 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 8 | 0.08 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 8 | 0.08 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD2 | 9 | 0.08 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD3 | 9 | 0.08 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD2 | 9 | 0.08 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD3 | 9 | 0.08 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD2 | 9 | 0.08 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD3 | 9 | 0.08 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 4 | 0.08 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 4 | 0.08 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 4 | 0.08 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 4 | 0.08 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 4 | 0.08 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 4 | 0.08 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 15 | 0.08 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 15 | 0.08 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 15 | 0.08 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 15 | 0.08 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 15 | 0.08 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 15 | 0.08 |
| (1,1527) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HA | 2 | 0.08 |
| (1,1527) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HA | 2 | 0.08 |
| (1,1527) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HA | 2 | 0.08 |
| (1,1527) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HA | 10 | 0.08 |
| (1,1527) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HA | 10 | 0.08 |
| (1,1527) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HA | 10 | 0.08 |
| (1,1456) | 1:B:3:ASP:HB2 | 1:B:53:VAL:H | 12 | 0.08 |
| (1,1338) | 1:B:77:ARG:H | 1:B:77:ARG:HB2 | 16 | 0.08 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 5 | 0.08 |
| (1,1242) | 1:B:69:VAL:HG11 | 1:B:71:GLY:H | 15 | 0.08 |
| (1,1242) | 1:B:69:VAL:HG12 | 1:B:71:GLY:H | 15 | 0.08 |
| (1,1242) | 1:B:69:VAL:HG13 | 1:B:71:GLY:H | 15 | 0.08 |
| (1,1222) | 1:B:69:VAL:H | 1:B:72:VAL:H | 14 | 0.08 |
| (1,1222) | 1:B:69:VAL:H | 1:B:72:VAL:H | 19 | 0.08 |
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 3 | 0.08 |
| (1,1160) | 1:B:67:ARG:H | 1:B:67:ARG:HD2 | 6 | 0.08 |
| (1,1160) | 1:B:67:ARG:H | 1:B:67:ARG:HD3 | 6 | 0.08 |
| (1,979) | 1:B:58:LYS:H | 1:B:58:LYS:HG3 | 20 | 0.07 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 6 | 0.07 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 9 | 0.07 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 10 | 0.07 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 4 | 0.07 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 13 | 0.07 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 1 | 0.07 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 12 | 0.07 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 13 | 0.07 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 14 | 0.07 |
| (1,752) | 1:A:41:LYS:HG2 | 1:A:43:GLY:H | 1 | 0.07 |
| (1,752) | 1:A:41:LYS:HG3 | 1:A:43:GLY:H | 1 | 0.07 |
| (1,735) | 1:B:41:LYS:H | 1:B:46:THR:H | 19 | 0.07 |
| (1,734) | 1:A:41:LYS:H | 1:A:46:THR:H | 1 | 0.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD1 | 9 | 0.07 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD2 | 9 | 0.07 |
| (1,712) | 1:A:41:LYS:H | 1:A:41:LYS:HG2 | 1 | 0.07 |
| (1,712) | 1:A:41:LYS:H | 1:A:41:LYS:HG3 | 1 | 0.07 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 9 | 0.07 |
| (1,7) | 1:A:4:PHE:H | 1:A:5:LEU:HB3 | 15 | 0.07 |
| (1,684) | 1:A:39:ASN:H | 1:A:48:ASN:H | 9 | 0.07 |
| (1,584) | 1:A:20:ASN:H | 1:B:32:ASN:HD21 | 2 | 0.07 |
| (1,584) | 1:A:20:ASN:H | 1:B:32:ASN:HD21 | 15 | 0.07 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD11 | 20 | 0.07 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD12 | 20 | 0.07 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD13 | 20 | 0.07 |
| (1,562) | 1:B:29:PHE:HD1 | 1:B:31:THR:H | 4 | 0.07 |
| (1,562) | 1:B:29:PHE:HD2 | 1:B:31:THR:H | 4 | 0.07 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 6 | 0.07 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 19 | 0.07 |
| (1,5220) | 1:B:64:ASP:HB3 | 1:B:65:LYS:HG2 | 20 | 0.07 |
| (1,5218) | 1:B:64:ASP:HA | 1:B:67:ARG:HG2 | 7 | 0.07 |
| (1,5170) | 1:B:54:LYS:HB2 | 1:B:55:ASN:HB2 | 4 | 0.07 |
| (1,5165) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HB2 | 16 | 0.07 |
| (1,5165) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HB2 | 16 | 0.07 |
| (1,5165) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HB2 | 16 | 0.07 |
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 1 | 0.07 |
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 4 | 0.07 |
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 13 | 0.07 |
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 16 | 0.07 |
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 19 | 0.07 |
| (1,5144) | 1:B:42:ASP:HB2 | 1:B:44:ILE:H | 14 | 0.07 |
| (1,5143) | 1:B:41:LYS:HG2 | 1:B:42:ASP:HB2 | 13 | 0.07 |
| (1,5143) | 1:B:41:LYS:HG3 | 1:B:42:ASP:HB2 | 13 | 0.07 |
| (1,5130) | 1:B:38:LEU:HD21 | 1:B:39:ASN:HD21 | 4 | 0.07 |
| (1,5130) | 1:B:38:LEU:HD22 | 1:B:39:ASN:HD21 | 4 | 0.07 |
| (1,5130) | 1:B:38:LEU:HD23 | 1:B:39:ASN:HD21 | 4 | 0.07 |
| (1,5105) | 1:B:34:ARG:HB2 | 1:B:35:THR:H | 10 | 0.07 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD11 | 5 | 0.07 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD12 | 5 | 0.07 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD13 | 5 | 0.07 |
| (1,5073) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HE2 | 11 | 0.07 |
| (1,5073) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HE3 | 11 | 0.07 |
| (1,5073) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HE2 | 12 | 0.07 |
| (1,5073) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HE3 | 12 | 0.07 |
| (1,5073) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HE2 | 17 | 0.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5073) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HE3 | 17 | 0.07 |
| (1,5067) | 1:B:28:LYS:H | 1:B:28:LYS:HG2 | 17 | 0.07 |
| (1,5067) | 1:B:28:LYS:H | 1:B:28:LYS:HG2 | 19 | 0.07 |
| (1,5067) | 1:B:28:LYS:H | 1:B:28:LYS:HG2 | 20 | 0.07 |
| (1,5056) | 1:B:26:ILE:HG12 | 1:B:27:SER:H | 10 | 0.07 |
| (1,5056) | 1:B:26:ILE:HG12 | 1:B:27:SER:H | 15 | 0.07 |
| (1,5056) | 1:B:26:ILE:HG12 | 1:B:27:SER:H | 16 | 0.07 |
| (1,5028) | 1:B:20:ASN:HB2 | 1:B:21:GLN:H | 18 | 0.07 |
| (1,4930) | 1:A:68:LYS:HA | 1:A:68:LYS:HG2 | 2 | 0.07 |
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 13 | 0.07 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD11 | 6 | 0.07 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD12 | 6 | 0.07 |
| (1,4891) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD13 | 6 | 0.07 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB2 | 17 | 0.07 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB3 | 17 | 0.07 |
| (1,4873) | 1:A:54:LYS:HE2 | 1:A:55:ASN:HD21 | 10 | 0.07 |
| (1,4873) | 1:A:54:LYS:HE3 | 1:A:55:ASN:HD21 | 10 | 0.07 |
| (1,4864) | 1:A:53:VAL:HG21 | 1:A:58:LYS:HB2 | 13 | 0.07 |
| (1,4864) | 1:A:53:VAL:HG22 | 1:A:58:LYS:HB2 | 13 | 0.07 |
| (1,4864) | 1:A:53:VAL:HG23 | 1:A:58:LYS:HB2 | 13 | 0.07 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD11 | 2 | 0.07 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD12 | 2 | 0.07 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD13 | 2 | 0.07 |
| (1,4826) | 1:A:38:LEU:HD21 | 1:A:39:ASN:HD21 | 11 | 0.07 |
| (1,4826) | 1:A:38:LEU:HD22 | 1:A:39:ASN:HD21 | 11 | 0.07 |
| (1,4826) | 1:A:38:LEU:HD23 | 1:A:39:ASN:HD21 | 11 | 0.07 |
| (1,4813) | 1:A:36:ILE:HG12 | 1:A:37:VAL:H | 6 | 0.07 |
| (1,4812) | 1:A:36:ILE:HG21 | 1:A:48:ASN:HB2 | 5 | 0.07 |
| (1,4812) | 1:A:36:ILE:HG22 | 1:A:48:ASN:HB2 | 5 | 0.07 |
| (1,4812) | 1:A:36:ILE:HG23 | 1:A:48:ASN:HB2 | 5 | 0.07 |
| (1,4812) | 1:A:36:ILE:HG21 | 1:A:48:ASN:HB2 | 16 | 0.07 |
| (1,4812) | 1:A:36:ILE:HG22 | 1:A:48:ASN:HB2 | 16 | 0.07 |
| (1,4812) | 1:A:36:ILE:HG23 | 1:A:48:ASN:HB2 | 16 | 0.07 |
| (1,4803) | 1:A:34:ARG:HB2 | 1:A:51:ILE:H | 16 | 0.07 |
| (1,4787) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HD2 | 3 | 0.07 |
| (1,4787) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HD2 | 13 | 0.07 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG21 | 8 | 0.07 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG22 | 8 | 0.07 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG23 | 8 | 0.07 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 6 | 0.07 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 13 | 0.07 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 15 | 0.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4737) | 1:A:24:GLY:HA2 | 1:A:25:VAL:HA | 13 | 0.07 |
| (1,4733) | 1:A:23:THR:HG21 | 1:A:27:SER:HB2 | 5 | 0.07 |
| (1,4733) | 1:A:23:THR:HG22 | 1:A:27:SER:HB2 | 5 | 0.07 |
| (1,4733) | 1:A:23:THR:HG23 | 1:A:27:SER:HB2 | 5 | 0.07 |
| (1,4733) | 1:A:23:THR:HG21 | 1:A:27:SER:HB2 | 9 | 0.07 |
| (1,4733) | 1:A:23:THR:HG22 | 1:A:27:SER:HB2 | 9 | 0.07 |
| (1,4733) | 1:A:23:THR:HG23 | 1:A:27:SER:HB2 | 9 | 0.07 |
| (1,4724) | 1:A:20:ASN:HB2 | 1:A:21:GLN:HE21 | 8 | 0.07 |
| (1,4696) | 1:A:16:ASN:HB2 | 1:A:18:MET:H | 10 | 0.07 |
| (1,4690) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD21 | 15 | 0.07 |
| (1,4690) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD21 | 15 | 0.07 |
| (1,4678) | 1:A:15:LYS:H | 1:A:18:MET:HG2 | 9 | 0.07 |
| (1,4667) | 1:A:14:ASP:HA | 1:A:15:LYS:HB2 | 2 | 0.07 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 2 | 0.07 |
| (1,4641) | 1:A:6:ALA:HB1 | 1:A:77:ARG:HG2 | 1 | 0.07 |
| (1,4641) | 1:A:6:ALA:HB2 | 1:A:77:ARG:HG2 | 1 | 0.07 |
| (1,4641) | 1:A:6:ALA:HB3 | 1:A:77:ARG:HG2 | 1 | 0.07 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 13 | 0.07 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 13 | 0.07 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 13 | 0.07 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 4 | 0.07 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 4 | 0.07 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 4 | 0.07 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 5 | 0.07 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 5 | 0.07 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 5 | 0.07 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 11 | 0.07 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 11 | 0.07 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 11 | 0.07 |
| (1,4609) | 1:A:81:LEU:HB3 | 1:A:83:HIS:HD2 | 14 | 0.07 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 5 | 0.07 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 6 | 0.07 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 14 | 0.07 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG21 | 8 | 0.07 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG22 | 8 | 0.07 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG23 | 8 | 0.07 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG21 | 14 | 0.07 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG22 | 14 | 0.07 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG23 | 14 | 0.07 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 9 | 0.07 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 9 | 0.07 |
| (1,4538) | 1:B:52:PHE:HD1 | 1:B:53:VAL:H | 15 | 0.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4538) | 1:B:52:PHE:HD2 | 1:B:53:VAL:H | 15 | 0.07 |
| (1,4538) | 1:B:52:PHE:HD1 | 1:B:53:VAL:H | 19 | 0.07 |
| (1,4538) | 1:B:52:PHE:HD2 | 1:B:53:VAL:H | 19 | 0.07 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 13 | 0.07 |
| (1,4495) | 1:A:12:GLY:H | 1:A:45:PHE:HE1 | 7 | 0.07 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 3 | 0.07 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 3 | 0.07 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 3 | 0.07 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 17 | 0.07 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 17 | 0.07 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 17 | 0.07 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 8 | 0.07 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 8 | 0.07 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 8 | 0.07 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 20 | 0.07 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 20 | 0.07 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 20 | 0.07 |
| (1,4325) | 1:B:80:ASN:HA | 1:B:81:LEU:HG | 5 | 0.07 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 12 | 0.07 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 12 | 0.07 |
| (1,4243) | 1:B:15:LYS:HA | 1:B:17:GLY:H | 9 | 0.07 |
| (1,4243) | 1:B:15:LYS:HA | 1:B:17:GLY:H | 20 | 0.07 |
| (1,4217) | 1:B:8:ILE:HA | 1:B:78:LEU:HB2 | 3 | 0.07 |
| (1,4217) | 1:B:8:ILE:HA | 1:B:78:LEU:HB2 | 11 | 0.07 |
| (1,4216) | 1:A:8:ILE:HA | 1:A:78:LEU:HB2 | 18 | 0.07 |
| (1,4216) | 1:A:8:ILE:HA | 1:A:78:LEU:HB2 | 20 | 0.07 |
| (1,4199) | 1:B:82:GLU:H | 1:B:83:HIS:HB3 | 4 | 0.07 |
| (1,4198) | 1:A:82:GLU:H | 1:A:83:HIS:HB3 | 19 | 0.07 |
| (1,4191) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HB3 | 6 | 0.07 |
| (1,4191) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HB3 | 6 | 0.07 |
| (1,4191) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HB3 | 6 | 0.07 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD11 | 17 | 0.07 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD12 | 17 | 0.07 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD13 | 17 | 0.07 |
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD11 | 17 | 0.07 |
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD12 | 17 | 0.07 |
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD13 | 17 | 0.07 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD11 | 17 | 0.07 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD12 | 17 | 0.07 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD13 | 17 | 0.07 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 2 | 0.07 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 2 | 0.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 2 | 0.07 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 15 | 0.07 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 15 | 0.07 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 15 | 0.07 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 1 | 0.07 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 1 | 0.07 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 1 | 0.07 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 5 | 0.07 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 5 | 0.07 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 5 | 0.07 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 15 | 0.07 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 15 | 0.07 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 15 | 0.07 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 7 | 0.07 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 7 | 0.07 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 7 | 0.07 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 18 | 0.07 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 18 | 0.07 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 18 | 0.07 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 20 | 0.07 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 20 | 0.07 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 20 | 0.07 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 1 | 0.07 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 1 | 0.07 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 1 | 0.07 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 4 | 0.07 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 4 | 0.07 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 4 | 0.07 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD11 | 5 | 0.07 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD12 | 5 | 0.07 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD13 | 5 | 0.07 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD11 | 6 | 0.07 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD12 | 6 | 0.07 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD13 | 6 | 0.07 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 18 | 0.07 |
| (1,4115) | 1:A:18:MET:HA | 1:A:21:GLN:HB2 | 1 | 0.07 |
| (1,4115) | 1:A:18:MET:HA | 1:A:21:GLN:HB2 | 12 | 0.07 |
| (1,4111) | 1:A:18:MET:HE1 | 1:A:21:GLN:HE21 | 17 | 0.07 |
| (1,4111) | 1:A:18:MET:HE2 | 1:A:21:GLN:HE21 | 17 | 0.07 |
| (1,4111) | 1:A:18:MET:HE3 | 1:A:21:GLN:HE21 | 17 | 0.07 |
| (1,4075) | 1:B:82:GLU:HA | 1:B:83:HIS:HB2 | 4 | 0.07 |
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD11 | 15 | 0.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD12 | 15 | 0.07 |
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD13 | 15 | 0.07 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD11 | 15 | 0.07 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD12 | 15 | 0.07 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD13 | 15 | 0.07 |
| (1,3937) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HB3 | 5 | 0.07 |
| (1,3921) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HD2 | 17 | 0.07 |
| (1,3921) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HD3 | 17 | 0.07 |
| (1,3921) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HD2 | 17 | 0.07 |
| (1,3921) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HD3 | 17 | 0.07 |
| (1,3921) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HD2 | 17 | 0.07 |
| (1,3921) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HD3 | 17 | 0.07 |
| (1,3921) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HD2 | 18 | 0.07 |
| (1,3921) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HD3 | 18 | 0.07 |
| (1,3921) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HD2 | 18 | 0.07 |
| (1,3921) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HD3 | 18 | 0.07 |
| (1,3921) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HD2 | 18 | 0.07 |
| (1,3921) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HD3 | 18 | 0.07 |
| (1,3896) | 1:A:74:THR:HA | 1:A:76:GLU:HG2 | 15 | 0.07 |
| (1,3896) | 1:A:74:THR:HA | 1:A:76:GLU:HG3 | 15 | 0.07 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 15 | 0.07 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 15 | 0.07 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 15 | 0.07 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 16 | 0.07 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 16 | 0.07 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 16 | 0.07 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 11 | 0.07 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 11 | 0.07 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 11 | 0.07 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 18 | 0.07 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 18 | 0.07 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 18 | 0.07 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 8 | 0.07 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 8 | 0.07 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 8 | 0.07 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 12 | 0.07 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 12 | 0.07 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 12 | 0.07 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 14 | 0.07 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 14 | 0.07 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 14 | 0.07 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG11 | 17 | 0.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG12 | 17 | 0.07 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG13 | 17 | 0.07 |
| (1,3756) | 1:B:69:VAL:H | 1:B:70:GLN:HB2 | 5 | 0.07 |
| (1,3756) | 1:B:69:VAL:H | 1:B:70:GLN:HB3 | 5 | 0.07 |
| (1,3756) | 1:B:69:VAL:H | 1:B:70:GLN:HB2 | 15 | 0.07 |
| (1,3756) | 1:B:69:VAL:H | 1:B:70:GLN:HB3 | 15 | 0.07 |
| (1,3755) | 1:A:69:VAL:H | 1:A:70:GLN:HB2 | 17 | 0.07 |
| (1,3755) | 1:A:69:VAL:H | 1:A:70:GLN:HB3 | 17 | 0.07 |
| (1,3735) | 1:A:66:LEU:HA | 1:A:69:VAL:HB | 18 | 0.07 |
| (1,3734) | 1:B:20:ASN:HA | 1:B:22:ILE:HB | 1 | 0.07 |
| (1,3734) | 1:B:20:ASN:HA | 1:B:22:ILE:HB | 5 | 0.07 |
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 3 | 0.07 |
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 4 | 0.07 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG11 | 11 | 0.07 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG12 | 11 | 0.07 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG13 | 11 | 0.07 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG11 | 11 | 0.07 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG12 | 11 | 0.07 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG13 | 11 | 0.07 |
| (1,3700) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD21 | 1 | 0.07 |
| (1,3700) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD21 | 1 | 0.07 |
| (1,3700) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD21 | 19 | 0.07 |
| (1,3700) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD21 | 19 | 0.07 |
| (1,3699) | 1:A:15:LYS:HE2 | 1:A:16:ASN:HD21 | 11 | 0.07 |
| (1,3699) | 1:A:15:LYS:HE3 | 1:A:16:ASN:HD21 | 11 | 0.07 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 9 | 0.07 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 9 | 0.07 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 9 | 0.07 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 16 | 0.07 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 16 | 0.07 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 16 | 0.07 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 19 | 0.07 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 19 | 0.07 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 19 | 0.07 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB2 | 18 | 0.07 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB3 | 18 | 0.07 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB2 | 17 | 0.07 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB3 | 17 | 0.07 |
| (1,3537) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HB2 | 14 | 0.07 |
| (1,3536) | 1:A:64:ASP:HB2 | 1:A:65:LYS:HB2 | 3 | 0.07 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE1 | 15 | 0.07 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE2 | 15 | 0.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE3 | 15 | 0.07 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 2 | 0.07 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 2 | 0.07 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 2 | 0.07 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 3 | 0.07 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 3 | 0.07 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 3 | 0.07 |
| (1,3519) | 1:A:63:MET:HE1 | 1:A:76:GLU:HA | 5 | 0.07 |
| (1,3519) | 1:A:63:MET:HE2 | 1:A:76:GLU:HA | 5 | 0.07 |
| (1,3519) | 1:A:63:MET:HE3 | 1:A:76:GLU:HA | 5 | 0.07 |
| (1,3519) | 1:A:63:MET:HE1 | 1:A:76:GLU:HA | 6 | 0.07 |
| (1,3519) | 1:A:63:MET:HE2 | 1:A:76:GLU:HA | 6 | 0.07 |
| (1,3519) | 1:A:63:MET:HE3 | 1:A:76:GLU:HA | 6 | 0.07 |
| (1,3519) | 1:A:63:MET:HE1 | 1:A:76:GLU:HA | 12 | 0.07 |
| (1,3519) | 1:A:63:MET:HE2 | 1:A:76:GLU:HA | 12 | 0.07 |
| (1,3519) | 1:A:63:MET:HE3 | 1:A:76:GLU:HA | 12 | 0.07 |
| (1,3518) | 1:B:63:MET:HE1 | 1:B:77:ARG:HA | 20 | 0.07 |
| (1,3518) | 1:B:63:MET:HE2 | 1:B:77:ARG:HA | 20 | 0.07 |
| (1,3518) | 1:B:63:MET:HE3 | 1:B:77:ARG:HA | 20 | 0.07 |
| (1,3517) | 1:A:63:MET:HE1 | 1:A:77:ARG:HA | 7 | 0.07 |
| (1,3517) | 1:A:63:MET:HE2 | 1:A:77:ARG:HA | 7 | 0.07 |
| (1,3517) | 1:A:63:MET:HE3 | 1:A:77:ARG:HA | 7 | 0.07 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE1 | 6 | 0.07 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE2 | 6 | 0.07 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE3 | 6 | 0.07 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE1 | 7 | 0.07 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE2 | 7 | 0.07 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE3 | 7 | 0.07 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE1 | 11 | 0.07 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE2 | 11 | 0.07 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE3 | 11 | 0.07 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE1 | 14 | 0.07 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE2 | 14 | 0.07 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE3 | 14 | 0.07 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE1 | 3 | 0.07 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE2 | 3 | 0.07 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE3 | 3 | 0.07 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE1 | 17 | 0.07 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE2 | 17 | 0.07 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE3 | 17 | 0.07 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE1 | 7 | 0.07 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE2 | 7 | 0.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE3 | 7 | 0.07 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE1 | 7 | 0.07 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE2 | 7 | 0.07 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE3 | 7 | 0.07 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE1 | 7 | 0.07 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE2 | 7 | 0.07 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE3 | 7 | 0.07 |
| (1,3465) | 1:A:30:ASP:H | 1:A:62:LEU:HD11 | 4 | 0.07 |
| (1,3465) | 1:A:30:ASP:H | 1:A:62:LEU:HD12 | 4 | 0.07 |
| (1,3465) | 1:A:30:ASP:H | 1:A:62:LEU:HD13 | 4 | 0.07 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 1 | 0.07 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 3 | 0.07 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 4 | 0.07 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 7 | 0.07 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 9 | 0.07 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 11 | 0.07 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 2 | 0.07 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 8 | 0.07 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 10 | 0.07 |
| (1,3195) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD21 | 14 | 0.07 |
| (1,3195) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD21 | 14 | 0.07 |
| (1,3185) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD22 | 10 | 0.07 |
| (1,3185) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD22 | 10 | 0.07 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD2 | 5 | 0.07 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD3 | 5 | 0.07 |
| (1,3182) | 1:A:54:LYS:HA | 1:A:54:LYS:HD2 | 14 | 0.07 |
| (1,3182) | 1:A:54:LYS:HA | 1:A:54:LYS:HD3 | 14 | 0.07 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 15 | 0.07 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 15 | 0.07 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 15 | 0.07 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 15 | 0.07 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 15 | 0.07 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 15 | 0.07 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 1 | 0.07 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 1 | 0.07 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 1 | 0.07 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 1 | 0.07 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 1 | 0.07 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 1 | 0.07 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 20 | 0.07 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 20 | 0.07 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 20 | 0.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 20 | 0.07 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 20 | 0.07 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 20 | 0.07 |
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD11 | 11 | 0.07 |
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD12 | 11 | 0.07 |
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD13 | 11 | 0.07 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD11 | 12 | 0.07 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD12 | 12 | 0.07 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD13 | 12 | 0.07 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD11 | 12 | 0.07 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD12 | 12 | 0.07 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD13 | 12 | 0.07 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD11 | 11 | 0.07 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD12 | 11 | 0.07 |
| (1,3033) | 1:B:7:GLY:HA3 | 1:B:51:ILE:HD13 | 11 | 0.07 |
| (1,3) | 1:A:2:THR:HG21 | 1:A:4:PHE:H | 20 | 0.07 |
| (1,3) | 1:A:2:THR:HG22 | 1:A:4:PHE:H | 20 | 0.07 |
| (1,3) | 1:A:2:THR:HG23 | 1:A:4:PHE:H | 20 | 0.07 |
| (1,292) | 1:B:20:ASN:H | 1:B:20:ASN:HD22 | 13 | 0.07 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 3 | 0.07 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 3 | 0.07 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 3 | 0.07 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 1 | 0.07 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 1 | 0.07 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 1 | 0.07 |
| (1,2878) | 1:A:8:ILE:H | 1:A:50:MET:HG3 | 6 | 0.07 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 10 | 0.07 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD21 | 4 | 0.07 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD22 | 4 | 0.07 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD23 | 4 | 0.07 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD21 | 4 | 0.07 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD22 | 4 | 0.07 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD23 | 4 | 0.07 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD21 | 4 | 0.07 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD22 | 4 | 0.07 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD23 | 4 | 0.07 |
| (1,2704) | 1:B:9:ARG:HD2 | 1:B:46:THR:HG21 | 20 | 0.07 |
| (1,2704) | 1:B:9:ARG:HD2 | 1:B:46:THR:HG22 | 20 | 0.07 |
| (1,2704) | 1:B:9:ARG:HD2 | 1:B:46:THR:HG23 | 20 | 0.07 |
| (1,2704) | 1:B:9:ARG:HD3 | 1:B:46:THR:HG21 | 20 | 0.07 |
| (1,2704) | 1:B:9:ARG:HD3 | 1:B:46:THR:HG22 | 20 | 0.07 |
| (1,2704) | 1:B:9:ARG:HD3 | 1:B:46:THR:HG23 | 20 | 0.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 2 | 0.07 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 2 | 0.07 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 2 | 0.07 |
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 5 | 0.07 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 5 | 0.07 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 5 | 0.07 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 6 | 0.07 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 6 | 0.07 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 6 | 0.07 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 19 | 0.07 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 19 | 0.07 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 19 | 0.07 |
| (1,2634) | 1:B:40:ALA:HA | 1:B:44:ILE:HG13 | 8 | 0.07 |
| (1,2633) | 1:A:40:ALA:HA | 1:A:44:ILE:HG13 | 7 | 0.07 |
| (1,2510) | 1:B:38:LEU:HD11 | 1:B:39:ASN:H | 19 | 0.07 |
| (1,2510) | 1:B:38:LEU:HD12 | 1:B:39:ASN:H | 19 | 0.07 |
| (1,2510) | 1:B:38:LEU:HD13 | 1:B:39:ASN:H | 19 | 0.07 |
| (1,2416) | 1:B:36:ILE:HD11 | 1:B:38:LEU:H | 10 | 0.07 |
| (1,2416) | 1:B:36:ILE:HD12 | 1:B:38:LEU:H | 10 | 0.07 |
| (1,2416) | 1:B:36:ILE:HD13 | 1:B:38:LEU:H | 10 | 0.07 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 1 | 0.07 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 1 | 0.07 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 1 | 0.07 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 10 | 0.07 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 10 | 0.07 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 10 | 0.07 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 17 | 0.07 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 17 | 0.07 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 17 | 0.07 |
| (1,2389) | 1:A:36:ILE:HG21 | 1:A:48:ASN:H | 6 | 0.07 |
| (1,2389) | 1:A:36:ILE:HG22 | 1:A:48:ASN:H | 6 | 0.07 |
| (1,2389) | 1:A:36:ILE:HG23 | 1:A:48:ASN:H | 6 | 0.07 |
| (1,2389) | 1:A:36:ILE:HG21 | 1:A:48:ASN:H | 19 | 0.07 |
| (1,2389) | 1:A:36:ILE:HG22 | 1:A:48:ASN:H | 19 | 0.07 |
| (1,2389) | 1:A:36:ILE:HG23 | 1:A:48:ASN:H | 19 | 0.07 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 15 | 0.07 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 15 | 0.07 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 15 | 0.07 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 18 | 0.07 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 18 | 0.07 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 18 | 0.07 |
| (1,2267) | 1:A:29:PHE:HD1 | 1:A:31:THR:HB | 10 | 0.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2267) | 1:A:29:PHE:HD2 | 1:A:31:THR:HB | 10 | 0.07 |
| (1,2259) | 1:A:68:LYS:HA | 1:A:68:LYS:HD2 | 11 | 0.07 |
| (1,2249) | 1:A:27:SER:HG | 1:A:28:LYS:HG2 | 7 | 0.07 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 5 | 0.07 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 5 | 0.07 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 5 | 0.07 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 11 | 0.07 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 11 | 0.07 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 11 | 0.07 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 16 | 0.07 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 16 | 0.07 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 16 | 0.07 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 17 | 0.07 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 17 | 0.07 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 17 | 0.07 |
| (1,216) | 1:B:16:ASN:HA | 1:B:17:GLY:H | 17 | 0.07 |
| (1,215) | 1:A:16:ASN:HA | 1:A:17:GLY:H | 8 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 6 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 6 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 6 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 7 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 7 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 7 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 8 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 8 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 8 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 13 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 13 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 13 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 14 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 14 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 14 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 16 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 16 | 0.07 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 16 | 0.07 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 4 | 0.07 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 4 | 0.07 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 4 | 0.07 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 14 | 0.07 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 14 | 0.07 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 14 | 0.07 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 2 | 0.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 2 | 0.07 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 2 | 0.07 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 6 | 0.07 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 6 | 0.07 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 6 | 0.07 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 15 | 0.07 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 15 | 0.07 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 15 | 0.07 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 17 | 0.07 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 17 | 0.07 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 17 | 0.07 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 1 | 0.07 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 1 | 0.07 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 1 | 0.07 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 9 | 0.07 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 9 | 0.07 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 9 | 0.07 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 12 | 0.07 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 12 | 0.07 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 12 | 0.07 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 13 | 0.07 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 13 | 0.07 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 13 | 0.07 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG21 | 15 | 0.07 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG22 | 15 | 0.07 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG23 | 15 | 0.07 |
| (1,1987) | 1:B:20:ASN:H | 1:B:21:GLN:HB2 | 6 | 0.07 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 3 | 0.07 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 3 | 0.07 |
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 3 | 0.07 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 1 | 0.07 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 1 | 0.07 |
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 1 | 0.07 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 14 | 0.07 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 14 | 0.07 |
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 14 | 0.07 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 11 | 0.07 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 6 | 0.07 |
| (1,1898) | 1:B:16:ASN:HB3 | 1:B:17:GLY:H | 2 | 0.07 |
| (1,1897) | 1:A:16:ASN:HB3 | 1:A:17:GLY:H | 5 | 0.07 |
| (1,1878) | 1:A:25:VAL:HG21 | 1:A:65:LYS:HE2 | 5 | 0.07 |
| (1,1878) | 1:A:25:VAL:HG21 | 1:A:65:LYS:HE3 | 5 | 0.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1878) | 1:A:25:VAL:HG22 | 1:A:65:LYS:HE2 | 5 | 0.07 |
| (1,1878) | 1:A:25:VAL:HG22 | 1:A:65:LYS:HE3 | 5 | 0.07 |
| (1,1878) | 1:A:25:VAL:HG23 | 1:A:65:LYS:HE2 | 5 | 0.07 |
| (1,1878) | 1:A:25:VAL:HG23 | 1:A:65:LYS:HE3 | 5 | 0.07 |
| (1,1876) | 1:A:41:LYS:HE2 | 1:A:44:ILE:HD11 | 12 | 0.07 |
| (1,1876) | 1:A:41:LYS:HE2 | 1:A:44:ILE:HD12 | 12 | 0.07 |
| (1,1876) | 1:A:41:LYS:HE2 | 1:A:44:ILE:HD13 | 12 | 0.07 |
| (1,1876) | 1:A:41:LYS:HE3 | 1:A:44:ILE:HD11 | 12 | 0.07 |
| (1,1876) | 1:A:41:LYS:HE3 | 1:A:44:ILE:HD12 | 12 | 0.07 |
| (1,1876) | 1:A:41:LYS:HE3 | 1:A:44:ILE:HD13 | 12 | 0.07 |
| (1,1862) | 1:A:13:GLU:HB2 | 1:A:15:LYS:HG2 | 16 | 0.07 |
| (1,1862) | 1:A:13:GLU:HB2 | 1:A:15:LYS:HG3 | 16 | 0.07 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG11 | 20 | 0.07 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG12 | 20 | 0.07 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG13 | 20 | 0.07 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG11 | 20 | 0.07 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG12 | 20 | 0.07 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG13 | 20 | 0.07 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG11 | 20 | 0.07 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG12 | 20 | 0.07 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG13 | 20 | 0.07 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG11 | 20 | 0.07 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG12 | 20 | 0.07 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG13 | 20 | 0.07 |
| (1,181) | 1:A:15:LYS:H | 1:A:18:MET:HG2 | 4 | 0.07 |
| (1,1802) | 1:A:13:GLU:HB3 | 1:A:71:GLY:HA3 | 8 | 0.07 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 16 | 0.07 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 16 | 0.07 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 16 | 0.07 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 20 | 0.07 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 20 | 0.07 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 20 | 0.07 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG21 | 12 | 0.07 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG22 | 12 | 0.07 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG23 | 12 | 0.07 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG21 | 12 | 0.07 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG22 | 12 | 0.07 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG23 | 12 | 0.07 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG21 | 12 | 0.07 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG22 | 12 | 0.07 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG23 | 12 | 0.07 |
| (1,172) | 1:B:15:LYS:H | 1:B:18:MET:HE1 | 20 | 0.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,172) | 1:B:15:LYS:H | 1:B:18:MET:HE2 | 20 | 0.07 |
| (1,172) | 1:B:15:LYS:H | 1:B:18:MET:HE3 | 20 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 7 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 7 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 7 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 7 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 7 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 7 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 7 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 7 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 7 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 8 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 8 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 8 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 8 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 8 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 8 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 8 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 8 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 8 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 14 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 14 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 14 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 14 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 14 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 14 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 14 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 14 | 0.07 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 14 | 0.07 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 12 | 0.07 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 12 | 0.07 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 12 | 0.07 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 12 | 0.07 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 12 | 0.07 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 12 | 0.07 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 12 | 0.07 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 12 | 0.07 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 12 | 0.07 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 13 | 0.07 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 13 | 0.07 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 13 | 0.07 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 13 | 0.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 13 | 0.07 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 13 | 0.07 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 13 | 0.07 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 13 | 0.07 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 13 | 0.07 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD2 | 4 | 0.07 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD3 | 4 | 0.07 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD2 | 4 | 0.07 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD3 | 4 | 0.07 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD2 | 4 | 0.07 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD3 | 4 | 0.07 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 14 | 0.07 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 14 | 0.07 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 14 | 0.07 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 14 | 0.07 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 14 | 0.07 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 14 | 0.07 |
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 5 | 0.07 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 5 | 0.07 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 5 | 0.07 |
| (1,1527) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HA | 1 | 0.07 |
| (1,1527) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HA | 1 | 0.07 |
| (1,1527) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HA | 1 | 0.07 |
| (1,1527) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HA | 4 | 0.07 |
| (1,1527) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HA | 4 | 0.07 |
| (1,1527) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HA | 4 | 0.07 |
| (1,1527) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HA | 9 | 0.07 |
| (1,1527) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HA | 9 | 0.07 |
| (1,1527) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HA | 9 | 0.07 |
| (1,1456) | 1:B:3:ASP:HB2 | 1:B:53:VAL:H | 4 | 0.07 |
| (1,1455) | 1:A:3:ASP:HB2 | 1:A:53:VAL:H | 17 | 0.07 |
| (1,1356) | 1:B:77:ARG:HG2 | 1:B:78:LEU:H | 16 | 0.07 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 3 | 0.07 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 6 | 0.07 |
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 8 | 0.07 |
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 12 | 0.07 |
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 15 | 0.07 |
| (1,1176) | 1:B:67:ARG:HE | 1:B:75:VAL:HB | 14 | 0.07 |
| (1,1131) | 1:A:62:LEU:HD11 | 1:A:66:LEU:H | 4 | 0.07 |
| (1,1131) | 1:A:62:LEU:HD12 | 1:A:66:LEU:H | 4 | 0.07 |
| (1,1131) | 1:A:62:LEU:HD13 | 1:A:66:LEU:H | 4 | 0.07 |
| (1,1130) | 1:B:62:LEU:HD11 | 1:B:65:LYS:H | 16 | 0.07 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1130) | 1:B:62:LEU:HD12 | 1:B:65:LYS:H | 16 | 0.07 |
| (1,1130) | 1:B:62:LEU:HD13 | 1:B:65:LYS:H | 16 | 0.07 |
| (1,978) | 1:A:58:LYS:H | 1:A:58:LYS:HG3 | 12 | 0.06 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 4 | 0.06 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 8 | 0.06 |
| (1,925) | 1:B:3:ASP:HB3 | 1:B:53:VAL:H | 12 | 0.06 |
| (1,924) | 1:A:3:ASP:HB3 | 1:A:53:VAL:H | 1 | 0.06 |
| (1,924) | 1:A:3:ASP:HB3 | 1:A:53:VAL:H | 17 | 0.06 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 1 | 0.06 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 16 | 0.06 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 17 | 0.06 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 19 | 0.06 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 2 | 0.06 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 3 | 0.06 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 5 | 0.06 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 8 | 0.06 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 17 | 0.06 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 18 | 0.06 |
| (1,742) | 1:A:41:LYS:HB2 | 1:A:42:ASP:H | 1 | 0.06 |
| (1,742) | 1:A:41:LYS:HB3 | 1:A:42:ASP:H | 1 | 0.06 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD1 | 8 | 0.06 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD2 | 8 | 0.06 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD1 | 13 | 0.06 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD2 | 13 | 0.06 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD1 | 17 | 0.06 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD2 | 17 | 0.06 |
| (1,630) | 1:A:35:THR:H | 1:A:83:HIS:HE1 | 3 | 0.06 |
| (1,579) | 1:A:32:ASN:HD21 | 1:A:33:ILE:HB | 4 | 0.06 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD11 | 15 | 0.06 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD12 | 15 | 0.06 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD13 | 15 | 0.06 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD11 | 19 | 0.06 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD12 | 19 | 0.06 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD13 | 19 | 0.06 |
| (1,561) | 1:A:29:PHE:HD1 | 1:A:31:THR:H | 16 | 0.06 |
| (1,561) | 1:A:29:PHE:HD2 | 1:A:31:THR:H | 16 | 0.06 |
| (1,5262) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HA | 9 | 0.06 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 8 | 0.06 |
| (1,5223) | 1:B:65:LYS:H | 1:B:65:LYS:HD2 | 8 | 0.06 |
| (1,5220) | 1:B:64:ASP:HB3 | 1:B:65:LYS:HG2 | 11 | 0.06 |
| (1,5218) | 1:B:64:ASP:HA | 1:B:67:ARG:HG2 | 2 | 0.06 |
| (1,5206) | 1:B:62:LEU:HA | 1:B:65:LYS:HG2 | 17 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 7 | 0.06 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 7 | 0.06 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 7 | 0.06 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB2 | 8 | 0.06 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB3 | 8 | 0.06 |
| (1,5165) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HB2 | 20 | 0.06 |
| (1,5165) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HB2 | 20 | 0.06 |
| (1,5165) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HB2 | 20 | 0.06 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG21 | 3 | 0.06 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG22 | 3 | 0.06 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG23 | 3 | 0.06 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD11 | 4 | 0.06 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD12 | 4 | 0.06 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD13 | 4 | 0.06 |
| (1,5076) | 1:B:28:LYS:HG2 | 1:B:29:PHE:H | 9 | 0.06 |
| (1,5056) | 1:B:26:ILE:HG12 | 1:B:27:SER:H | 8 | 0.06 |
| (1,5056) | 1:B:26:ILE:HG12 | 1:B:27:SER:H | 11 | 0.06 |
| (1,5036) | 1:B:24:GLY:HA2 | 1:B:25:VAL:HA | 14 | 0.06 |
| (1,5008) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD21 | 6 | 0.06 |
| (1,5008) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD21 | 6 | 0.06 |
| (1,4980) | 1:B:9:ARG:H | 1:B:9:ARG:HG2 | 5 | 0.06 |
| (1,4968) | 1:B:8:ILE:H | 1:B:8:ILE:HG12 | 9 | 0.06 |
| (1,4953) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HD1 | 4 | 0.06 |
| (1,4953) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HD2 | 4 | 0.06 |
| (1,4948) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HA | 19 | 0.06 |
| (1,4946) | 1:A:82:GLU:H | 1:A:82:GLU:HG2 | 9 | 0.06 |
| (1,4915) | 1:A:65:LYS:HA | 1:A:68:LYS:HD2 | 4 | 0.06 |
| (1,4912) | 1:A:65:LYS:H | 1:A:65:LYS:HD2 | 17 | 0.06 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD11 | 20 | 0.06 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD12 | 20 | 0.06 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD13 | 20 | 0.06 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 8 | 0.06 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 9 | 0.06 |
| (1,4842) | 1:A:42:ASP:HB2 | 1:A:44:ILE:HG12 | 4 | 0.06 |
| (1,4836) | 1:A:39:ASN:HD21 | 1:A:48:ASN:HD21 | 5 | 0.06 |
| (1,4803) | 1:A:34:ARG:HB2 | 1:A:51:ILE:H | 9 | 0.06 |
| (1,4789) | 1:A:31:THR:HG21 | 1:A:58:LYS:HE2 | 8 | 0.06 |
| (1,4789) | 1:A:31:THR:HG22 | 1:A:58:LYS:HE2 | 8 | 0.06 |
| (1,4789) | 1:A:31:THR:HG23 | 1:A:58:LYS:HE2 | 8 | 0.06 |
| (1,4769) | 1:A:28:LYS:H | 1:A:28:LYS:HG2 | 11 | 0.06 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG21 | 1 | 0.06 |
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG22 | 1 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4765) | 1:A:27:SER:HB2 | 1:B:23:THR:HG23 | 1 | 0.06 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 5 | 0.06 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 16 | 0.06 |
| (1,4728) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HG12 | 12 | 0.06 |
| (1,4726) | 1:A:20:ASN:HB2 | 1:B:33:ILE:HD11 | 11 | 0.06 |
| (1,4726) | 1:A:20:ASN:HB2 | 1:B:33:ILE:HD12 | 11 | 0.06 |
| (1,4726) | 1:A:20:ASN:HB2 | 1:B:33:ILE:HD13 | 11 | 0.06 |
| (1,4703) | 1:A:17:GLY:HA2 | 1:A:21:GLN:HE22 | 19 | 0.06 |
| (1,4670) | 1:A:14:ASP:HB2 | 1:A:40:ALA:HB1 | 15 | 0.06 |
| (1,4670) | 1:A:14:ASP:HB2 | 1:A:40:ALA:HB2 | 15 | 0.06 |
| (1,4670) | 1:A:14:ASP:HB2 | 1:A:40:ALA:HB3 | 15 | 0.06 |
| (1,4661) | 1:A:9:ARG:HD2 | 1:A:48:ASN:HD21 | 16 | 0.06 |
| (1,4661) | 1:A:9:ARG:HD3 | 1:A:48:ASN:HD21 | 16 | 0.06 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 18 | 0.06 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 7 | 0.06 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 7 | 0.06 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 7 | 0.06 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 3 | 0.06 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 3 | 0.06 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 3 | 0.06 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 9 | 0.06 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 9 | 0.06 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 9 | 0.06 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 14 | 0.06 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 14 | 0.06 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 14 | 0.06 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 15 | 0.06 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 15 | 0.06 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 15 | 0.06 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 16 | 0.06 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 16 | 0.06 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 16 | 0.06 |
| (1,4614) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HD2 | 10 | 0.06 |
| (1,4614) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HD2 | 13 | 0.06 |
| (1,4609) | 1:A:81:LEU:HB3 | 1:A:83:HIS:HD2 | 5 | 0.06 |
| (1,4607) | 1:A:5:LEU:HG | 1:A:83:HIS:HD2 | 2 | 0.06 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 1 | 0.06 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 4 | 0.06 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 13 | 0.06 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 5 | 0.06 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 7 | 0.06 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 19 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG21 | 3 | 0.06 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG22 | 3 | 0.06 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG23 | 3 | 0.06 |
| (1,4572) | 1:B:44:ILE:HG13 | 1:B:73:PHE:HE1 | 10 | 0.06 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 5 | 0.06 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 5 | 0.06 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 7 | 0.06 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 7 | 0.06 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 8 | 0.06 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 8 | 0.06 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 18 | 0.06 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 18 | 0.06 |
| (1,4538) | 1:B:52:PHE:HD1 | 1:B:53:VAL:H | 5 | 0.06 |
| (1,4538) | 1:B:52:PHE:HD2 | 1:B:53:VAL:H | 5 | 0.06 |
| (1,4537) | 1:A:52:PHE:HD1 | 1:A:53:VAL:H | 12 | 0.06 |
| (1,4537) | 1:A:52:PHE:HD2 | 1:A:53:VAL:H | 12 | 0.06 |
| (1,4475) | 1:A:22:ILE:HD11 | 1:A:45:PHE:HE1 | 3 | 0.06 |
| (1,4475) | 1:A:22:ILE:HD12 | 1:A:45:PHE:HE1 | 3 | 0.06 |
| (1,4475) | 1:A:22:ILE:HD13 | 1:A:45:PHE:HE1 | 3 | 0.06 |
| (1,4444) | 1:A:45:PHE:HD1 | 1:A:47:CYS:HG | 15 | 0.06 |
| (1,4444) | 1:A:45:PHE:HD2 | 1:A:47:CYS:HG | 15 | 0.06 |
| (1,4419) | 1:B:29:PHE:H | 1:B:29:PHE:HD1 | 4 | 0.06 |
| (1,4419) | 1:B:29:PHE:H | 1:B:29:PHE:HD2 | 4 | 0.06 |
| (1,4413) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 12 | 0.06 |
| (1,4413) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 12 | 0.06 |
| (1,4413) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 14 | 0.06 |
| (1,4413) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 14 | 0.06 |
| (1,4412) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 8 | 0.06 |
| (1,4412) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 8 | 0.06 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 9 | 0.06 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 9 | 0.06 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 9 | 0.06 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 13 | 0.06 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 13 | 0.06 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 13 | 0.06 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 2 | 0.06 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 2 | 0.06 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 2 | 0.06 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 9 | 0.06 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 9 | 0.06 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 9 | 0.06 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 12 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 12 | 0.06 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 12 | 0.06 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 13 | 0.06 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 13 | 0.06 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 13 | 0.06 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 16 | 0.06 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 16 | 0.06 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 16 | 0.06 |
| (1,4334) | 1:A:83:HIS:HA | 1:A:83:HIS:HD2 | 2 | 0.06 |
| (1,4325) | 1:B:80:ASN:HA | 1:B:81:LEU:HG | 13 | 0.06 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 5 | 0.06 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 5 | 0.06 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 10 | 0.06 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 10 | 0.06 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 15 | 0.06 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 15 | 0.06 |
| (1,4242) | 1:A:15:LYS:HA | 1:A:17:GLY:H | 5 | 0.06 |
| (1,4217) | 1:B:8:ILE:HA | 1:B:78:LEU:HB2 | 10 | 0.06 |
| (1,4217) | 1:B:8:ILE:HA | 1:B:78:LEU:HB2 | 12 | 0.06 |
| (1,4199) | 1:B:82:GLU:H | 1:B:83:HIS:HB3 | 10 | 0.06 |
| (1,4199) | 1:B:82:GLU:H | 1:B:83:HIS:HB3 | 12 | 0.06 |
| (1,4191) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HB3 | 16 | 0.06 |
| (1,4191) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HB3 | 16 | 0.06 |
| (1,4191) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HB3 | 16 | 0.06 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD11 | 12 | 0.06 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD12 | 12 | 0.06 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD13 | 12 | 0.06 |
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD11 | 12 | 0.06 |
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD12 | 12 | 0.06 |
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD13 | 12 | 0.06 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD11 | 12 | 0.06 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD12 | 12 | 0.06 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD13 | 12 | 0.06 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 5 | 0.06 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 5 | 0.06 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 5 | 0.06 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 12 | 0.06 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 12 | 0.06 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 12 | 0.06 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 12 | 0.06 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 12 | 0.06 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 12 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 16 | 0.06 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 16 | 0.06 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 16 | 0.06 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 2 | 0.06 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 2 | 0.06 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 2 | 0.06 |
| (1,4147) | 1:B:61:THR:HG21 | 1:B:65:LYS:HB3 | 15 | 0.06 |
| (1,4147) | 1:B:61:THR:HG22 | 1:B:65:LYS:HB3 | 15 | 0.06 |
| (1,4147) | 1:B:61:THR:HG23 | 1:B:65:LYS:HB3 | 15 | 0.06 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD11 | 1 | 0.06 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD12 | 1 | 0.06 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD13 | 1 | 0.06 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD11 | 8 | 0.06 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD12 | 8 | 0.06 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD13 | 8 | 0.06 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD11 | 10 | 0.06 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD12 | 10 | 0.06 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD13 | 10 | 0.06 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 4 | 0.06 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 5 | 0.06 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 8 | 0.06 |
| (1,4115) | 1:A:18:MET:HA | 1:A:21:GLN:HB2 | 3 | 0.06 |
| (1,4115) | 1:A:18:MET:HA | 1:A:21:GLN:HB2 | 14 | 0.06 |
| (1,4106) | 1:B:15:LYS:HB3 | 1:B:18:MET:HB3 | 11 | 0.06 |
| (1,4106) | 1:B:15:LYS:HB3 | 1:B:18:MET:HB3 | 17 | 0.06 |
| (1,4106) | 1:B:15:LYS:HB3 | 1:B:18:MET:HB3 | 20 | 0.06 |
| (1,4075) | 1:B:82:GLU:HA | 1:B:83:HIS:HB2 | 15 | 0.06 |
| (1,4074) | 1:A:82:GLU:HA | 1:A:83:HIS:HB2 | 1 | 0.06 |
| (1,4074) | 1:A:82:GLU:HA | 1:A:83:HIS:HB2 | 11 | 0.06 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD21 | 12 | 0.06 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD22 | 12 | 0.06 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD23 | 12 | 0.06 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD21 | 17 | 0.06 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD22 | 17 | 0.06 |
| (1,4060) | 1:A:7:GLY:HA2 | 1:A:81:LEU:HD23 | 17 | 0.06 |
| (1,3952) | 1:A:78:LEU:HB2 | 1:A:80:ASN:H | 16 | 0.06 |
| (1,3936) | 1:A:7:GLY:HA2 | 1:A:78:LEU:HB3 | 5 | 0.06 |
| (1,3917) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HD2 | 4 | 0.06 |
| (1,3917) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HD3 | 4 | 0.06 |
| (1,3917) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HD2 | 4 | 0.06 |
| (1,3917) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HD3 | 4 | 0.06 |
| (1,3917) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HD2 | 4 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3917) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HD3 | 4 | 0.06 |
| (1,3917) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HD2 | 6 | 0.06 |
| (1,3917) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HD3 | 6 | 0.06 |
| (1,3917) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HD2 | 6 | 0.06 |
| (1,3917) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HD3 | 6 | 0.06 |
| (1,3917) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HD2 | 6 | 0.06 |
| (1,3917) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HD3 | 6 | 0.06 |
| (1,3897) | 1:B:74:THR:HA | 1:B:76:GLU:HG2 | 12 | 0.06 |
| (1,3897) | 1:B:74:THR:HA | 1:B:76:GLU:HG3 | 12 | 0.06 |
| (1,3896) | 1:A:74:THR:HA | 1:A:76:GLU:HG2 | 14 | 0.06 |
| (1,3896) | 1:A:74:THR:HA | 1:A:76:GLU:HG3 | 14 | 0.06 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 10 | 0.06 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 10 | 0.06 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 10 | 0.06 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 14 | 0.06 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 14 | 0.06 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 14 | 0.06 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 16 | 0.06 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 16 | 0.06 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 16 | 0.06 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 20 | 0.06 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 20 | 0.06 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 20 | 0.06 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 3 | 0.06 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 3 | 0.06 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 3 | 0.06 |
| (1,3840) | 1:B:72:VAL:HG11 | 1:B:74:THR:HB | 13 | 0.06 |
| (1,3840) | 1:B:72:VAL:HG12 | 1:B:74:THR:HB | 13 | 0.06 |
| (1,3840) | 1:B:72:VAL:HG13 | 1:B:74:THR:HB | 13 | 0.06 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 7 | 0.06 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 7 | 0.06 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 7 | 0.06 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 8 | 0.06 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 8 | 0.06 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 8 | 0.06 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 9 | 0.06 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 9 | 0.06 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 9 | 0.06 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 16 | 0.06 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 16 | 0.06 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 16 | 0.06 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 17 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 17 | 0.06 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 17 | 0.06 |
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 18 | 0.06 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 18 | 0.06 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 18 | 0.06 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG11 | 4 | 0.06 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG12 | 4 | 0.06 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG13 | 4 | 0.06 |
| (1,3734) | 1:B:20:ASN:HA | 1:B:22:ILE:HB | 13 | 0.06 |
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 2 | 0.06 |
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 10 | 0.06 |
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 19 | 0.06 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 5 | 0.06 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 5 | 0.06 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 5 | 0.06 |
| (1,3702) | 1:B:15:LYS:HE2 | 1:B:18:MET:H | 5 | 0.06 |
| (1,3702) | 1:B:15:LYS:HE3 | 1:B:18:MET:H | 5 | 0.06 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE2 | 3 | 0.06 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE3 | 3 | 0.06 |
| (1,3691) | 1:A:68:LYS:HA | 1:A:68:LYS:HE2 | 6 | 0.06 |
| (1,3691) | 1:A:68:LYS:HA | 1:A:68:LYS:HE3 | 6 | 0.06 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 10 | 0.06 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 10 | 0.06 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 10 | 0.06 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 18 | 0.06 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 18 | 0.06 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 18 | 0.06 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 1 | 0.06 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 1 | 0.06 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 1 | 0.06 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 6 | 0.06 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 6 | 0.06 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 6 | 0.06 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 8 | 0.06 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 8 | 0.06 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 8 | 0.06 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 12 | 0.06 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 12 | 0.06 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 12 | 0.06 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 16 | 0.06 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 16 | 0.06 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 16 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB2 | 12 | 0.06 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB3 | 12 | 0.06 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB2 | 3 | 0.06 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB3 | 3 | 0.06 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB2 | 14 | 0.06 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB3 | 14 | 0.06 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB2 | 20 | 0.06 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB3 | 20 | 0.06 |
| (1,3537) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HB2 | 7 | 0.06 |
| (1,3536) | 1:A:64:ASP:HB2 | 1:A:65:LYS:HB2 | 2 | 0.06 |
| (1,3536) | 1:A:64:ASP:HB2 | 1:A:65:LYS:HB2 | 15 | 0.06 |
| (1,3536) | 1:A:64:ASP:HB2 | 1:A:65:LYS:HB2 | 16 | 0.06 |
| (1,3528) | 1:B:63:MET:HE1 | 1:B:77:ARG:H | 2 | 0.06 |
| (1,3528) | 1:B:63:MET:HE2 | 1:B:77:ARG:H | 2 | 0.06 |
| (1,3528) | 1:B:63:MET:HE3 | 1:B:77:ARG:H | 2 | 0.06 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 1 | 0.06 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 1 | 0.06 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 1 | 0.06 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 9 | 0.06 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 9 | 0.06 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 9 | 0.06 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 13 | 0.06 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 13 | 0.06 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 13 | 0.06 |
| (1,3519) | 1:A:63:MET:HE1 | 1:A:76:GLU:HA | 1 | 0.06 |
| (1,3519) | 1:A:63:MET:HE2 | 1:A:76:GLU:HA | 1 | 0.06 |
| (1,3519) | 1:A:63:MET:HE3 | 1:A:76:GLU:HA | 1 | 0.06 |
| (1,3519) | 1:A:63:MET:HE1 | 1:A:76:GLU:HA | 3 | 0.06 |
| (1,3519) | 1:A:63:MET:HE2 | 1:A:76:GLU:HA | 3 | 0.06 |
| (1,3519) | 1:A:63:MET:HE3 | 1:A:76:GLU:HA | 3 | 0.06 |
| (1,3519) | 1:A:63:MET:HE1 | 1:A:76:GLU:HA | 14 | 0.06 |
| (1,3519) | 1:A:63:MET:HE2 | 1:A:76:GLU:HA | 14 | 0.06 |
| (1,3519) | 1:A:63:MET:HE3 | 1:A:76:GLU:HA | 14 | 0.06 |
| (1,3518) | 1:B:63:MET:HE1 | 1:B:77:ARG:HA | 4 | 0.06 |
| (1,3518) | 1:B:63:MET:HE2 | 1:B:77:ARG:HA | 4 | 0.06 |
| (1,3518) | 1:B:63:MET:HE3 | 1:B:77:ARG:HA | 4 | 0.06 |
| (1,3517) | 1:A:63:MET:HE1 | 1:A:77:ARG:HA | 19 | 0.06 |
| (1,3517) | 1:A:63:MET:HE2 | 1:A:77:ARG:HA | 19 | 0.06 |
| (1,3517) | 1:A:63:MET:HE3 | 1:A:77:ARG:HA | 19 | 0.06 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE1 | 12 | 0.06 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE2 | 12 | 0.06 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE3 | 12 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE1 | 10 | 0.06 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE2 | 10 | 0.06 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE3 | 10 | 0.06 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE1 | 10 | 0.06 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE2 | 10 | 0.06 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE3 | 10 | 0.06 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE1 | 10 | 0.06 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE2 | 10 | 0.06 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE3 | 10 | 0.06 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 13 | 0.06 |
| (1,3419) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HB2 | 15 | 0.06 |
| (1,3386) | 1:A:61:THR:HG21 | 1:A:65:LYS:HE2 | 19 | 0.06 |
| (1,3386) | 1:A:61:THR:HG21 | 1:A:65:LYS:HE3 | 19 | 0.06 |
| (1,3386) | 1:A:61:THR:HG22 | 1:A:65:LYS:HE2 | 19 | 0.06 |
| (1,3386) | 1:A:61:THR:HG22 | 1:A:65:LYS:HE3 | 19 | 0.06 |
| (1,3386) | 1:A:61:THR:HG23 | 1:A:65:LYS:HE2 | 19 | 0.06 |
| (1,3386) | 1:A:61:THR:HG23 | 1:A:65:LYS:HE3 | 19 | 0.06 |
| (1,3285) | 1:B:58:LYS:H | 1:B:58:LYS:HD2 | 3 | 0.06 |
| (1,3285) | 1:B:58:LYS:H | 1:B:58:LYS:HD3 | 3 | 0.06 |
| (1,3285) | 1:B:58:LYS:H | 1:B:58:LYS:HD2 | 18 | 0.06 |
| (1,3285) | 1:B:58:LYS:H | 1:B:58:LYS:HD3 | 18 | 0.06 |
| (1,3274) | 1:A:30:ASP:HB2 | 1:A:58:LYS:HD2 | 15 | 0.06 |
| (1,3274) | 1:A:30:ASP:HB2 | 1:A:58:LYS:HD3 | 15 | 0.06 |
| (1,3274) | 1:A:30:ASP:HB3 | 1:A:58:LYS:HD2 | 15 | 0.06 |
| (1,3274) | 1:A:30:ASP:HB3 | 1:A:58:LYS:HD3 | 15 | 0.06 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 12 | 0.06 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 17 | 0.06 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 20 | 0.06 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG21 | 3 | 0.06 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG22 | 3 | 0.06 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG23 | 3 | 0.06 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG21 | 3 | 0.06 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG22 | 3 | 0.06 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG23 | 3 | 0.06 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG21 | 15 | 0.06 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG22 | 15 | 0.06 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG23 | 15 | 0.06 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG21 | 15 | 0.06 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG22 | 15 | 0.06 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG23 | 15 | 0.06 |
| (1,3191) | 1:B:54:LYS:H | 1:B:54:LYS:HD2 | 14 | 0.06 |
| (1,3191) | 1:B:54:LYS:H | 1:B:54:LYS:HD3 | 14 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3185) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD22 | 8 | 0.06 |
| (1,3185) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD22 | 8 | 0.06 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD2 | 15 | 0.06 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD3 | 15 | 0.06 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD2 | 19 | 0.06 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD3 | 19 | 0.06 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD2 | 20 | 0.06 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD3 | 20 | 0.06 |
| (1,3094) | 1:A:53:VAL:HG11 | 1:A:58:LYS:HZ1 | 7 | 0.06 |
| (1,3094) | 1:A:53:VAL:HG12 | 1:A:58:LYS:HZ1 | 7 | 0.06 |
| (1,3094) | 1:A:53:VAL:HG13 | 1:A:58:LYS:HZ1 | 7 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 7 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 7 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 7 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 7 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 7 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 7 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 8 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 8 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 8 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 8 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 8 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 8 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 9 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 9 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 9 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 9 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 9 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 9 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 11 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 11 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 11 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 11 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 11 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 11 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 17 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 17 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 17 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 17 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 17 | 0.06 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 17 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 11 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 11 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 11 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 11 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 11 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 11 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 12 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 12 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 12 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 12 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 12 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 12 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 16 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 16 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 16 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 16 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 16 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 16 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 17 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 17 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 17 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 17 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 17 | 0.06 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 17 | 0.06 |
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD11 | 12 | 0.06 |
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD12 | 12 | 0.06 |
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD13 | 12 | 0.06 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD11 | 16 | 0.06 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD12 | 16 | 0.06 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD13 | 16 | 0.06 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD11 | 20 | 0.06 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD12 | 20 | 0.06 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD13 | 20 | 0.06 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD11 | 4 | 0.06 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD12 | 4 | 0.06 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD13 | 4 | 0.06 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD11 | 4 | 0.06 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD12 | 4 | 0.06 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD13 | 4 | 0.06 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD11 | 9 | 0.06 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD12 | 9 | 0.06 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD13 | 9 | 0.06 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD11 | 9 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD12 | 9 | 0.06 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD13 | 9 | 0.06 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD11 | 18 | 0.06 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD12 | 18 | 0.06 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD13 | 18 | 0.06 |
| (1,2991) | 1:A:51:ILE:HG21 | 1:B:20:ASN:HD22 | 11 | 0.06 |
| (1,2991) | 1:A:51:ILE:HG22 | 1:B:20:ASN:HD22 | 11 | 0.06 |
| (1,2991) | 1:A:51:ILE:HG23 | 1:B:20:ASN:HD22 | 11 | 0.06 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG21 | 5 | 0.06 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG22 | 5 | 0.06 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG23 | 5 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG21 | 1:B:62:LEU:HD11 | 17 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG21 | 1:B:62:LEU:HD12 | 17 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG21 | 1:B:62:LEU:HD13 | 17 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG22 | 1:B:62:LEU:HD11 | 17 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG22 | 1:B:62:LEU:HD12 | 17 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG22 | 1:B:62:LEU:HD13 | 17 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG23 | 1:B:62:LEU:HD11 | 17 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG23 | 1:B:62:LEU:HD12 | 17 | 0.06 |
| (1,2971) | 1:B:8:ILE:HG23 | 1:B:62:LEU:HD13 | 17 | 0.06 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 8 | 0.06 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 8 | 0.06 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 8 | 0.06 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 14 | 0.06 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 14 | 0.06 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 14 | 0.06 |
| (1,2879) | 1:B:8:ILE:H | 1:B:50:MET:HG3 | 5 | 0.06 |
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 5 | 0.06 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 1 | 0.06 |
| (1,2754) | 1:B:23:THR:HG1 | 1:B:47:CYS:HB3 | 20 | 0.06 |
| (1,2753) | 1:A:23:THR:HG1 | 1:A:47:CYS:HB3 | 4 | 0.06 |
| (1,2669) | 1:A:44:ILE:HD11 | 1:A:46:THR:HB | 11 | 0.06 |
| (1,2669) | 1:A:44:ILE:HD12 | 1:A:46:THR:HB | 11 | 0.06 |
| (1,2669) | 1:A:44:ILE:HD13 | 1:A:46:THR:HB | 11 | 0.06 |
| (1,2661) | 1:A:44:ILE:HG21 | 1:A:45:PHE:H | 20 | 0.06 |
| (1,2661) | 1:A:44:ILE:HG22 | 1:A:45:PHE:H | 20 | 0.06 |
| (1,2661) | 1:A:44:ILE:HG23 | 1:A:45:PHE:H | 20 | 0.06 |
| (1,2658) | 1:B:14:ASP:H | 1:B:44:ILE:HG21 | 8 | 0.06 |
| (1,2658) | 1:B:14:ASP:H | 1:B:44:ILE:HG22 | 8 | 0.06 |
| (1,2658) | 1:B:14:ASP:H | 1:B:44:ILE:HG23 | 8 | 0.06 |
| (1,2637) | 1:A:44:ILE:HG13 | 1:A:45:PHE:H | 7 | 0.06 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD21 | 13 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD22 | 13 | 0.06 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD23 | 13 | 0.06 |
| (1,2509) | 1:A:38:LEU:HD11 | 1:A:39:ASN:H | 12 | 0.06 |
| (1,2509) | 1:A:38:LEU:HD12 | 1:A:39:ASN:H | 12 | 0.06 |
| (1,2509) | 1:A:38:LEU:HD13 | 1:A:39:ASN:H | 12 | 0.06 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 2 | 0.06 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 2 | 0.06 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 2 | 0.06 |
| (1,2402) | 1:B:23:THR:HG1 | 1:B:36:ILE:HD11 | 9 | 0.06 |
| (1,2402) | 1:B:23:THR:HG1 | 1:B:36:ILE:HD12 | 9 | 0.06 |
| (1,2402) | 1:B:23:THR:HG1 | 1:B:36:ILE:HD13 | 9 | 0.06 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 12 | 0.06 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 12 | 0.06 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 12 | 0.06 |
| (1,2390) | 1:B:36:ILE:HG21 | 1:B:48:ASN:H | 13 | 0.06 |
| (1,2390) | 1:B:36:ILE:HG22 | 1:B:48:ASN:H | 13 | 0.06 |
| (1,2390) | 1:B:36:ILE:HG23 | 1:B:48:ASN:H | 13 | 0.06 |
| (1,2389) | 1:A:36:ILE:HG21 | 1:A:48:ASN:H | 5 | 0.06 |
| (1,2389) | 1:A:36:ILE:HG22 | 1:A:48:ASN:H | 5 | 0.06 |
| (1,2389) | 1:A:36:ILE:HG23 | 1:A:48:ASN:H | 5 | 0.06 |
| (1,2389) | 1:A:36:ILE:HG21 | 1:A:48:ASN:H | 17 | 0.06 |
| (1,2389) | 1:A:36:ILE:HG22 | 1:A:48:ASN:H | 17 | 0.06 |
| (1,2389) | 1:A:36:ILE:HG23 | 1:A:48:ASN:H | 17 | 0.06 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 3 | 0.06 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 3 | 0.06 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 3 | 0.06 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 6 | 0.06 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 6 | 0.06 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 6 | 0.06 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 17 | 0.06 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 17 | 0.06 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 17 | 0.06 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 1 | 0.06 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 1 | 0.06 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 1 | 0.06 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 6 | 0.06 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 6 | 0.06 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 6 | 0.06 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 20 | 0.06 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 20 | 0.06 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 20 | 0.06 |
| (1,2267) | 1:A:29:PHE:HD1 | 1:A:31:THR:HB | 12 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2267) | 1:A:29:PHE:HD2 | 1:A:31:THR:HB | 12 | 0.06 |
| (1,2249) | 1:A:27:SER:HG | 1:A:28:LYS:HG2 | 9 | 0.06 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 1 | 0.06 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 1 | 0.06 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 1 | 0.06 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 2 | 0.06 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 2 | 0.06 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 2 | 0.06 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 6 | 0.06 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 6 | 0.06 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 6 | 0.06 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 20 | 0.06 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 20 | 0.06 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 20 | 0.06 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 9 | 0.06 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 9 | 0.06 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 9 | 0.06 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 19 | 0.06 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 19 | 0.06 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 19 | 0.06 |
| (1,216) | 1:B:16:ASN:HA | 1:B:17:GLY:H | 4 | 0.06 |
| (1,216) | 1:B:16:ASN:HA | 1:B:17:GLY:H | 7 | 0.06 |
| (1,216) | 1:B:16:ASN:HA | 1:B:17:GLY:H | 11 | 0.06 |
| (1,216) | 1:B:16:ASN:HA | 1:B:17:GLY:H | 14 | 0.06 |
| (1,216) | 1:B:16:ASN:HA | 1:B:17:GLY:H | 20 | 0.06 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 3 | 0.06 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 3 | 0.06 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 3 | 0.06 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 10 | 0.06 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 10 | 0.06 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 10 | 0.06 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 11 | 0.06 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 11 | 0.06 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 11 | 0.06 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 15 | 0.06 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 15 | 0.06 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 15 | 0.06 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 1 | 0.06 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 1 | 0.06 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 1 | 0.06 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 10 | 0.06 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 10 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 10 | 0.06 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 12 | 0.06 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 12 | 0.06 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 12 | 0.06 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 19 | 0.06 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 19 | 0.06 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 19 | 0.06 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 1 | 0.06 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 1 | 0.06 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 1 | 0.06 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 7 | 0.06 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 7 | 0.06 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 7 | 0.06 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 8 | 0.06 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 8 | 0.06 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 8 | 0.06 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 19 | 0.06 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 19 | 0.06 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 19 | 0.06 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 8 | 0.06 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 8 | 0.06 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 8 | 0.06 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 10 | 0.06 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 10 | 0.06 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 10 | 0.06 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 14 | 0.06 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 14 | 0.06 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 14 | 0.06 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 16 | 0.06 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 16 | 0.06 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 16 | 0.06 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 18 | 0.06 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 18 | 0.06 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 18 | 0.06 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 6 | 0.06 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 6 | 0.06 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 6 | 0.06 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG21 | 7 | 0.06 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG22 | 7 | 0.06 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG23 | 7 | 0.06 |
| (1,206) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD22 | 4 | 0.06 |
| (1,206) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD22 | 4 | 0.06 |

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wwPDB NMR Structure Validation Summary Report

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,206) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD22 | 7 | 0.06 |
| (1,206) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD22 | 7 | 0.06 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 5 | 0.06 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 5 | 0.06 |
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 5 | 0.06 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 14 | 0.06 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 14 | 0.06 |
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 14 | 0.06 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 3 | 0.06 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 17 | 0.06 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 10 | 0.06 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 19 | 0.06 |
| (1,1898) | 1:B:16:ASN:HB3 | 1:B:17:GLY:H | 13 | 0.06 |
| (1,1898) | 1:B:16:ASN:HB3 | 1:B:17:GLY:H | 16 | 0.06 |
| (1,1897) | 1:A:16:ASN:HB3 | 1:A:17:GLY:H | 6 | 0.06 |
| (1,1897) | 1:A:16:ASN:HB3 | 1:A:17:GLY:H | 12 | 0.06 |
| (1,1875) | 1:B:11:VAL:HG21 | 1:B:41:LYS:HE2 | 1 | 0.06 |
| (1,1875) | 1:B:11:VAL:HG21 | 1:B:41:LYS:HE3 | 1 | 0.06 |
| (1,1875) | 1:B:11:VAL:HG22 | 1:B:41:LYS:HE2 | 1 | 0.06 |
| (1,1875) | 1:B:11:VAL:HG22 | 1:B:41:LYS:HE3 | 1 | 0.06 |
| (1,1875) | 1:B:11:VAL:HG23 | 1:B:41:LYS:HE2 | 1 | 0.06 |
| (1,1875) | 1:B:11:VAL:HG23 | 1:B:41:LYS:HE3 | 1 | 0.06 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG11 | 18 | 0.06 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG12 | 18 | 0.06 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG13 | 18 | 0.06 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG11 | 18 | 0.06 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG12 | 18 | 0.06 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG13 | 18 | 0.06 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG11 | 8 | 0.06 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG12 | 8 | 0.06 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG13 | 8 | 0.06 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG11 | 8 | 0.06 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG12 | 8 | 0.06 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG13 | 8 | 0.06 |
| (1,1799) | 1:B:13:GLU:HB3 | 1:B:15:LYS:HD2 | 15 | 0.06 |
| (1,1799) | 1:B:13:GLU:HB3 | 1:B:15:LYS:HD3 | 15 | 0.06 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 4 | 0.06 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 4 | 0.06 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 4 | 0.06 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 12 | 0.06 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 12 | 0.06 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 12 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG21 | 8 | 0.06 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG22 | 8 | 0.06 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG23 | 8 | 0.06 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG21 | 8 | 0.06 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG22 | 8 | 0.06 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG23 | 8 | 0.06 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG21 | 8 | 0.06 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG22 | 8 | 0.06 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG23 | 8 | 0.06 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG21 | 17 | 0.06 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG22 | 17 | 0.06 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG23 | 17 | 0.06 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG21 | 17 | 0.06 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG22 | 17 | 0.06 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG23 | 17 | 0.06 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG21 | 17 | 0.06 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG22 | 17 | 0.06 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG23 | 17 | 0.06 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD11 | 4 | 0.06 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD12 | 4 | 0.06 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD13 | 4 | 0.06 |
| (1,1612) | 1:B:24:GLY:H | 1:B:26:ILE:HD11 | 4 | 0.06 |
| (1,1612) | 1:B:24:GLY:H | 1:B:26:ILE:HD12 | 4 | 0.06 |
| (1,1612) | 1:B:24:GLY:H | 1:B:26:ILE:HD13 | 4 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 2 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 2 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 2 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 2 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 2 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 2 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 2 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 2 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 2 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 3 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 3 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 3 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 3 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 3 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 3 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 3 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 3 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 3 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 13 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 13 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 13 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 13 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 13 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 13 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 13 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 13 | 0.06 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 13 | 0.06 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD2 | 7 | 0.06 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD3 | 7 | 0.06 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD2 | 7 | 0.06 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD3 | 7 | 0.06 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD2 | 7 | 0.06 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD3 | 7 | 0.06 |
| (1,1542) | 1:B:6:ALA:HB1 | 1:B:7:GLY:HA3 | 7 | 0.06 |
| (1,1542) | 1:B:6:ALA:HB2 | 1:B:7:GLY:HA3 | 7 | 0.06 |
| (1,1542) | 1:B:6:ALA:HB3 | 1:B:7:GLY:HA3 | 7 | 0.06 |
| (1,1542) | 1:B:6:ALA:HB1 | 1:B:7:GLY:HA3 | 8 | 0.06 |
| (1,1542) | 1:B:6:ALA:HB2 | 1:B:7:GLY:HA3 | 8 | 0.06 |
| (1,1542) | 1:B:6:ALA:HB3 | 1:B:7:GLY:HA3 | 8 | 0.06 |
| (1,1541) | 1:A:6:ALA:HB1 | 1:A:7:GLY:HA3 | 1 | 0.06 |
| (1,1541) | 1:A:6:ALA:HB2 | 1:A:7:GLY:HA3 | 1 | 0.06 |
| (1,1541) | 1:A:6:ALA:HB3 | 1:A:7:GLY:HA3 | 1 | 0.06 |
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 19 | 0.06 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 19 | 0.06 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 19 | 0.06 |
| (1,1527) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HA | 16 | 0.06 |
| (1,1527) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HA | 16 | 0.06 |
| (1,1527) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HA | 16 | 0.06 |
| (1,1527) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HA | 17 | 0.06 |
| (1,1527) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HA | 17 | 0.06 |
| (1,1527) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HA | 17 | 0.06 |
| (1,1419) | 1:A:40:ALA:H | 1:A:41:LYS:HD2 | 9 | 0.06 |
| (1,1419) | 1:A:40:ALA:H | 1:A:41:LYS:HD3 | 9 | 0.06 |
| (1,1338) | 1:B:77:ARG:H | 1:B:77:ARG:HB2 | 8 | 0.06 |
| (1,1225) | 1:A:69:VAL:H | 1:A:70:GLN:H | 11 | 0.06 |
| (1,1222) | 1:B:69:VAL:H | 1:B:72:VAL:H | 1 | 0.06 |
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 6 | 0.06 |
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 13 | 0.06 |
| (1,1131) | 1:A:62:LEU:HD11 | 1:A:66:LEU:H | 19 | 0.06 |
| (1,1131) | 1:A:62:LEU:HD12 | 1:A:66:LEU:H | 19 | 0.06 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1131) | 1:A:62:LEU:HD13 | 1:A:66:LEU:H | 19 | 0.06 |
| (1,1091) | 1:B:64:ASP:H | 1:B:75:VAL:HG11 | 14 | 0.06 |
| (1,1091) | 1:B:64:ASP:H | 1:B:75:VAL:HG12 | 14 | 0.06 |
| (1,1091) | 1:B:64:ASP:H | 1:B:75:VAL:HG13 | 14 | 0.06 |
| (1,979) | 1:B:58:LYS:H | 1:B:58:LYS:HG3 | 13 | 0.05 |
| (1,978) | 1:A:58:LYS:H | 1:A:58:LYS:HG3 | 18 | 0.05 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 9 | 0.05 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 10 | 0.05 |
| (1,958) | 1:A:57:ASP:H | 1:A:58:LYS:HG3 | 15 | 0.05 |
| (1,915) | 1:B:51:ILE:HG12 | 1:B:52:PHE:H | 14 | 0.05 |
| (1,914) | 1:A:51:ILE:HG12 | 1:A:52:PHE:H | 13 | 0.05 |
| (1,914) | 1:A:51:ILE:HG12 | 1:A:52:PHE:H | 19 | 0.05 |
| (1,84) | 1:A:9:ARG:HE | 1:A:11:VAL:HG21 | 14 | 0.05 |
| (1,84) | 1:A:9:ARG:HE | 1:A:11:VAL:HG22 | 14 | 0.05 |
| (1,84) | 1:A:9:ARG:HE | 1:A:11:VAL:HG23 | 14 | 0.05 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 2 | 0.05 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 3 | 0.05 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 4 | 0.05 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 5 | 0.05 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 8 | 0.05 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 12 | 0.05 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 18 | 0.05 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 12 | 0.05 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 16 | 0.05 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 19 | 0.05 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 20 | 0.05 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 6 | 0.05 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 10 | 0.05 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 17 | 0.05 |
| (1,777) | 1:B:43:GLY:H | 1:B:44:ILE:H | 4 | 0.05 |
| (1,735) | 1:B:41:LYS:H | 1:B:46:THR:H | 17 | 0.05 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD1 | 11 | 0.05 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD2 | 11 | 0.05 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD1 | 4 | 0.05 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD2 | 4 | 0.05 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD1 | 7 | 0.05 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD2 | 7 | 0.05 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD1 | 8 | 0.05 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD2 | 8 | 0.05 |
| (1,631) | 1:B:35:THR:H | 1:B:83:HIS:HE1 | 9 | 0.05 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD11 | 6 | 0.05 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD12 | 6 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD13 | 6 | 0.05 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD11 | 15 | 0.05 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD12 | 15 | 0.05 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD13 | 15 | 0.05 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD11 | 17 | 0.05 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD12 | 17 | 0.05 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD13 | 17 | 0.05 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD11 | 18 | 0.05 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD12 | 18 | 0.05 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD13 | 18 | 0.05 |
| (1,564) | 1:A:31:THR:H | 1:B:20:ASN:HD21 | 13 | 0.05 |
| (1,5260) | 1:B:82:GLU:H | 1:B:82:GLU:HG2 | 11 | 0.05 |
| (1,5259) | 1:B:81:LEU:H | 1:B:82:GLU:HG2 | 16 | 0.05 |
| (1,5248) | 1:B:76:GLU:HB2 | 1:B:77:ARG:H | 19 | 0.05 |
| (1,5243) | 1:B:68:LYS:HA | 1:B:68:LYS:HD2 | 1 | 0.05 |
| (1,5223) | 1:B:65:LYS:H | 1:B:65:LYS:HD2 | 5 | 0.05 |
| (1,5222) | 1:B:65:LYS:H | 1:B:65:LYS:HG2 | 13 | 0.05 |
| (1,5220) | 1:B:64:ASP:HB3 | 1:B:65:LYS:HG2 | 17 | 0.05 |
| (1,5206) | 1:B:62:LEU:HA | 1:B:65:LYS:HG2 | 2 | 0.05 |
| (1,5206) | 1:B:62:LEU:HA | 1:B:65:LYS:HG2 | 10 | 0.05 |
| (1,5199) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 9 | 0.05 |
| (1,5199) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 9 | 0.05 |
| (1,5199) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 9 | 0.05 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB2 | 9 | 0.05 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB3 | 9 | 0.05 |
| (1,5167) | 1:B:53:VAL:HG21 | 1:B:58:LYS:HB2 | 2 | 0.05 |
| (1,5167) | 1:B:53:VAL:HG22 | 1:B:58:LYS:HB2 | 2 | 0.05 |
| (1,5167) | 1:B:53:VAL:HG23 | 1:B:58:LYS:HB2 | 2 | 0.05 |
| (1,5151) | 1:B:46:THR:HG1 | 1:B:48:ASN:HD21 | 2 | 0.05 |
| (1,5145) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG12 | 9 | 0.05 |
| (1,5126) | 1:B:37:VAL:HG11 | 1:B:48:ASN:HD21 | 16 | 0.05 |
| (1,5126) | 1:B:37:VAL:HG12 | 1:B:48:ASN:HD21 | 16 | 0.05 |
| (1,5126) | 1:B:37:VAL:HG13 | 1:B:48:ASN:HD21 | 16 | 0.05 |
| (1,5114) | 1:B:35:THR:HB | 1:B:50:MET:HB2 | 11 | 0.05 |
| (1,5099) | 1:B:32:ASN:HD21 | 1:B:33:ILE:HB | 4 | 0.05 |
| (1,5099) | 1:B:32:ASN:HD21 | 1:B:33:ILE:HB | 19 | 0.05 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD11 | 20 | 0.05 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD12 | 20 | 0.05 |
| (1,5082) | 1:B:29:PHE:HB2 | 1:B:62:LEU:HD13 | 20 | 0.05 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD11 | 10 | 0.05 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD12 | 10 | 0.05 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD13 | 10 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5063) | 1:B:27:SER:HB2 | 1:B:28:LYS:H | 18 | 0.05 |
| (1,5056) | 1:B:26:ILE:HG12 | 1:B:27:SER:H | 1 | 0.05 |
| (1,5056) | 1:B:26:ILE:HG12 | 1:B:27:SER:H | 2 | 0.05 |
| (1,5056) | 1:B:26:ILE:HG12 | 1:B:27:SER:H | 7 | 0.05 |
| (1,5056) | 1:B:26:ILE:HG12 | 1:B:27:SER:H | 18 | 0.05 |
| (1,5056) | 1:B:26:ILE:HG12 | 1:B:27:SER:H | 19 | 0.05 |
| (1,5013) | 1:B:16:ASN:HB2 | 1:B:18:MET:H | 20 | 0.05 |
| (1,5001) | 1:B:15:LYS:HA | 1:B:16:ASN:HD21 | 14 | 0.05 |
| (1,4993) | 1:B:14:ASP:HB2 | 1:B:43:GLY:H | 13 | 0.05 |
| (1,4986) | 1:B:9:ARG:HD2 | 1:B:76:GLU:HB2 | 8 | 0.05 |
| (1,4986) | 1:B:9:ARG:HD3 | 1:B:76:GLU:HB2 | 8 | 0.05 |
| (1,4985) | 1:B:9:ARG:HD2 | 1:B:48:ASN:HD21 | 8 | 0.05 |
| (1,4985) | 1:B:9:ARG:HD3 | 1:B:48:ASN:HD21 | 8 | 0.05 |
| (1,4947) | 1:A:82:GLU:HA | 1:A:82:GLU:HG2 | 14 | 0.05 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 16 | 0.05 |
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 15 | 0.05 |
| (1,4912) | 1:A:65:LYS:H | 1:A:65:LYS:HD2 | 7 | 0.05 |
| (1,4882) | 1:A:56:THR:HG21 | 1:A:59:LEU:HB2 | 10 | 0.05 |
| (1,4882) | 1:A:56:THR:HG22 | 1:A:59:LEU:HB2 | 10 | 0.05 |
| (1,4882) | 1:A:56:THR:HG23 | 1:A:59:LEU:HB2 | 10 | 0.05 |
| (1,4882) | 1:A:56:THR:HG21 | 1:A:59:LEU:HB2 | 17 | 0.05 |
| (1,4882) | 1:A:56:THR:HG22 | 1:A:59:LEU:HB2 | 17 | 0.05 |
| (1,4882) | 1:A:56:THR:HG23 | 1:A:59:LEU:HB2 | 17 | 0.05 |
| (1,4871) | 1:A:54:LYS:HD2 | 1:A:55:ASN:HB2 | 19 | 0.05 |
| (1,4871) | 1:A:54:LYS:HD3 | 1:A:55:ASN:HB2 | 19 | 0.05 |
| (1,4868) | 1:A:54:LYS:HB2 | 1:A:55:ASN:HD21 | 12 | 0.05 |
| (1,4865) | 1:A:54:LYS:H | 1:A:54:LYS:HG2 | 9 | 0.05 |
| (1,4864) | 1:A:53:VAL:HG21 | 1:A:58:LYS:HB2 | 15 | 0.05 |
| (1,4864) | 1:A:53:VAL:HG22 | 1:A:58:LYS:HB2 | 15 | 0.05 |
| (1,4864) | 1:A:53:VAL:HG23 | 1:A:58:LYS:HB2 | 15 | 0.05 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 11 | 0.05 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 17 | 0.05 |
| (1,4834) | 1:A:39:ASN:HD21 | 1:A:46:THR:HB | 18 | 0.05 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE2 | 1 | 0.05 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE3 | 1 | 0.05 |
| (1,4819) | 1:A:37:VAL:HB | 1:A:48:ASN:HD21 | 2 | 0.05 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG21 | 14 | 0.05 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG22 | 14 | 0.05 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG23 | 14 | 0.05 |
| (1,4812) | 1:A:36:ILE:HG21 | 1:A:48:ASN:HB2 | 14 | 0.05 |
| (1,4812) | 1:A:36:ILE:HG22 | 1:A:48:ASN:HB2 | 14 | 0.05 |
| (1,4812) | 1:A:36:ILE:HG23 | 1:A:48:ASN:HB2 | 14 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4792) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG13 | 11 | 0.05 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG21 | 18 | 0.05 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG22 | 18 | 0.05 |
| (1,4791) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG23 | 18 | 0.05 |
| (1,4787) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HD2 | 2 | 0.05 |
| (1,4787) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HD2 | 20 | 0.05 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD11 | 11 | 0.05 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD12 | 11 | 0.05 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD13 | 11 | 0.05 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD11 | 20 | 0.05 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD12 | 20 | 0.05 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD13 | 20 | 0.05 |
| (1,4769) | 1:A:28:LYS:H | 1:A:28:LYS:HG2 | 3 | 0.05 |
| (1,4769) | 1:A:28:LYS:H | 1:A:28:LYS:HG2 | 12 | 0.05 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 3 | 0.05 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 7 | 0.05 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 11 | 0.05 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 12 | 0.05 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 18 | 0.05 |
| (1,4753) | 1:A:25:VAL:HG21 | 1:A:28:LYS:HG2 | 13 | 0.05 |
| (1,4753) | 1:A:25:VAL:HG22 | 1:A:28:LYS:HG2 | 13 | 0.05 |
| (1,4753) | 1:A:25:VAL:HG23 | 1:A:28:LYS:HG2 | 13 | 0.05 |
| (1,4728) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HG12 | 3 | 0.05 |
| (1,4724) | 1:A:20:ASN:HB2 | 1:A:21:GLN:HE21 | 5 | 0.05 |
| (1,4723) | 1:A:20:ASN:HB2 | 1:A:21:GLN:H | 7 | 0.05 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 8 | 0.05 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 8 | 0.05 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 8 | 0.05 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 9 | 0.05 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 9 | 0.05 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 9 | 0.05 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 12 | 0.05 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 12 | 0.05 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 12 | 0.05 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 6 | 0.05 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 6 | 0.05 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 6 | 0.05 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 10 | 0.05 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 10 | 0.05 |
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 10 | 0.05 |
| (1,4623) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HE1 | 17 | 0.05 |
| (1,4623) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HE1 | 17 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4623) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HE1 | 17 | 0.05 |
| (1,4620) | 1:B:82:GLU:HA | 1:B:83:HIS:HD2 | 7 | 0.05 |
| (1,4609) | 1:A:81:LEU:HB3 | 1:A:83:HIS:HD2 | 3 | 0.05 |
| (1,4608) | 1:B:5:LEU:HG | 1:B:83:HIS:HD2 | 15 | 0.05 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 11 | 0.05 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 12 | 0.05 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 8 | 0.05 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 11 | 0.05 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 17 | 0.05 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG21 | 14 | 0.05 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG22 | 14 | 0.05 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG23 | 14 | 0.05 |
| (1,4567) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HE1 | 4 | 0.05 |
| (1,4567) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HE1 | 4 | 0.05 |
| (1,4567) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HE1 | 4 | 0.05 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 15 | 0.05 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 15 | 0.05 |
| (1,4550) | 1:B:4:PHE:HB2 | 1:B:52:PHE:HE1 | 19 | 0.05 |
| (1,4550) | 1:B:4:PHE:HB3 | 1:B:52:PHE:HE1 | 19 | 0.05 |
| (1,4549) | 1:A:4:PHE:HB2 | 1:A:52:PHE:HE1 | 12 | 0.05 |
| (1,4549) | 1:A:4:PHE:HB3 | 1:A:52:PHE:HE1 | 12 | 0.05 |
| (1,4537) | 1:A:52:PHE:HD1 | 1:A:53:VAL:H | 5 | 0.05 |
| (1,4537) | 1:A:52:PHE:HD2 | 1:A:53:VAL:H | 5 | 0.05 |
| (1,4537) | 1:A:52:PHE:HD1 | 1:A:53:VAL:H | 11 | 0.05 |
| (1,4537) | 1:A:52:PHE:HD2 | 1:A:53:VAL:H | 11 | 0.05 |
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD1 | 17 | 0.05 |
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD2 | 17 | 0.05 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 2 | 0.05 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 9 | 0.05 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 10 | 0.05 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 1 | 0.05 |
| (1,4496) | 1:B:12:GLY:H | 1:B:45:PHE:HE1 | 15 | 0.05 |
| (1,4496) | 1:B:12:GLY:H | 1:B:45:PHE:HE1 | 19 | 0.05 |
| (1,4493) | 1:A:12:GLY:HA2 | 1:A:45:PHE:HE1 | 1 | 0.05 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 3 | 0.05 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 3 | 0.05 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 3 | 0.05 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 8 | 0.05 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 8 | 0.05 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 8 | 0.05 |
| (1,4416) | 1:A:29:PHE:HA | 1:A:29:PHE:HD1 | 20 | 0.05 |
| (1,4416) | 1:A:29:PHE:HA | 1:A:29:PHE:HD2 | 20 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4413) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 5 | 0.05 |
| (1,4413) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 5 | 0.05 |
| (1,4413) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 10 | 0.05 |
| (1,4413) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 10 | 0.05 |
| (1,4412) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 2 | 0.05 |
| (1,4412) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 2 | 0.05 |
| (1,4412) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 7 | 0.05 |
| (1,4412) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 7 | 0.05 |
| (1,4412) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 14 | 0.05 |
| (1,4412) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 14 | 0.05 |
| (1,4393) | 1:B:4:PHE:HZ | 1:B:6:ALA:HA | 2 | 0.05 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG11 | 7 | 0.05 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG12 | 7 | 0.05 |
| (1,4383) | 1:B:4:PHE:HZ | 1:B:53:VAL:HG13 | 7 | 0.05 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 7 | 0.05 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 7 | 0.05 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 7 | 0.05 |
| (1,4335) | 1:B:83:HIS:HA | 1:B:83:HIS:HD2 | 15 | 0.05 |
| (1,4335) | 1:B:83:HIS:HA | 1:B:83:HIS:HD2 | 17 | 0.05 |
| (1,4325) | 1:B:80:ASN:HA | 1:B:81:LEU:HG | 18 | 0.05 |
| (1,4293) | 1:B:73:PHE:HA | 1:B:75:VAL:HG21 | 14 | 0.05 |
| (1,4293) | 1:B:73:PHE:HA | 1:B:75:VAL:HG22 | 14 | 0.05 |
| (1,4293) | 1:B:73:PHE:HA | 1:B:75:VAL:HG23 | 14 | 0.05 |
| (1,4259) | 1:B:41:LYS:HG2 | 1:B:42:ASP:HA | 19 | 0.05 |
| (1,4259) | 1:B:41:LYS:HG3 | 1:B:42:ASP:HA | 19 | 0.05 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG2 | 7 | 0.05 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG3 | 7 | 0.05 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG2 | 16 | 0.05 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG3 | 16 | 0.05 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG2 | 19 | 0.05 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG3 | 19 | 0.05 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 2 | 0.05 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 2 | 0.05 |
| (1,4217) | 1:B:8:ILE:HA | 1:B:78:LEU:HB2 | 18 | 0.05 |
| (1,4216) | 1:A:8:ILE:HA | 1:A:78:LEU:HB2 | 16 | 0.05 |
| (1,4199) | 1:B:82:GLU:H | 1:B:83:HIS:HB3 | 8 | 0.05 |
| (1,4198) | 1:A:82:GLU:H | 1:A:83:HIS:HB3 | 10 | 0.05 |
| (1,4198) | 1:A:82:GLU:H | 1:A:83:HIS:HB3 | 11 | 0.05 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD11 | 5 | 0.05 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD12 | 5 | 0.05 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD13 | 5 | 0.05 |
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD11 | 5 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD12 | 5 | 0.05 |
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD13 | 5 | 0.05 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD11 | 5 | 0.05 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD12 | 5 | 0.05 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD13 | 5 | 0.05 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD11 | 8 | 0.05 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD12 | 8 | 0.05 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD13 | 8 | 0.05 |
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD11 | 8 | 0.05 |
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD12 | 8 | 0.05 |
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD13 | 8 | 0.05 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD11 | 8 | 0.05 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD12 | 8 | 0.05 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD13 | 8 | 0.05 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 19 | 0.05 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 19 | 0.05 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 19 | 0.05 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 17 | 0.05 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 17 | 0.05 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 17 | 0.05 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 4 | 0.05 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 4 | 0.05 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 4 | 0.05 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 12 | 0.05 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 12 | 0.05 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 12 | 0.05 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 13 | 0.05 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 13 | 0.05 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 13 | 0.05 |
| (1,4152) | 1:A:41:LYS:HE2 | 1:A:44:ILE:HB | 15 | 0.05 |
| (1,4152) | 1:A:41:LYS:HE3 | 1:A:44:ILE:HB | 15 | 0.05 |
| (1,4146) | 1:A:61:THR:HG21 | 1:A:65:LYS:HB3 | 5 | 0.05 |
| (1,4146) | 1:A:61:THR:HG22 | 1:A:65:LYS:HB3 | 5 | 0.05 |
| (1,4146) | 1:A:61:THR:HG23 | 1:A:65:LYS:HB3 | 5 | 0.05 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD11 | 3 | 0.05 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD12 | 3 | 0.05 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD13 | 3 | 0.05 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD11 | 18 | 0.05 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD12 | 18 | 0.05 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD13 | 18 | 0.05 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD11 | 9 | 0.05 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD12 | 9 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD13 | 9 | 0.05 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 6 | 0.05 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 13 | 0.05 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 15 | 0.05 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 16 | 0.05 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 19 | 0.05 |
| (1,4115) | 1:A:18:MET:HA | 1:A:21:GLN:HB2 | 7 | 0.05 |
| (1,4115) | 1:A:18:MET:HA | 1:A:21:GLN:HB2 | 8 | 0.05 |
| (1,4115) | 1:A:18:MET:HA | 1:A:21:GLN:HB2 | 16 | 0.05 |
| (1,4115) | 1:A:18:MET:HA | 1:A:21:GLN:HB2 | 19 | 0.05 |
| (1,4081) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HA | 1 | 0.05 |
| (1,4074) | 1:A:82:GLU:HA | 1:A:83:HIS:HB2 | 7 | 0.05 |
| (1,4054) | 1:A:6:ALA:H | 1:A:81:LEU:HD11 | 4 | 0.05 |
| (1,4054) | 1:A:6:ALA:H | 1:A:81:LEU:HD12 | 4 | 0.05 |
| (1,4054) | 1:A:6:ALA:H | 1:A:81:LEU:HD13 | 4 | 0.05 |
| (1,4015) | 1:B:78:LEU:HB3 | 1:B:79:SER:HB2 | 9 | 0.05 |
| (1,4015) | 1:B:78:LEU:HB3 | 1:B:79:SER:HB3 | 9 | 0.05 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD21 | 8 | 0.05 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD22 | 8 | 0.05 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD23 | 8 | 0.05 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD21 | 8 | 0.05 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD22 | 8 | 0.05 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD23 | 8 | 0.05 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD11 | 2 | 0.05 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD12 | 2 | 0.05 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD13 | 2 | 0.05 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD11 | 16 | 0.05 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD12 | 16 | 0.05 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD13 | 16 | 0.05 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD11 | 7 | 0.05 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD12 | 7 | 0.05 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD13 | 7 | 0.05 |
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD11 | 6 | 0.05 |
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD12 | 6 | 0.05 |
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD13 | 6 | 0.05 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD11 | 6 | 0.05 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD12 | 6 | 0.05 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD13 | 6 | 0.05 |
| (1,3921) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HD2 | 1 | 0.05 |
| (1,3921) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HD3 | 1 | 0.05 |
| (1,3921) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HD2 | 1 | 0.05 |
| (1,3921) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HD3 | 1 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3921) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HD2 | 1 | 0.05 |
| (1,3921) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HD3 | 1 | 0.05 |
| (1,3896) | 1:A:74:THR:HA | 1:A:76:GLU:HG2 | 5 | 0.05 |
| (1,3896) | 1:A:74:THR:HA | 1:A:76:GLU:HG3 | 5 | 0.05 |
| (1,3896) | 1:A:74:THR:HA | 1:A:76:GLU:HG2 | 20 | 0.05 |
| (1,3896) | 1:A:74:THR:HA | 1:A:76:GLU:HG3 | 20 | 0.05 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 1 | 0.05 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 1 | 0.05 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 1 | 0.05 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 4 | 0.05 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 4 | 0.05 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 4 | 0.05 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 12 | 0.05 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 12 | 0.05 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 12 | 0.05 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 2 | 0.05 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 2 | 0.05 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 2 | 0.05 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 5 | 0.05 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 5 | 0.05 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 5 | 0.05 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 8 | 0.05 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 8 | 0.05 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 8 | 0.05 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 12 | 0.05 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 12 | 0.05 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 12 | 0.05 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG21 | 10 | 0.05 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG22 | 10 | 0.05 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG23 | 10 | 0.05 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG21 | 10 | 0.05 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG22 | 10 | 0.05 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG23 | 10 | 0.05 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG21 | 19 | 0.05 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG22 | 19 | 0.05 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG23 | 19 | 0.05 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG21 | 3 | 0.05 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG22 | 3 | 0.05 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG23 | 3 | 0.05 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG21 | 16 | 0.05 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG22 | 16 | 0.05 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG23 | 16 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3839) | 1:A:72:VAL:HG11 | 1:A:74:THR:HB | 19 | 0.05 |
| (1,3839) | 1:A:72:VAL:HG12 | 1:A:74:THR:HB | 19 | 0.05 |
| (1,3839) | 1:A:72:VAL:HG13 | 1:A:74:THR:HB | 19 | 0.05 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG11 | 3 | 0.05 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG12 | 3 | 0.05 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG13 | 3 | 0.05 |
| (1,3775) | 1:A:70:GLN:HG2 | 1:A:72:VAL:H | 19 | 0.05 |
| (1,3775) | 1:A:70:GLN:HG3 | 1:A:72:VAL:H | 19 | 0.05 |
| (1,3756) | 1:B:69:VAL:H | 1:B:70:GLN:HB2 | 10 | 0.05 |
| (1,3756) | 1:B:69:VAL:H | 1:B:70:GLN:HB3 | 10 | 0.05 |
| (1,3735) | 1:A:66:LEU:HA | 1:A:69:VAL:HB | 15 | 0.05 |
| (1,3735) | 1:A:66:LEU:HA | 1:A:69:VAL:HB | 19 | 0.05 |
| (1,3734) | 1:B:20:ASN:HA | 1:B:22:ILE:HB | 2 | 0.05 |
| (1,3734) | 1:B:20:ASN:HA | 1:B:22:ILE:HB | 12 | 0.05 |
| (1,3734) | 1:B:20:ASN:HA | 1:B:22:ILE:HB | 20 | 0.05 |
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 11 | 0.05 |
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 12 | 0.05 |
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 17 | 0.05 |
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 20 | 0.05 |
| (1,3701) | 1:A:15:LYS:HE2 | 1:A:18:MET:H | 5 | 0.05 |
| (1,3701) | 1:A:15:LYS:HE3 | 1:A:18:MET:H | 5 | 0.05 |
| (1,3701) | 1:A:15:LYS:HE2 | 1:A:18:MET:H | 12 | 0.05 |
| (1,3701) | 1:A:15:LYS:HE3 | 1:A:18:MET:H | 12 | 0.05 |
| (1,3699) | 1:A:15:LYS:HE2 | 1:A:16:ASN:HD21 | 12 | 0.05 |
| (1,3699) | 1:A:15:LYS:HE3 | 1:A:16:ASN:HD21 | 12 | 0.05 |
| (1,3620) | 1:A:41:LYS:HE2 | 1:A:44:ILE:H | 14 | 0.05 |
| (1,3620) | 1:A:41:LYS:HE3 | 1:A:44:ILE:H | 14 | 0.05 |
| (1,3620) | 1:A:41:LYS:HE2 | 1:A:44:ILE:H | 20 | 0.05 |
| (1,3620) | 1:A:41:LYS:HE3 | 1:A:44:ILE:H | 20 | 0.05 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 12 | 0.05 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 12 | 0.05 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 12 | 0.05 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 13 | 0.05 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 13 | 0.05 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 13 | 0.05 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 15 | 0.05 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 15 | 0.05 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 15 | 0.05 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 18 | 0.05 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 18 | 0.05 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 18 | 0.05 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB2 | 9 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB3 | 9 | 0.05 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB2 | 17 | 0.05 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB3 | 17 | 0.05 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB2 | 19 | 0.05 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB3 | 19 | 0.05 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB2 | 4 | 0.05 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB3 | 4 | 0.05 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB2 | 8 | 0.05 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB3 | 8 | 0.05 |
| (1,3536) | 1:A:64:ASP:HB2 | 1:A:65:LYS:HB2 | 9 | 0.05 |
| (1,3536) | 1:A:64:ASP:HB2 | 1:A:65:LYS:HB2 | 10 | 0.05 |
| (1,3535) | 1:B:64:ASP:HB2 | 1:B:67:ARG:HB2 | 20 | 0.05 |
| (1,3535) | 1:B:64:ASP:HB2 | 1:B:67:ARG:HB3 | 20 | 0.05 |
| (1,3530) | 1:B:9:ARG:H | 1:B:63:MET:HE1 | 17 | 0.05 |
| (1,3530) | 1:B:9:ARG:H | 1:B:63:MET:HE2 | 17 | 0.05 |
| (1,3530) | 1:B:9:ARG:H | 1:B:63:MET:HE3 | 17 | 0.05 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE1 | 19 | 0.05 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE2 | 19 | 0.05 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE3 | 19 | 0.05 |
| (1,3528) | 1:B:63:MET:HE1 | 1:B:77:ARG:H | 5 | 0.05 |
| (1,3528) | 1:B:63:MET:HE2 | 1:B:77:ARG:H | 5 | 0.05 |
| (1,3528) | 1:B:63:MET:HE3 | 1:B:77:ARG:H | 5 | 0.05 |
| (1,3528) | 1:B:63:MET:HE1 | 1:B:77:ARG:H | 6 | 0.05 |
| (1,3528) | 1:B:63:MET:HE2 | 1:B:77:ARG:H | 6 | 0.05 |
| (1,3528) | 1:B:63:MET:HE3 | 1:B:77:ARG:H | 6 | 0.05 |
| (1,3527) | 1:A:63:MET:HE1 | 1:A:77:ARG:H | 14 | 0.05 |
| (1,3527) | 1:A:63:MET:HE2 | 1:A:77:ARG:H | 14 | 0.05 |
| (1,3527) | 1:A:63:MET:HE3 | 1:A:77:ARG:H | 14 | 0.05 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 10 | 0.05 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 10 | 0.05 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 10 | 0.05 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 14 | 0.05 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 14 | 0.05 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 14 | 0.05 |
| (1,3519) | 1:A:63:MET:HE1 | 1:A:76:GLU:HA | 9 | 0.05 |
| (1,3519) | 1:A:63:MET:HE2 | 1:A:76:GLU:HA | 9 | 0.05 |
| (1,3519) | 1:A:63:MET:HE3 | 1:A:76:GLU:HA | 9 | 0.05 |
| (1,3517) | 1:A:63:MET:HE1 | 1:A:77:ARG:HA | 10 | 0.05 |
| (1,3517) | 1:A:63:MET:HE2 | 1:A:77:ARG:HA | 10 | 0.05 |
| (1,3517) | 1:A:63:MET:HE3 | 1:A:77:ARG:HA | 10 | 0.05 |
| (1,3517) | 1:A:63:MET:HE1 | 1:A:77:ARG:HA | 11 | 0.05 |
| (1,3517) | 1:A:63:MET:HE2 | 1:A:77:ARG:HA | 11 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3517) | 1:A:63:MET:HE3 | 1:A:77:ARG:HA | 11 | 0.05 |
| (1,3517) | 1:A:63:MET:HE1 | 1:A:77:ARG:HA | 15 | 0.05 |
| (1,3517) | 1:A:63:MET:HE2 | 1:A:77:ARG:HA | 15 | 0.05 |
| (1,3517) | 1:A:63:MET:HE3 | 1:A:77:ARG:HA | 15 | 0.05 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE1 | 1 | 0.05 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE2 | 1 | 0.05 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE3 | 1 | 0.05 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE1 | 9 | 0.05 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE2 | 9 | 0.05 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE3 | 9 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE1 | 11 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE2 | 11 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE3 | 11 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE1 | 11 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE2 | 11 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE3 | 11 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE1 | 11 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE2 | 11 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE3 | 11 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE1 | 13 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE2 | 13 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE3 | 13 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE1 | 13 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE2 | 13 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE3 | 13 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE1 | 13 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE2 | 13 | 0.05 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE3 | 13 | 0.05 |
| (1,3440) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD11 | 20 | 0.05 |
| (1,3440) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD12 | 20 | 0.05 |
| (1,3440) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD13 | 20 | 0.05 |
| (1,3357) | 1:B:60:THR:HA | 1:B:60:THR:HG21 | 3 | 0.05 |
| (1,3357) | 1:B:60:THR:HA | 1:B:60:THR:HG22 | 3 | 0.05 |
| (1,3357) | 1:B:60:THR:HA | 1:B:60:THR:HG23 | 3 | 0.05 |
| (1,3356) | 1:A:60:THR:HA | 1:A:60:THR:HG21 | 2 | 0.05 |
| (1,3356) | 1:A:60:THR:HA | 1:A:60:THR:HG22 | 2 | 0.05 |
| (1,3356) | 1:A:60:THR:HA | 1:A:60:THR:HG23 | 2 | 0.05 |
| (1,3356) | 1:A:60:THR:HA | 1:A:60:THR:HG21 | 14 | 0.05 |
| (1,3356) | 1:A:60:THR:HA | 1:A:60:THR:HG22 | 14 | 0.05 |
| (1,3356) | 1:A:60:THR:HA | 1:A:60:THR:HG23 | 14 | 0.05 |
| (1,3274) | 1:A:30:ASP:HB2 | 1:A:58:LYS:HD2 | 11 | 0.05 |
| (1,3274) | 1:A:30:ASP:HB2 | 1:A:58:LYS:HD3 | 11 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3274) | 1:A:30:ASP:HB3 | 1:A:58:LYS:HD2 | 11 | 0.05 |
| (1,3274) | 1:A:30:ASP:HB3 | 1:A:58:LYS:HD3 | 11 | 0.05 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 8 | 0.05 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 3 | 0.05 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 9 | 0.05 |
| (1,3252) | 1:A:4:PHE:HZ | 1:A:58:LYS:HG3 | 11 | 0.05 |
| (1,3190) | 1:A:54:LYS:H | 1:A:54:LYS:HD2 | 8 | 0.05 |
| (1,3190) | 1:A:54:LYS:H | 1:A:54:LYS:HD3 | 8 | 0.05 |
| (1,3184) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD22 | 14 | 0.05 |
| (1,3184) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD22 | 14 | 0.05 |
| (1,3184) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD22 | 19 | 0.05 |
| (1,3184) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD22 | 19 | 0.05 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG11 | 2 | 0.05 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG12 | 2 | 0.05 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG13 | 2 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 1 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 1 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 1 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 1 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 1 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 1 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 4 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 4 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 4 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 4 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 4 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 4 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 14 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 14 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 14 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 14 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 14 | 0.05 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 14 | 0.05 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 7 | 0.05 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 7 | 0.05 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 7 | 0.05 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 7 | 0.05 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 7 | 0.05 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 7 | 0.05 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD11 | 12 | 0.05 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD12 | 12 | 0.05 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD13 | 12 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3013) | 1:B:51:ILE:HD11 | 1:B:62:LEU:HD21 | 16 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD11 | 1:B:62:LEU:HD22 | 16 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD11 | 1:B:62:LEU:HD23 | 16 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD12 | 1:B:62:LEU:HD21 | 16 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD12 | 1:B:62:LEU:HD22 | 16 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD12 | 1:B:62:LEU:HD23 | 16 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD13 | 1:B:62:LEU:HD21 | 16 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD13 | 1:B:62:LEU:HD22 | 16 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD13 | 1:B:62:LEU:HD23 | 16 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD11 | 1:B:62:LEU:HD21 | 20 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD11 | 1:B:62:LEU:HD22 | 20 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD11 | 1:B:62:LEU:HD23 | 20 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD12 | 1:B:62:LEU:HD21 | 20 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD12 | 1:B:62:LEU:HD22 | 20 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD12 | 1:B:62:LEU:HD23 | 20 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD13 | 1:B:62:LEU:HD21 | 20 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD13 | 1:B:62:LEU:HD22 | 20 | 0.05 |
| (1,3013) | 1:B:51:ILE:HD13 | 1:B:62:LEU:HD23 | 20 | 0.05 |
| (1,2991) | 1:A:51:ILE:HG21 | 1:B:20:ASN:HD22 | 12 | 0.05 |
| (1,2991) | 1:A:51:ILE:HG22 | 1:B:20:ASN:HD22 | 12 | 0.05 |
| (1,2991) | 1:A:51:ILE:HG23 | 1:B:20:ASN:HD22 | 12 | 0.05 |
| (1,2990) | 1:A:20:ASN:HD22 | 1:B:51:ILE:HG21 | 7 | 0.05 |
| (1,2990) | 1:A:20:ASN:HD22 | 1:B:51:ILE:HG22 | 7 | 0.05 |
| (1,2990) | 1:A:20:ASN:HD22 | 1:B:51:ILE:HG23 | 7 | 0.05 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG21 | 3 | 0.05 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG22 | 3 | 0.05 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG23 | 3 | 0.05 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG21 | 19 | 0.05 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG22 | 19 | 0.05 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG23 | 19 | 0.05 |
| (1,2971) | 1:B:8:ILE:HG21 | 1:B:62:LEU:HD11 | 12 | 0.05 |
| (1,2971) | 1:B:8:ILE:HG21 | 1:B:62:LEU:HD12 | 12 | 0.05 |
| (1,2971) | 1:B:8:ILE:HG21 | 1:B:62:LEU:HD13 | 12 | 0.05 |
| (1,2971) | 1:B:8:ILE:HG22 | 1:B:62:LEU:HD11 | 12 | 0.05 |
| (1,2971) | 1:B:8:ILE:HG22 | 1:B:62:LEU:HD12 | 12 | 0.05 |
| (1,2971) | 1:B:8:ILE:HG22 | 1:B:62:LEU:HD13 | 12 | 0.05 |
| (1,2971) | 1:B:8:ILE:HG23 | 1:B:62:LEU:HD11 | 12 | 0.05 |
| (1,2971) | 1:B:8:ILE:HG23 | 1:B:62:LEU:HD12 | 12 | 0.05 |
| (1,2971) | 1:B:8:ILE:HG23 | 1:B:62:LEU:HD13 | 12 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD11 | 10 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD12 | 10 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD13 | 10 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD11 | 10 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD12 | 10 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD13 | 10 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD11 | 10 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD12 | 10 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD13 | 10 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD11 | 11 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD12 | 11 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD13 | 11 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD11 | 11 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD12 | 11 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD13 | 11 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD11 | 11 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD12 | 11 | 0.05 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD13 | 11 | 0.05 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 10 | 0.05 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 10 | 0.05 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 10 | 0.05 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 5 | 0.05 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 5 | 0.05 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 5 | 0.05 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 9 | 0.05 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 9 | 0.05 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 9 | 0.05 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 11 | 0.05 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 11 | 0.05 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 11 | 0.05 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 19 | 0.05 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 19 | 0.05 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 19 | 0.05 |
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 8 | 0.05 |
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 14 | 0.05 |
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 19 | 0.05 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 5 | 0.05 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 6 | 0.05 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 7 | 0.05 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 9 | 0.05 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 14 | 0.05 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 16 | 0.05 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 17 | 0.05 |
| (1,2754) | 1:B:23:THR:HG1 | 1:B:47:CYS:HB3 | 1 | 0.05 |
| (1,2754) | 1:B:23:THR:HG1 | 1:B:47:CYS:HB3 | 18 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2753) | 1:A:23:THR:HG1 | 1:A:47:CYS:HB3 | 19 | 0.05 |
| (1,2704) | 1:B:9:ARG:HD2 | 1:B:46:THR:HG21 | 2 | 0.05 |
| (1,2704) | 1:B:9:ARG:HD2 | 1:B:46:THR:HG22 | 2 | 0.05 |
| (1,2704) | 1:B:9:ARG:HD2 | 1:B:46:THR:HG23 | 2 | 0.05 |
| (1,2704) | 1:B:9:ARG:HD3 | 1:B:46:THR:HG21 | 2 | 0.05 |
| (1,2704) | 1:B:9:ARG:HD3 | 1:B:46:THR:HG22 | 2 | 0.05 |
| (1,2704) | 1:B:9:ARG:HD3 | 1:B:46:THR:HG23 | 2 | 0.05 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG21 | 6 | 0.05 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG22 | 6 | 0.05 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG23 | 6 | 0.05 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 5 | 0.05 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 5 | 0.05 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 5 | 0.05 |
| (1,2666) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HD11 | 1 | 0.05 |
| (1,2666) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HD12 | 1 | 0.05 |
| (1,2666) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HD13 | 1 | 0.05 |
| (1,2662) | 1:B:44:ILE:HG21 | 1:B:45:PHE:H | 12 | 0.05 |
| (1,2662) | 1:B:44:ILE:HG22 | 1:B:45:PHE:H | 12 | 0.05 |
| (1,2662) | 1:B:44:ILE:HG23 | 1:B:45:PHE:H | 12 | 0.05 |
| (1,2638) | 1:B:44:ILE:HG13 | 1:B:45:PHE:H | 3 | 0.05 |
| (1,2587) | 1:A:15:LYS:H | 1:A:40:ALA:HB1 | 4 | 0.05 |
| (1,2587) | 1:A:15:LYS:H | 1:A:40:ALA:HB2 | 4 | 0.05 |
| (1,2587) | 1:A:15:LYS:H | 1:A:40:ALA:HB3 | 4 | 0.05 |
| (1,2587) | 1:A:15:LYS:H | 1:A:40:ALA:HB1 | 19 | 0.05 |
| (1,2587) | 1:A:15:LYS:H | 1:A:40:ALA:HB2 | 19 | 0.05 |
| (1,2587) | 1:A:15:LYS:H | 1:A:40:ALA:HB3 | 19 | 0.05 |
| (1,2549) | 1:A:38:LEU:HD21 | 1:A:45:PHE:HE1 | 11 | 0.05 |
| (1,2549) | 1:A:38:LEU:HD22 | 1:A:45:PHE:HE1 | 11 | 0.05 |
| (1,2549) | 1:A:38:LEU:HD23 | 1:A:45:PHE:HE1 | 11 | 0.05 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD21 | 16 | 0.05 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD22 | 16 | 0.05 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD23 | 16 | 0.05 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD21 | 17 | 0.05 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD22 | 17 | 0.05 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD23 | 17 | 0.05 |
| (1,2534) | 1:B:23:THR:HG1 | 1:B:38:LEU:HD21 | 2 | 0.05 |
| (1,2534) | 1:B:23:THR:HG1 | 1:B:38:LEU:HD22 | 2 | 0.05 |
| (1,2534) | 1:B:23:THR:HG1 | 1:B:38:LEU:HD23 | 2 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 3 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 3 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 3 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 5 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 5 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 5 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 9 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 9 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 9 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 10 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 10 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 10 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 11 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 11 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 11 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 13 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 13 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 13 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 18 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 18 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 18 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 20 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 20 | 0.05 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 20 | 0.05 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 5 | 0.05 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 5 | 0.05 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 5 | 0.05 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 6 | 0.05 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 6 | 0.05 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 6 | 0.05 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 8 | 0.05 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 8 | 0.05 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 8 | 0.05 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 16 | 0.05 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 16 | 0.05 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 16 | 0.05 |
| (1,2344) | 1:B:35:THR:HB | 1:B:50:MET:HB2 | 11 | 0.05 |
| (1,2334) | 1:B:33:ILE:HD11 | 1:B:34:ARG:H | 14 | 0.05 |
| (1,2334) | 1:B:33:ILE:HD12 | 1:B:34:ARG:H | 14 | 0.05 |
| (1,2334) | 1:B:33:ILE:HD13 | 1:B:34:ARG:H | 14 | 0.05 |
| (1,2268) | 1:B:29:PHE:HD1 | 1:B:31:THR:HB | 3 | 0.05 |
| (1,2268) | 1:B:29:PHE:HD2 | 1:B:31:THR:HB | 3 | 0.05 |
| (1,2268) | 1:B:29:PHE:HD1 | 1:B:31:THR:HB | 18 | 0.05 |
| (1,2268) | 1:B:29:PHE:HD2 | 1:B:31:THR:HB | 18 | 0.05 |
| (1,2267) | 1:A:29:PHE:HD1 | 1:A:31:THR:HB | 7 | 0.05 |
| (1,2267) | 1:A:29:PHE:HD2 | 1:A:31:THR:HB | 7 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2260) | 1:B:68:LYS:HA | 1:B:68:LYS:HD2 | 4 | 0.05 |
| (1,2259) | 1:A:68:LYS:HA | 1:A:68:LYS:HD2 | 19 | 0.05 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 4 | 0.05 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 4 | 0.05 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 4 | 0.05 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 6 | 0.05 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 6 | 0.05 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 6 | 0.05 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 15 | 0.05 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 15 | 0.05 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 15 | 0.05 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 20 | 0.05 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 20 | 0.05 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 20 | 0.05 |
| (1,2180) | 1:B:22:ILE:HA | 1:B:25:VAL:HG21 | 18 | 0.05 |
| (1,2180) | 1:B:22:ILE:HA | 1:B:25:VAL:HG22 | 18 | 0.05 |
| (1,2180) | 1:B:22:ILE:HA | 1:B:25:VAL:HG23 | 18 | 0.05 |
| (1,216) | 1:B:16:ASN:HA | 1:B:17:GLY:H | 5 | 0.05 |
| (1,216) | 1:B:16:ASN:HA | 1:B:17:GLY:H | 19 | 0.05 |
| (1,215) | 1:A:16:ASN:HA | 1:A:17:GLY:H | 7 | 0.05 |
| (1,215) | 1:A:16:ASN:HA | 1:A:17:GLY:H | 9 | 0.05 |
| (1,215) | 1:A:16:ASN:HA | 1:A:17:GLY:H | 15 | 0.05 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 17 | 0.05 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 17 | 0.05 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 17 | 0.05 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 20 | 0.05 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 20 | 0.05 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 20 | 0.05 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 5 | 0.05 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 5 | 0.05 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 5 | 0.05 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 6 | 0.05 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 6 | 0.05 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 6 | 0.05 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 7 | 0.05 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 7 | 0.05 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 7 | 0.05 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 8 | 0.05 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 8 | 0.05 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 8 | 0.05 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 11 | 0.05 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 11 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 11 | 0.05 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 3 | 0.05 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 3 | 0.05 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 3 | 0.05 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 12 | 0.05 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 12 | 0.05 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 12 | 0.05 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 16 | 0.05 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 16 | 0.05 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 16 | 0.05 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 20 | 0.05 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 20 | 0.05 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 20 | 0.05 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 5 | 0.05 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 5 | 0.05 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 5 | 0.05 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 7 | 0.05 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 7 | 0.05 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 7 | 0.05 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 19 | 0.05 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 19 | 0.05 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 19 | 0.05 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 8 | 0.05 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 8 | 0.05 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 8 | 0.05 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG21 | 1 | 0.05 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG22 | 1 | 0.05 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG23 | 1 | 0.05 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG21 | 2 | 0.05 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG22 | 2 | 0.05 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG23 | 2 | 0.05 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG21 | 5 | 0.05 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG22 | 5 | 0.05 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG23 | 5 | 0.05 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG21 | 13 | 0.05 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG22 | 13 | 0.05 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG23 | 13 | 0.05 |
| (1,1989) | 1:B:21:GLN:HG2 | 1:B:69:VAL:HG11 | 14 | 0.05 |
| (1,1989) | 1:B:21:GLN:HG2 | 1:B:69:VAL:HG12 | 14 | 0.05 |
| (1,1989) | 1:B:21:GLN:HG2 | 1:B:69:VAL:HG13 | 14 | 0.05 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 2 | 0.05 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 2 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 2 | 0.05 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 18 | 0.05 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 18 | 0.05 |
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 18 | 0.05 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 2 | 0.05 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 2 | 0.05 |
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 2 | 0.05 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 2 | 0.05 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 15 | 0.05 |
| (1,1898) | 1:B:16:ASN:HB3 | 1:B:17:GLY:H | 6 | 0.05 |
| (1,1880) | 1:A:68:LYS:HE2 | 1:A:69:VAL:HG21 | 4 | 0.05 |
| (1,1880) | 1:A:68:LYS:HE2 | 1:A:69:VAL:HG22 | 4 | 0.05 |
| (1,1880) | 1:A:68:LYS:HE2 | 1:A:69:VAL:HG23 | 4 | 0.05 |
| (1,1880) | 1:A:68:LYS:HE3 | 1:A:69:VAL:HG21 | 4 | 0.05 |
| (1,1880) | 1:A:68:LYS:HE3 | 1:A:69:VAL:HG22 | 4 | 0.05 |
| (1,1880) | 1:A:68:LYS:HE3 | 1:A:69:VAL:HG23 | 4 | 0.05 |
| (1,1877) | 1:B:41:LYS:HE2 | 1:B:44:ILE:HD11 | 13 | 0.05 |
| (1,1877) | 1:B:41:LYS:HE2 | 1:B:44:ILE:HD12 | 13 | 0.05 |
| (1,1877) | 1:B:41:LYS:HE2 | 1:B:44:ILE:HD13 | 13 | 0.05 |
| (1,1877) | 1:B:41:LYS:HE3 | 1:B:44:ILE:HD11 | 13 | 0.05 |
| (1,1877) | 1:B:41:LYS:HE3 | 1:B:44:ILE:HD12 | 13 | 0.05 |
| (1,1877) | 1:B:41:LYS:HE3 | 1:B:44:ILE:HD13 | 13 | 0.05 |
| (1,1876) | 1:A:41:LYS:HE2 | 1:A:44:ILE:HD11 | 13 | 0.05 |
| (1,1876) | 1:A:41:LYS:HE2 | 1:A:44:ILE:HD12 | 13 | 0.05 |
| (1,1876) | 1:A:41:LYS:HE2 | 1:A:44:ILE:HD13 | 13 | 0.05 |
| (1,1876) | 1:A:41:LYS:HE3 | 1:A:44:ILE:HD11 | 13 | 0.05 |
| (1,1876) | 1:A:41:LYS:HE3 | 1:A:44:ILE:HD12 | 13 | 0.05 |
| (1,1876) | 1:A:41:LYS:HE3 | 1:A:44:ILE:HD13 | 13 | 0.05 |
| (1,1875) | 1:B:11:VAL:HG21 | 1:B:41:LYS:HE2 | 6 | 0.05 |
| (1,1875) | 1:B:11:VAL:HG21 | 1:B:41:LYS:HE3 | 6 | 0.05 |
| (1,1875) | 1:B:11:VAL:HG22 | 1:B:41:LYS:HE2 | 6 | 0.05 |
| (1,1875) | 1:B:11:VAL:HG22 | 1:B:41:LYS:HE3 | 6 | 0.05 |
| (1,1875) | 1:B:11:VAL:HG23 | 1:B:41:LYS:HE2 | 6 | 0.05 |
| (1,1875) | 1:B:11:VAL:HG23 | 1:B:41:LYS:HE3 | 6 | 0.05 |
| (1,1875) | 1:B:11:VAL:HG21 | 1:B:41:LYS:HE2 | 13 | 0.05 |
| (1,1875) | 1:B:11:VAL:HG21 | 1:B:41:LYS:HE3 | 13 | 0.05 |
| (1,1875) | 1:B:11:VAL:HG22 | 1:B:41:LYS:HE2 | 13 | 0.05 |
| (1,1875) | 1:B:11:VAL:HG22 | 1:B:41:LYS:HE3 | 13 | 0.05 |
| (1,1875) | 1:B:11:VAL:HG23 | 1:B:41:LYS:HE2 | 13 | 0.05 |
| (1,1875) | 1:B:11:VAL:HG23 | 1:B:41:LYS:HE3 | 13 | 0.05 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG11 | 3 | 0.05 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG12 | 3 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG13 | 3 | 0.05 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG11 | 3 | 0.05 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG12 | 3 | 0.05 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG13 | 3 | 0.05 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG11 | 6 | 0.05 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG12 | 6 | 0.05 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG13 | 6 | 0.05 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG11 | 6 | 0.05 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG12 | 6 | 0.05 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG13 | 6 | 0.05 |
| (1,1819) | 1:B:13:GLU:HB2 | 1:B:73:PHE:HE1 | 6 | 0.05 |
| (1,1803) | 1:B:13:GLU:HB3 | 1:B:71:GLY:HA3 | 8 | 0.05 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 19 | 0.05 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 19 | 0.05 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 19 | 0.05 |
| (1,1745) | 1:B:11:VAL:HG21 | 1:B:46:THR:HB | 14 | 0.05 |
| (1,1745) | 1:B:11:VAL:HG22 | 1:B:46:THR:HB | 14 | 0.05 |
| (1,1745) | 1:B:11:VAL:HG23 | 1:B:46:THR:HB | 14 | 0.05 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG21 | 13 | 0.05 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG22 | 13 | 0.05 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG23 | 13 | 0.05 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG21 | 13 | 0.05 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG22 | 13 | 0.05 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG23 | 13 | 0.05 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG21 | 13 | 0.05 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG22 | 13 | 0.05 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG23 | 13 | 0.05 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD11 | 7 | 0.05 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD12 | 7 | 0.05 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD13 | 7 | 0.05 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD11 | 11 | 0.05 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD12 | 11 | 0.05 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD13 | 11 | 0.05 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD11 | 17 | 0.05 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD12 | 17 | 0.05 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD13 | 17 | 0.05 |
| (1,165) | 1:B:13:GLU:H | 1:B:73:PHE:H | 19 | 0.05 |
| (1,1633) | 1:B:9:ARG:HD2 | 1:B:76:GLU:HG2 | 8 | 0.05 |
| (1,1633) | 1:B:9:ARG:HD2 | 1:B:76:GLU:HG3 | 8 | 0.05 |
| (1,1633) | 1:B:9:ARG:HD3 | 1:B:76:GLU:HG2 | 8 | 0.05 |
| (1,1633) | 1:B:9:ARG:HD3 | 1:B:76:GLU:HG3 | 8 | 0.05 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 17 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 17 | 0.05 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 17 | 0.05 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 17 | 0.05 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 17 | 0.05 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 17 | 0.05 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 17 | 0.05 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 17 | 0.05 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 17 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 1 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 1 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 1 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 1 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 1 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 1 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 1 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 1 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 1 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 16 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 16 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 16 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 16 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 16 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 16 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 16 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 16 | 0.05 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 16 | 0.05 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD2 | 15 | 0.05 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD3 | 15 | 0.05 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD2 | 15 | 0.05 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD3 | 15 | 0.05 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD2 | 15 | 0.05 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD3 | 15 | 0.05 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 2 | 0.05 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 2 | 0.05 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 2 | 0.05 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 2 | 0.05 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 2 | 0.05 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 2 | 0.05 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 5 | 0.05 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 5 | 0.05 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 5 | 0.05 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 5 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 5 | 0.05 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 5 | 0.05 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 11 | 0.05 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 11 | 0.05 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 11 | 0.05 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 11 | 0.05 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 11 | 0.05 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 11 | 0.05 |
| (1,1541) | 1:A:6:ALA:HB1 | 1:A:7:GLY:HA3 | 15 | 0.05 |
| (1,1541) | 1:A:6:ALA:HB2 | 1:A:7:GLY:HA3 | 15 | 0.05 |
| (1,1541) | 1:A:6:ALA:HB3 | 1:A:7:GLY:HA3 | 15 | 0.05 |
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 1 | 0.05 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 1 | 0.05 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 1 | 0.05 |
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 12 | 0.05 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 12 | 0.05 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 12 | 0.05 |
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 18 | 0.05 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 18 | 0.05 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 18 | 0.05 |
| (1,1527) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HA | 5 | 0.05 |
| (1,1527) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HA | 5 | 0.05 |
| (1,1527) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HA | 5 | 0.05 |
| (1,1527) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HA | 14 | 0.05 |
| (1,1527) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HA | 14 | 0.05 |
| (1,1527) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HA | 14 | 0.05 |
| (1,1527) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HA | 19 | 0.05 |
| (1,1527) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HA | 19 | 0.05 |
| (1,1527) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HA | 19 | 0.05 |
| (1,1455) | 1:A:3:ASP:HB2 | 1:A:53:VAL:H | 20 | 0.05 |
| (1,1430) | 1:B:45:PHE:H | 1:B:45:PHE:HE1 | 2 | 0.05 |
| (1,1400) | 1:B:81:LEU:HA | 1:B:82:GLU:H | 5 | 0.05 |
| (1,1370) | 1:B:78:LEU:HD21 | 1:B:79:SER:H | 19 | 0.05 |
| (1,1370) | 1:B:78:LEU:HD22 | 1:B:79:SER:H | 19 | 0.05 |
| (1,1370) | 1:B:78:LEU:HD23 | 1:B:79:SER:H | 19 | 0.05 |
| (1,13) | 1:A:4:PHE:H | 1:A:54:LYS:HA | 16 | 0.05 |
| (1,1242) | 1:B:69:VAL:HG11 | 1:B:71:GLY:H | 17 | 0.05 |
| (1,1242) | 1:B:69:VAL:HG12 | 1:B:71:GLY:H | 17 | 0.05 |
| (1,1242) | 1:B:69:VAL:HG13 | 1:B:71:GLY:H | 17 | 0.05 |
| (1,1226) | 1:B:69:VAL:H | 1:B:70:GLN:H | 6 | 0.05 |
| (1,1225) | 1:A:69:VAL:H | 1:A:70:GLN:H | 9 | 0.05 |
| (1,1222) | 1:B:69:VAL:H | 1:B:72:VAL:H | 9 | 0.05 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1222) | 1:B:69:VAL:H | 1:B:72:VAL:H | 11 | 0.05 |
| (1,1222) | 1:B:69:VAL:H | 1:B:72:VAL:H | 18 | 0.05 |
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 4 | 0.05 |
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 19 | 0.05 |
| (1,1176) | 1:B:67:ARG:HE | 1:B:75:VAL:HB | 7 | 0.05 |
| (1,1176) | 1:B:67:ARG:HE | 1:B:75:VAL:HB | 11 | 0.05 |
| (1,1132) | 1:B:62:LEU:HD11 | 1:B:66:LEU:H | 14 | 0.05 |
| (1,1132) | 1:B:62:LEU:HD12 | 1:B:66:LEU:H | 14 | 0.05 |
| (1,1132) | 1:B:62:LEU:HD13 | 1:B:66:LEU:H | 14 | 0.05 |
| (1,1131) | 1:A:62:LEU:HD11 | 1:A:66:LEU:H | 15 | 0.05 |
| (1,1131) | 1:A:62:LEU:HD12 | 1:A:66:LEU:H | 15 | 0.05 |
| (1,1131) | 1:A:62:LEU:HD13 | 1:A:66:LEU:H | 15 | 0.05 |
| (1,1130) | 1:B:62:LEU:HD11 | 1:B:65:LYS:H | 15 | 0.05 |
| (1,1130) | 1:B:62:LEU:HD12 | 1:B:65:LYS:H | 15 | 0.05 |
| (1,1130) | 1:B:62:LEU:HD13 | 1:B:65:LYS:H | 15 | 0.05 |
| (1,979) | 1:B:58:LYS:H | 1:B:58:LYS:HG3 | 7 | 0.04 |
| (1,978) | 1:A:58:LYS:H | 1:A:58:LYS:HG3 | 1 | 0.04 |
| (1,978) | 1:A:58:LYS:H | 1:A:58:LYS:HG3 | 14 | 0.04 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 14 | 0.04 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 15 | 0.04 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 18 | 0.04 |
| (1,957) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD22 | 4 | 0.04 |
| (1,957) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD22 | 4 | 0.04 |
| (1,957) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD22 | 20 | 0.04 |
| (1,957) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD22 | 20 | 0.04 |
| (1,956) | 1:A:54:LYS:HE2 | 1:A:55:ASN:HD22 | 11 | 0.04 |
| (1,956) | 1:A:54:LYS:HE3 | 1:A:55:ASN:HD22 | 11 | 0.04 |
| (1,915) | 1:B:51:ILE:HG12 | 1:B:52:PHE:H | 4 | 0.04 |
| (1,915) | 1:B:51:ILE:HG12 | 1:B:52:PHE:H | 12 | 0.04 |
| (1,915) | 1:B:51:ILE:HG12 | 1:B:52:PHE:H | 16 | 0.04 |
| (1,915) | 1:B:51:ILE:HG12 | 1:B:52:PHE:H | 18 | 0.04 |
| (1,914) | 1:A:51:ILE:HG12 | 1:A:52:PHE:H | 6 | 0.04 |
| (1,849) | 1:B:47:CYS:HG | 1:B:48:ASN:H | 1 | 0.04 |
| (1,849) | 1:B:47:CYS:HG | 1:B:48:ASN:H | 7 | 0.04 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 7 | 0.04 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 11 | 0.04 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 15 | 0.04 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 6 | 0.04 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 14 | 0.04 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 15 | 0.04 |
| (1,8) | 1:B:4:PHE:H | 1:B:5:LEU:HB3 | 7 | 0.04 |
| (1,735) | 1:B:41:LYS:H | 1:B:46:THR:H | 15 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,734) | 1:A:41:LYS:H | 1:A:46:THR:H | 2 | 0.04 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD1 | 2 | 0.04 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD2 | 2 | 0.04 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD1 | 4 | 0.04 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD2 | 4 | 0.04 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD1 | 3 | 0.04 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD2 | 3 | 0.04 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD1 | 9 | 0.04 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD2 | 9 | 0.04 |
| (1,73) | 1:A:9:ARG:H | 1:A:76:GLU:HB2 | 19 | 0.04 |
| (1,631) | 1:B:35:THR:H | 1:B:83:HIS:HE1 | 5 | 0.04 |
| (1,579) | 1:A:32:ASN:HD21 | 1:A:33:ILE:HB | 12 | 0.04 |
| (1,579) | 1:A:32:ASN:HD21 | 1:A:33:ILE:HB | 17 | 0.04 |
| (1,561) | 1:A:29:PHE:HD1 | 1:A:31:THR:H | 6 | 0.04 |
| (1,561) | 1:A:29:PHE:HD2 | 1:A:31:THR:H | 6 | 0.04 |
| (1,561) | 1:A:29:PHE:HD1 | 1:A:31:THR:H | 18 | 0.04 |
| (1,561) | 1:A:29:PHE:HD2 | 1:A:31:THR:H | 18 | 0.04 |
| (1,557) | 1:A:30:ASP:HA | 1:A:31:THR:H | 14 | 0.04 |
| (1,5262) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HA | 16 | 0.04 |
| (1,5262) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HA | 17 | 0.04 |
| (1,5261) | 1:B:82:GLU:HA | 1:B:82:GLU:HG2 | 7 | 0.04 |
| (1,5242) | 1:B:68:LYS:HA | 1:B:68:LYS:HG2 | 14 | 0.04 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 3 | 0.04 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 12 | 0.04 |
| (1,5216) | 1:B:63:MET:HE1 | 1:B:77:ARG:HB2 | 16 | 0.04 |
| (1,5216) | 1:B:63:MET:HE2 | 1:B:77:ARG:HB2 | 16 | 0.04 |
| (1,5216) | 1:B:63:MET:HE3 | 1:B:77:ARG:HB2 | 16 | 0.04 |
| (1,5216) | 1:B:63:MET:HE1 | 1:B:77:ARG:HB2 | 18 | 0.04 |
| (1,5216) | 1:B:63:MET:HE2 | 1:B:77:ARG:HB2 | 18 | 0.04 |
| (1,5216) | 1:B:63:MET:HE3 | 1:B:77:ARG:HB2 | 18 | 0.04 |
| (1,5206) | 1:B:62:LEU:HA | 1:B:65:LYS:HG2 | 5 | 0.04 |
| (1,5193) | 1:B:58:LYS:HE2 | 1:B:62:LEU:H | 18 | 0.04 |
| (1,5191) | 1:B:58:LYS:HG2 | 1:B:58:LYS:HE2 | 20 | 0.04 |
| (1,5162) | 1:B:53:VAL:HA | 1:B:54:LYS:HB2 | 13 | 0.04 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD11 | 9 | 0.04 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD12 | 9 | 0.04 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD13 | 9 | 0.04 |
| (1,5123) | 1:B:37:VAL:HB | 1:B:48:ASN:HD21 | 20 | 0.04 |
| (1,5114) | 1:B:35:THR:HB | 1:B:50:MET:HB2 | 1 | 0.04 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD11 | 2 | 0.04 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD12 | 2 | 0.04 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD13 | 2 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5063) | 1:B:27:SER:HB2 | 1:B:28:LYS:H | 16 | 0.04 |
| (1,5044) | 1:B:25:VAL:H | 1:B:28:LYS:HG2 | 12 | 0.04 |
| (1,5024) | 1:B:18:MET:HG2 | 1:B:45:PHE:HZ | 11 | 0.04 |
| (1,5023) | 1:B:18:MET:HG2 | 1:B:45:PHE:HE1 | 9 | 0.04 |
| (1,4998) | 1:B:14:ASP:HB2 | 1:B:45:PHE:HD1 | 19 | 0.04 |
| (1,4998) | 1:B:14:ASP:HB2 | 1:B:45:PHE:HD2 | 19 | 0.04 |
| (1,4994) | 1:B:14:ASP:HB2 | 1:B:43:GLY:HA2 | 16 | 0.04 |
| (1,4985) | 1:B:9:ARG:HD2 | 1:B:48:ASN:HD21 | 18 | 0.04 |
| (1,4985) | 1:B:9:ARG:HD3 | 1:B:48:ASN:HD21 | 18 | 0.04 |
| (1,4981) | 1:B:9:ARG:H | 1:B:76:GLU:HB2 | 17 | 0.04 |
| (1,4968) | 1:B:8:ILE:H | 1:B:8:ILE:HG12 | 4 | 0.04 |
| (1,4968) | 1:B:8:ILE:H | 1:B:8:ILE:HG12 | 17 | 0.04 |
| (1,4955) | 1:B:4:PHE:H | 1:B:52:PHE:HB2 | 10 | 0.04 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 12 | 0.04 |
| (1,4934) | 1:A:76:GLU:HA | 1:A:77:ARG:HB2 | 4 | 0.04 |
| (1,4934) | 1:A:76:GLU:HA | 1:A:77:ARG:HB2 | 7 | 0.04 |
| (1,4930) | 1:A:68:LYS:HA | 1:A:68:LYS:HG2 | 12 | 0.04 |
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 17 | 0.04 |
| (1,4910) | 1:A:64:ASP:HA | 1:A:67:ARG:HG2 | 6 | 0.04 |
| (1,4889) | 1:A:58:LYS:HE2 | 1:A:59:LEU:HA | 16 | 0.04 |
| (1,4888) | 1:A:58:LYS:HG2 | 1:A:58:LYS:HE2 | 12 | 0.04 |
| (1,4888) | 1:A:58:LYS:HG2 | 1:A:58:LYS:HE2 | 18 | 0.04 |
| (1,4858) | 1:A:52:PHE:HB2 | 1:A:53:VAL:H | 17 | 0.04 |
| (1,4822) | 1:A:37:VAL:HG11 | 1:A:48:ASN:HD21 | 18 | 0.04 |
| (1,4822) | 1:A:37:VAL:HG12 | 1:A:48:ASN:HD21 | 18 | 0.04 |
| (1,4822) | 1:A:37:VAL:HG13 | 1:A:48:ASN:HD21 | 18 | 0.04 |
| (1,4809) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 17 | 0.04 |
| (1,4774) | 1:A:28:LYS:HB2 | 1:A:28:LYS:HD2 | 17 | 0.04 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 8 | 0.04 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 9 | 0.04 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 14 | 0.04 |
| (1,4727) | 1:A:20:ASN:HD21 | 1:B:33:ILE:HG12 | 15 | 0.04 |
| (1,4696) | 1:A:16:ASN:HB2 | 1:A:18:MET:H | 9 | 0.04 |
| (1,4690) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD21 | 4 | 0.04 |
| (1,4690) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD21 | 4 | 0.04 |
| (1,4667) | 1:A:14:ASP:HA | 1:A:15:LYS:HB2 | 13 | 0.04 |
| (1,4630) | 1:A:3:ASP:HB2 | 1:A:52:PHE:HD1 | 19 | 0.04 |
| (1,4630) | 1:A:3:ASP:HB2 | 1:A:52:PHE:HD2 | 19 | 0.04 |
| (1,4620) | 1:B:82:GLU:HA | 1:B:83:HIS:HD2 | 11 | 0.04 |
| (1,4614) | 1:B:82:GLU:HG2 | 1:B:83:HIS:HD2 | 11 | 0.04 |
| (1,4610) | 1:B:81:LEU:HB3 | 1:B:83:HIS:HD2 | 11 | 0.04 |
| (1,4608) | 1:B:5:LEU:HG | 1:B:83:HIS:HD2 | 14 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 10 | 0.04 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 14 | 0.04 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 4 | 0.04 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 6 | 0.04 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 16 | 0.04 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 18 | 0.04 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG21 | 5 | 0.04 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG22 | 5 | 0.04 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG23 | 5 | 0.04 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG21 | 16 | 0.04 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG22 | 16 | 0.04 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG23 | 16 | 0.04 |
| (1,4562) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HE2 | 15 | 0.04 |
| (1,4562) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HE3 | 15 | 0.04 |
| (1,4538) | 1:B:52:PHE:HD1 | 1:B:53:VAL:H | 2 | 0.04 |
| (1,4538) | 1:B:52:PHE:HD2 | 1:B:53:VAL:H | 2 | 0.04 |
| (1,4538) | 1:B:52:PHE:HD1 | 1:B:53:VAL:H | 3 | 0.04 |
| (1,4538) | 1:B:52:PHE:HD2 | 1:B:53:VAL:H | 3 | 0.04 |
| (1,4538) | 1:B:52:PHE:HD1 | 1:B:53:VAL:H | 11 | 0.04 |
| (1,4538) | 1:B:52:PHE:HD2 | 1:B:53:VAL:H | 11 | 0.04 |
| (1,4537) | 1:A:52:PHE:HD1 | 1:A:53:VAL:H | 4 | 0.04 |
| (1,4537) | 1:A:52:PHE:HD2 | 1:A:53:VAL:H | 4 | 0.04 |
| (1,4537) | 1:A:52:PHE:HD1 | 1:A:53:VAL:H | 7 | 0.04 |
| (1,4537) | 1:A:52:PHE:HD2 | 1:A:53:VAL:H | 7 | 0.04 |
| (1,4537) | 1:A:52:PHE:HD1 | 1:A:53:VAL:H | 16 | 0.04 |
| (1,4537) | 1:A:52:PHE:HD2 | 1:A:53:VAL:H | 16 | 0.04 |
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD1 | 1 | 0.04 |
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD2 | 1 | 0.04 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 9 | 0.04 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 10 | 0.04 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 13 | 0.04 |
| (1,4413) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 3 | 0.04 |
| (1,4413) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 3 | 0.04 |
| (1,4413) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 9 | 0.04 |
| (1,4413) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 9 | 0.04 |
| (1,4413) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 11 | 0.04 |
| (1,4413) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 11 | 0.04 |
| (1,4413) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 16 | 0.04 |
| (1,4413) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 16 | 0.04 |
| (1,4412) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 10 | 0.04 |
| (1,4412) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 10 | 0.04 |
| (1,4393) | 1:B:4:PHE:HZ | 1:B:6:ALA:HA | 11 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4392) | 1:A:4:PHE:HZ | 1:A:6:ALA:HA | 2 | 0.04 |
| (1,4392) | 1:A:4:PHE:HZ | 1:A:6:ALA:HA | 14 | 0.04 |
| (1,4371) | 1:B:4:PHE:HE1 | 1:B:55:ASN:HA | 18 | 0.04 |
| (1,4366) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HA | 14 | 0.04 |
| (1,4351) | 1:B:4:PHE:HD1 | 1:B:5:LEU:H | 13 | 0.04 |
| (1,4351) | 1:B:4:PHE:HD2 | 1:B:5:LEU:H | 13 | 0.04 |
| (1,4350) | 1:A:4:PHE:HD1 | 1:A:5:LEU:H | 13 | 0.04 |
| (1,4350) | 1:A:4:PHE:HD2 | 1:A:5:LEU:H | 13 | 0.04 |
| (1,4344) | 1:A:4:PHE:HD1 | 1:A:54:LYS:HA | 13 | 0.04 |
| (1,4344) | 1:A:4:PHE:HD2 | 1:A:54:LYS:HA | 13 | 0.04 |
| (1,4325) | 1:B:80:ASN:HA | 1:B:81:LEU:HG | 4 | 0.04 |
| (1,4324) | 1:A:80:ASN:HA | 1:A:81:LEU:HG | 5 | 0.04 |
| (1,4324) | 1:A:80:ASN:HA | 1:A:81:LEU:HG | 17 | 0.04 |
| (1,4318) | 1:A:77:ARG:HG3 | 1:A:79:SER:HA | 11 | 0.04 |
| (1,4317) | 1:B:79:SER:HA | 1:B:81:LEU:HG | 12 | 0.04 |
| (1,4316) | 1:A:79:SER:HA | 1:A:81:LEU:HG | 7 | 0.04 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG2 | 3 | 0.04 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG3 | 3 | 0.04 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 14 | 0.04 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 14 | 0.04 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 16 | 0.04 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 16 | 0.04 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 19 | 0.04 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 19 | 0.04 |
| (1,4243) | 1:B:15:LYS:HA | 1:B:17:GLY:H | 11 | 0.04 |
| (1,4242) | 1:A:15:LYS:HA | 1:A:17:GLY:H | 9 | 0.04 |
| (1,4217) | 1:B:8:ILE:HA | 1:B:78:LEU:HB2 | 2 | 0.04 |
| (1,4217) | 1:B:8:ILE:HA | 1:B:78:LEU:HB2 | 14 | 0.04 |
| (1,4192) | 1:A:5:LEU:HB2 | 1:A:83:HIS:HB3 | 10 | 0.04 |
| (1,4192) | 1:A:5:LEU:HB2 | 1:A:83:HIS:HB3 | 14 | 0.04 |
| (1,4190) | 1:A:81:LEU:HD11 | 1:A:83:HIS:HB3 | 3 | 0.04 |
| (1,4190) | 1:A:81:LEU:HD12 | 1:A:83:HIS:HB3 | 3 | 0.04 |
| (1,4190) | 1:A:81:LEU:HD13 | 1:A:83:HIS:HB3 | 3 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD11 | 6 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD12 | 6 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD13 | 6 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD11 | 6 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD12 | 6 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD13 | 6 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD11 | 6 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD12 | 6 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD13 | 6 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD11 | 20 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD12 | 20 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD13 | 20 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD11 | 20 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD12 | 20 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD13 | 20 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD11 | 20 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD12 | 20 | 0.04 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD13 | 20 | 0.04 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 3 | 0.04 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 3 | 0.04 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 3 | 0.04 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 4 | 0.04 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 4 | 0.04 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 4 | 0.04 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG21 | 19 | 0.04 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG22 | 19 | 0.04 |
| (1,4172) | 1:A:73:PHE:HB3 | 1:A:75:VAL:HG23 | 19 | 0.04 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 9 | 0.04 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 9 | 0.04 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 9 | 0.04 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 15 | 0.04 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 15 | 0.04 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 15 | 0.04 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 16 | 0.04 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 16 | 0.04 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 16 | 0.04 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 19 | 0.04 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 19 | 0.04 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 19 | 0.04 |
| (1,4146) | 1:A:61:THR:HG21 | 1:A:65:LYS:HB3 | 8 | 0.04 |
| (1,4146) | 1:A:61:THR:HG22 | 1:A:65:LYS:HB3 | 8 | 0.04 |
| (1,4146) | 1:A:61:THR:HG23 | 1:A:65:LYS:HB3 | 8 | 0.04 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD11 | 1 | 0.04 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD12 | 1 | 0.04 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD13 | 1 | 0.04 |
| (1,4123) | 1:B:23:THR:H | 1:B:26:ILE:HD11 | 5 | 0.04 |
| (1,4123) | 1:B:23:THR:H | 1:B:26:ILE:HD12 | 5 | 0.04 |
| (1,4123) | 1:B:23:THR:H | 1:B:26:ILE:HD13 | 5 | 0.04 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 1 | 0.04 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 2 | 0.04 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 12 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 17 | 0.04 |
| (1,4115) | 1:A:18:MET:HA | 1:A:21:GLN:HB2 | 6 | 0.04 |
| (1,4115) | 1:A:18:MET:HA | 1:A:21:GLN:HB2 | 11 | 0.04 |
| (1,4106) | 1:B:15:LYS:HB3 | 1:B:18:MET:HB3 | 16 | 0.04 |
| (1,4084) | 1:A:82:GLU:HG3 | 1:A:83:HIS:HA | 9 | 0.04 |
| (1,4074) | 1:A:82:GLU:HA | 1:A:83:HIS:HB2 | 4 | 0.04 |
| (1,4074) | 1:A:82:GLU:HA | 1:A:83:HIS:HB2 | 19 | 0.04 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD21 | 3 | 0.04 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD22 | 3 | 0.04 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD23 | 3 | 0.04 |
| (1,4018) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD21 | 10 | 0.04 |
| (1,4018) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD22 | 10 | 0.04 |
| (1,4018) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD23 | 10 | 0.04 |
| (1,4014) | 1:A:78:LEU:HB3 | 1:A:79:SER:HB2 | 3 | 0.04 |
| (1,4014) | 1:A:78:LEU:HB3 | 1:A:79:SER:HB3 | 3 | 0.04 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD21 | 15 | 0.04 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD22 | 15 | 0.04 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD23 | 15 | 0.04 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD21 | 15 | 0.04 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD22 | 15 | 0.04 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD23 | 15 | 0.04 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD11 | 12 | 0.04 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD12 | 12 | 0.04 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD13 | 12 | 0.04 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD11 | 5 | 0.04 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD12 | 5 | 0.04 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD13 | 5 | 0.04 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD11 | 16 | 0.04 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD12 | 16 | 0.04 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD13 | 16 | 0.04 |
| (1,3972) | 1:A:9:ARG:HD2 | 1:A:78:LEU:HD11 | 10 | 0.04 |
| (1,3972) | 1:A:9:ARG:HD2 | 1:A:78:LEU:HD12 | 10 | 0.04 |
| (1,3972) | 1:A:9:ARG:HD2 | 1:A:78:LEU:HD13 | 10 | 0.04 |
| (1,3972) | 1:A:9:ARG:HD3 | 1:A:78:LEU:HD11 | 10 | 0.04 |
| (1,3972) | 1:A:9:ARG:HD3 | 1:A:78:LEU:HD12 | 10 | 0.04 |
| (1,3972) | 1:A:9:ARG:HD3 | 1:A:78:LEU:HD13 | 10 | 0.04 |
| (1,397) | 1:B:22:ILE:H | 1:B:23:THR:HG1 | 8 | 0.04 |
| (1,3967) | 1:B:50:MET:HE1 | 1:B:78:LEU:HD11 | 13 | 0.04 |
| (1,3967) | 1:B:50:MET:HE1 | 1:B:78:LEU:HD12 | 13 | 0.04 |
| (1,3967) | 1:B:50:MET:HE1 | 1:B:78:LEU:HD13 | 13 | 0.04 |
| (1,3967) | 1:B:50:MET:HE2 | 1:B:78:LEU:HD11 | 13 | 0.04 |
| (1,3967) | 1:B:50:MET:HE2 | 1:B:78:LEU:HD12 | 13 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3967) | 1:B:50:MET:HE2 | 1:B:78:LEU:HD13 | 13 | 0.04 |
| (1,3967) | 1:B:50:MET:HE3 | 1:B:78:LEU:HD11 | 13 | 0.04 |
| (1,3967) | 1:B:50:MET:HE3 | 1:B:78:LEU:HD12 | 13 | 0.04 |
| (1,3967) | 1:B:50:MET:HE3 | 1:B:78:LEU:HD13 | 13 | 0.04 |
| (1,3952) | 1:A:78:LEU:HB2 | 1:A:80:ASN:H | 6 | 0.04 |
| (1,3927) | 1:B:4:PHE:HZ | 1:B:77:ARG:HD2 | 10 | 0.04 |
| (1,3927) | 1:B:4:PHE:HZ | 1:B:77:ARG:HD3 | 10 | 0.04 |
| (1,3917) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HD2 | 9 | 0.04 |
| (1,3917) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HD3 | 9 | 0.04 |
| (1,3917) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HD2 | 9 | 0.04 |
| (1,3917) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HD3 | 9 | 0.04 |
| (1,3917) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HD2 | 9 | 0.04 |
| (1,3917) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HD3 | 9 | 0.04 |
| (1,3901) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 15 | 0.04 |
| (1,3901) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 15 | 0.04 |
| (1,3901) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 15 | 0.04 |
| (1,3896) | 1:A:74:THR:HA | 1:A:76:GLU:HG2 | 19 | 0.04 |
| (1,3896) | 1:A:74:THR:HA | 1:A:76:GLU:HG3 | 19 | 0.04 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 5 | 0.04 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 5 | 0.04 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 5 | 0.04 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 14 | 0.04 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 14 | 0.04 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 14 | 0.04 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 17 | 0.04 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 17 | 0.04 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 17 | 0.04 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG21 | 4 | 0.04 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG22 | 4 | 0.04 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG23 | 4 | 0.04 |
| (1,3857) | 1:A:73:PHE:HA | 1:A:74:THR:HG21 | 10 | 0.04 |
| (1,3857) | 1:A:73:PHE:HA | 1:A:74:THR:HG22 | 10 | 0.04 |
| (1,3857) | 1:A:73:PHE:HA | 1:A:74:THR:HG23 | 10 | 0.04 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG21 | 18 | 0.04 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG22 | 18 | 0.04 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG23 | 18 | 0.04 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG11 | 1 | 0.04 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG12 | 1 | 0.04 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG13 | 1 | 0.04 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG11 | 1 | 0.04 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG12 | 1 | 0.04 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG13 | 1 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3776) | 1:B:70:GLN:HG2 | 1:B:72:VAL:H | 5 | 0.04 |
| (1,3776) | 1:B:70:GLN:HG3 | 1:B:72:VAL:H | 5 | 0.04 |
| (1,3755) | 1:A:69:VAL:H | 1:A:70:GLN:HB2 | 3 | 0.04 |
| (1,3755) | 1:A:69:VAL:H | 1:A:70:GLN:HB3 | 3 | 0.04 |
| (1,3736) | 1:B:66:LEU:HA | 1:B:69:VAL:HB | 14 | 0.04 |
| (1,3735) | 1:A:66:LEU:HA | 1:A:69:VAL:HB | 8 | 0.04 |
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 5 | 0.04 |
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 9 | 0.04 |
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 16 | 0.04 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG21 | 19 | 0.04 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG22 | 19 | 0.04 |
| (1,3726) | 1:B:45:PHE:HE1 | 1:B:69:VAL:HG23 | 19 | 0.04 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG21 | 8 | 0.04 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG22 | 8 | 0.04 |
| (1,3725) | 1:A:45:PHE:HE1 | 1:A:69:VAL:HG23 | 8 | 0.04 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG11 | 14 | 0.04 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG12 | 14 | 0.04 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG13 | 14 | 0.04 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG11 | 14 | 0.04 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG12 | 14 | 0.04 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG13 | 14 | 0.04 |
| (1,3702) | 1:B:15:LYS:HE2 | 1:B:18:MET:H | 12 | 0.04 |
| (1,3702) | 1:B:15:LYS:HE3 | 1:B:18:MET:H | 12 | 0.04 |
| (1,3702) | 1:B:15:LYS:HE2 | 1:B:18:MET:H | 19 | 0.04 |
| (1,3702) | 1:B:15:LYS:HE3 | 1:B:18:MET:H | 19 | 0.04 |
| (1,3701) | 1:A:15:LYS:HE2 | 1:A:18:MET:H | 2 | 0.04 |
| (1,3701) | 1:A:15:LYS:HE3 | 1:A:18:MET:H | 2 | 0.04 |
| (1,369) | 1:B:21:GLN:HE22 | 1:B:69:VAL:HA | 7 | 0.04 |
| (1,3653) | 1:B:67:ARG:HD2 | 1:B:75:VAL:HG11 | 2 | 0.04 |
| (1,3653) | 1:B:67:ARG:HD2 | 1:B:75:VAL:HG12 | 2 | 0.04 |
| (1,3653) | 1:B:67:ARG:HD2 | 1:B:75:VAL:HG13 | 2 | 0.04 |
| (1,3653) | 1:B:67:ARG:HD3 | 1:B:75:VAL:HG11 | 2 | 0.04 |
| (1,3653) | 1:B:67:ARG:HD3 | 1:B:75:VAL:HG12 | 2 | 0.04 |
| (1,3653) | 1:B:67:ARG:HD3 | 1:B:75:VAL:HG13 | 2 | 0.04 |
| (1,362) | 1:A:21:GLN:HE22 | 1:A:69:VAL:HG21 | 11 | 0.04 |
| (1,362) | 1:A:21:GLN:HE22 | 1:A:69:VAL:HG22 | 11 | 0.04 |
| (1,362) | 1:A:21:GLN:HE22 | 1:A:69:VAL:HG23 | 11 | 0.04 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 7 | 0.04 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 7 | 0.04 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 7 | 0.04 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 3 | 0.04 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 3 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 3 | 0.04 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 9 | 0.04 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 9 | 0.04 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 9 | 0.04 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB2 | 4 | 0.04 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB3 | 4 | 0.04 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB2 | 5 | 0.04 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB3 | 5 | 0.04 |
| (1,3537) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HB2 | 2 | 0.04 |
| (1,3537) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HB2 | 10 | 0.04 |
| (1,3537) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HB2 | 12 | 0.04 |
| (1,3536) | 1:A:64:ASP:HB2 | 1:A:65:LYS:HB2 | 1 | 0.04 |
| (1,3536) | 1:A:64:ASP:HB2 | 1:A:65:LYS:HB2 | 6 | 0.04 |
| (1,3536) | 1:A:64:ASP:HB2 | 1:A:65:LYS:HB2 | 13 | 0.04 |
| (1,3531) | 1:A:61:THR:HG21 | 1:A:64:ASP:HB2 | 20 | 0.04 |
| (1,3531) | 1:A:61:THR:HG22 | 1:A:64:ASP:HB2 | 20 | 0.04 |
| (1,3531) | 1:A:61:THR:HG23 | 1:A:64:ASP:HB2 | 20 | 0.04 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE1 | 10 | 0.04 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE2 | 10 | 0.04 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE3 | 10 | 0.04 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE1 | 13 | 0.04 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE2 | 13 | 0.04 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE3 | 13 | 0.04 |
| (1,3527) | 1:A:63:MET:HE1 | 1:A:77:ARG:H | 1 | 0.04 |
| (1,3527) | 1:A:63:MET:HE2 | 1:A:77:ARG:H | 1 | 0.04 |
| (1,3527) | 1:A:63:MET:HE3 | 1:A:77:ARG:H | 1 | 0.04 |
| (1,3527) | 1:A:63:MET:HE1 | 1:A:77:ARG:H | 9 | 0.04 |
| (1,3527) | 1:A:63:MET:HE2 | 1:A:77:ARG:H | 9 | 0.04 |
| (1,3527) | 1:A:63:MET:HE3 | 1:A:77:ARG:H | 9 | 0.04 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 5 | 0.04 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 5 | 0.04 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 5 | 0.04 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 6 | 0.04 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 6 | 0.04 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 6 | 0.04 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 8 | 0.04 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 8 | 0.04 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 8 | 0.04 |
| (1,3519) | 1:A:63:MET:HE1 | 1:A:76:GLU:HA | 7 | 0.04 |
| (1,3519) | 1:A:63:MET:HE2 | 1:A:76:GLU:HA | 7 | 0.04 |
| (1,3519) | 1:A:63:MET:HE3 | 1:A:76:GLU:HA | 7 | 0.04 |
| (1,3519) | 1:A:63:MET:HE1 | 1:A:76:GLU:HA | 16 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3519) | 1:A:63:MET:HE2 | 1:A:76:GLU:HA | 16 | 0.04 |
| (1,3519) | 1:A:63:MET:HE3 | 1:A:76:GLU:HA | 16 | 0.04 |
| (1,3519) | 1:A:63:MET:HE1 | 1:A:76:GLU:HA | 17 | 0.04 |
| (1,3519) | 1:A:63:MET:HE2 | 1:A:76:GLU:HA | 17 | 0.04 |
| (1,3519) | 1:A:63:MET:HE3 | 1:A:76:GLU:HA | 17 | 0.04 |
| (1,3519) | 1:A:63:MET:HE1 | 1:A:76:GLU:HA | 20 | 0.04 |
| (1,3519) | 1:A:63:MET:HE2 | 1:A:76:GLU:HA | 20 | 0.04 |
| (1,3519) | 1:A:63:MET:HE3 | 1:A:76:GLU:HA | 20 | 0.04 |
| (1,3518) | 1:B:63:MET:HE1 | 1:B:77:ARG:HA | 17 | 0.04 |
| (1,3518) | 1:B:63:MET:HE2 | 1:B:77:ARG:HA | 17 | 0.04 |
| (1,3518) | 1:B:63:MET:HE3 | 1:B:77:ARG:HA | 17 | 0.04 |
| (1,3517) | 1:A:63:MET:HE1 | 1:A:77:ARG:HA | 13 | 0.04 |
| (1,3517) | 1:A:63:MET:HE2 | 1:A:77:ARG:HA | 13 | 0.04 |
| (1,3517) | 1:A:63:MET:HE3 | 1:A:77:ARG:HA | 13 | 0.04 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE1 | 18 | 0.04 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE2 | 18 | 0.04 |
| (1,3514) | 1:B:61:THR:HA | 1:B:63:MET:HE3 | 18 | 0.04 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE1 | 8 | 0.04 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE2 | 8 | 0.04 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE3 | 8 | 0.04 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE1 | 19 | 0.04 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE2 | 19 | 0.04 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE3 | 19 | 0.04 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE1 | 19 | 0.04 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE2 | 19 | 0.04 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE3 | 19 | 0.04 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE1 | 19 | 0.04 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE2 | 19 | 0.04 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE3 | 19 | 0.04 |
| (1,3386) | 1:A:61:THR:HG21 | 1:A:65:LYS:HE2 | 8 | 0.04 |
| (1,3386) | 1:A:61:THR:HG21 | 1:A:65:LYS:HE3 | 8 | 0.04 |
| (1,3386) | 1:A:61:THR:HG22 | 1:A:65:LYS:HE2 | 8 | 0.04 |
| (1,3386) | 1:A:61:THR:HG22 | 1:A:65:LYS:HE3 | 8 | 0.04 |
| (1,3386) | 1:A:61:THR:HG23 | 1:A:65:LYS:HE2 | 8 | 0.04 |
| (1,3386) | 1:A:61:THR:HG23 | 1:A:65:LYS:HE3 | 8 | 0.04 |
| (1,3323) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD21 | 17 | 0.04 |
| (1,3323) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD22 | 17 | 0.04 |
| (1,3323) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD23 | 17 | 0.04 |
| (1,3323) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD21 | 17 | 0.04 |
| (1,3323) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD22 | 17 | 0.04 |
| (1,3323) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD23 | 17 | 0.04 |
| (1,3323) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD21 | 17 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3323) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD22 | 17 | 0.04 |
| (1,3323) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD23 | 17 | 0.04 |
| (1,3311) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD11 | 7 | 0.04 |
| (1,3311) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD12 | 7 | 0.04 |
| (1,3311) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD13 | 7 | 0.04 |
| (1,3311) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD11 | 7 | 0.04 |
| (1,3311) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD12 | 7 | 0.04 |
| (1,3311) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD13 | 7 | 0.04 |
| (1,3311) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD11 | 7 | 0.04 |
| (1,3311) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD12 | 7 | 0.04 |
| (1,3311) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD13 | 7 | 0.04 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD11 | 15 | 0.04 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD12 | 15 | 0.04 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD13 | 15 | 0.04 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD11 | 15 | 0.04 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD12 | 15 | 0.04 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD13 | 15 | 0.04 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD11 | 15 | 0.04 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD12 | 15 | 0.04 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD13 | 15 | 0.04 |
| (1,3285) | 1:B:58:LYS:H | 1:B:58:LYS:HD2 | 14 | 0.04 |
| (1,3285) | 1:B:58:LYS:H | 1:B:58:LYS:HD3 | 14 | 0.04 |
| (1,3284) | 1:A:58:LYS:H | 1:A:58:LYS:HD2 | 10 | 0.04 |
| (1,3284) | 1:A:58:LYS:H | 1:A:58:LYS:HD3 | 10 | 0.04 |
| (1,3275) | 1:B:30:ASP:HB2 | 1:B:58:LYS:HD2 | 3 | 0.04 |
| (1,3275) | 1:B:30:ASP:HB2 | 1:B:58:LYS:HD3 | 3 | 0.04 |
| (1,3275) | 1:B:30:ASP:HB3 | 1:B:58:LYS:HD2 | 3 | 0.04 |
| (1,3275) | 1:B:30:ASP:HB3 | 1:B:58:LYS:HD3 | 3 | 0.04 |
| (1,3253) | 1:B:4:PHE:HZ | 1:B:58:LYS:HG3 | 10 | 0.04 |
| (1,3231) | 1:B:57:ASP:HB2 | 1:B:58:LYS:HG3 | 5 | 0.04 |
| (1,3231) | 1:B:57:ASP:HB3 | 1:B:58:LYS:HG3 | 5 | 0.04 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG21 | 13 | 0.04 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG22 | 13 | 0.04 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG23 | 13 | 0.04 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG21 | 13 | 0.04 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG22 | 13 | 0.04 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG23 | 13 | 0.04 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG21 | 17 | 0.04 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG22 | 17 | 0.04 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG23 | 17 | 0.04 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG21 | 17 | 0.04 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG22 | 17 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG23 | 17 | 0.04 |
| (1,3193) | 1:B:54:LYS:HA | 1:B:54:LYS:HE2 | 14 | 0.04 |
| (1,3193) | 1:B:54:LYS:HA | 1:B:54:LYS:HE3 | 14 | 0.04 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD2 | 2 | 0.04 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD3 | 2 | 0.04 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD2 | 18 | 0.04 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD3 | 18 | 0.04 |
| (1,3128) | 1:A:53:VAL:HG21 | 1:A:58:LYS:HA | 6 | 0.04 |
| (1,3128) | 1:A:53:VAL:HG22 | 1:A:58:LYS:HA | 6 | 0.04 |
| (1,3128) | 1:A:53:VAL:HG23 | 1:A:58:LYS:HA | 6 | 0.04 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG11 | 13 | 0.04 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG12 | 13 | 0.04 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG13 | 13 | 0.04 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG11 | 18 | 0.04 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG12 | 18 | 0.04 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG13 | 18 | 0.04 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 12 | 0.04 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 12 | 0.04 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 12 | 0.04 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 12 | 0.04 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 12 | 0.04 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 12 | 0.04 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 19 | 0.04 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 19 | 0.04 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 19 | 0.04 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 19 | 0.04 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 19 | 0.04 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 19 | 0.04 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 3 | 0.04 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 3 | 0.04 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 3 | 0.04 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 3 | 0.04 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 3 | 0.04 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 3 | 0.04 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 4 | 0.04 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 4 | 0.04 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 4 | 0.04 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 4 | 0.04 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 4 | 0.04 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 4 | 0.04 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 13 | 0.04 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 13 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 13 | 0.04 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 13 | 0.04 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 13 | 0.04 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 13 | 0.04 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD11 | 1 | 0.04 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD12 | 1 | 0.04 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD13 | 1 | 0.04 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD11 | 15 | 0.04 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD12 | 15 | 0.04 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD13 | 15 | 0.04 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD11 | 1 | 0.04 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD12 | 1 | 0.04 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD13 | 1 | 0.04 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD11 | 1 | 0.04 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD12 | 1 | 0.04 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD13 | 1 | 0.04 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD21 | 6 | 0.04 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD22 | 6 | 0.04 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD23 | 6 | 0.04 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD21 | 6 | 0.04 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD22 | 6 | 0.04 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD23 | 6 | 0.04 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD21 | 6 | 0.04 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD22 | 6 | 0.04 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD23 | 6 | 0.04 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG21 | 20 | 0.04 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG22 | 20 | 0.04 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG23 | 20 | 0.04 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG21 | 2 | 0.04 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG22 | 2 | 0.04 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG23 | 2 | 0.04 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG21 | 14 | 0.04 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG22 | 14 | 0.04 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG23 | 14 | 0.04 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG21 | 15 | 0.04 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG22 | 15 | 0.04 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG23 | 15 | 0.04 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG21 | 18 | 0.04 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG22 | 18 | 0.04 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG23 | 18 | 0.04 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD11 | 19 | 0.04 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD12 | 19 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD13 | 19 | 0.04 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD11 | 19 | 0.04 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD12 | 19 | 0.04 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD13 | 19 | 0.04 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD11 | 19 | 0.04 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD12 | 19 | 0.04 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD13 | 19 | 0.04 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 2 | 0.04 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 2 | 0.04 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 2 | 0.04 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 5 | 0.04 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 5 | 0.04 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 5 | 0.04 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 6 | 0.04 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 6 | 0.04 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 6 | 0.04 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 11 | 0.04 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 11 | 0.04 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 11 | 0.04 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 12 | 0.04 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 12 | 0.04 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 12 | 0.04 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 15 | 0.04 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 15 | 0.04 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 15 | 0.04 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 18 | 0.04 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 18 | 0.04 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 18 | 0.04 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 3 | 0.04 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 3 | 0.04 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 3 | 0.04 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 12 | 0.04 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 12 | 0.04 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 12 | 0.04 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 17 | 0.04 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 17 | 0.04 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 17 | 0.04 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 18 | 0.04 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 18 | 0.04 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 18 | 0.04 |
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 2 | 0.04 |
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 4 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 7 | 0.04 |
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 9 | 0.04 |
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 13 | 0.04 |
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 18 | 0.04 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 19 | 0.04 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 20 | 0.04 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD21 | 10 | 0.04 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD22 | 10 | 0.04 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD23 | 10 | 0.04 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD21 | 10 | 0.04 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD22 | 10 | 0.04 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD23 | 10 | 0.04 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD21 | 10 | 0.04 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD22 | 10 | 0.04 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD23 | 10 | 0.04 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD21 | 7 | 0.04 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD22 | 7 | 0.04 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD23 | 7 | 0.04 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD21 | 7 | 0.04 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD22 | 7 | 0.04 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD23 | 7 | 0.04 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD21 | 7 | 0.04 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD22 | 7 | 0.04 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD23 | 7 | 0.04 |
| (1,2754) | 1:B:23:THR:HG1 | 1:B:47:CYS:HB3 | 11 | 0.04 |
| (1,2754) | 1:B:23:THR:HG1 | 1:B:47:CYS:HB3 | 17 | 0.04 |
| (1,2753) | 1:A:23:THR:HG1 | 1:A:47:CYS:HB3 | 3 | 0.04 |
| (1,2753) | 1:A:23:THR:HG1 | 1:A:47:CYS:HB3 | 6 | 0.04 |
| (1,2753) | 1:A:23:THR:HG1 | 1:A:47:CYS:HB3 | 8 | 0.04 |
| (1,2753) | 1:A:23:THR:HG1 | 1:A:47:CYS:HB3 | 12 | 0.04 |
| (1,2753) | 1:A:23:THR:HG1 | 1:A:47:CYS:HB3 | 13 | 0.04 |
| (1,2725) | 1:A:46:THR:HG21 | 1:A:47:CYS:H | 12 | 0.04 |
| (1,2725) | 1:A:46:THR:HG22 | 1:A:47:CYS:H | 12 | 0.04 |
| (1,2725) | 1:A:46:THR:HG23 | 1:A:47:CYS:H | 12 | 0.04 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG21 | 3 | 0.04 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG22 | 3 | 0.04 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG23 | 3 | 0.04 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG21 | 11 | 0.04 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG22 | 11 | 0.04 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG23 | 11 | 0.04 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG21 | 18 | 0.04 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG22 | 18 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG23 | 18 | 0.04 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG21 | 19 | 0.04 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG22 | 19 | 0.04 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG23 | 19 | 0.04 |
| (1,2681) | 1:A:44:ILE:H | 1:A:44:ILE:HD11 | 7 | 0.04 |
| (1,2681) | 1:A:44:ILE:H | 1:A:44:ILE:HD12 | 7 | 0.04 |
| (1,2681) | 1:A:44:ILE:H | 1:A:44:ILE:HD13 | 7 | 0.04 |
| (1,2676) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HD1 | 7 | 0.04 |
| (1,2676) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HD2 | 7 | 0.04 |
| (1,2676) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HD1 | 7 | 0.04 |
| (1,2676) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HD2 | 7 | 0.04 |
| (1,2676) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HD1 | 7 | 0.04 |
| (1,2676) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HD2 | 7 | 0.04 |
| (1,2672) | 1:B:13:GLU:HA | 1:B:44:ILE:HD11 | 12 | 0.04 |
| (1,2672) | 1:B:13:GLU:HA | 1:B:44:ILE:HD12 | 12 | 0.04 |
| (1,2672) | 1:B:13:GLU:HA | 1:B:44:ILE:HD13 | 12 | 0.04 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD11 | 10 | 0.04 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD12 | 10 | 0.04 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD13 | 10 | 0.04 |
| (1,2670) | 1:B:44:ILE:HD11 | 1:B:46:THR:HB | 8 | 0.04 |
| (1,2670) | 1:B:44:ILE:HD12 | 1:B:46:THR:HB | 8 | 0.04 |
| (1,2670) | 1:B:44:ILE:HD13 | 1:B:46:THR:HB | 8 | 0.04 |
| (1,2670) | 1:B:44:ILE:HD11 | 1:B:46:THR:HB | 19 | 0.04 |
| (1,2670) | 1:B:44:ILE:HD12 | 1:B:46:THR:HB | 19 | 0.04 |
| (1,2670) | 1:B:44:ILE:HD13 | 1:B:46:THR:HB | 19 | 0.04 |
| (1,2669) | 1:A:44:ILE:HD11 | 1:A:46:THR:HB | 7 | 0.04 |
| (1,2669) | 1:A:44:ILE:HD12 | 1:A:46:THR:HB | 7 | 0.04 |
| (1,2669) | 1:A:44:ILE:HD13 | 1:A:46:THR:HB | 7 | 0.04 |
| (1,2669) | 1:A:44:ILE:HD11 | 1:A:46:THR:HB | 18 | 0.04 |
| (1,2669) | 1:A:44:ILE:HD12 | 1:A:46:THR:HB | 18 | 0.04 |
| (1,2669) | 1:A:44:ILE:HD13 | 1:A:46:THR:HB | 18 | 0.04 |
| (1,2661) | 1:A:44:ILE:HG21 | 1:A:45:PHE:H | 16 | 0.04 |
| (1,2661) | 1:A:44:ILE:HG22 | 1:A:45:PHE:H | 16 | 0.04 |
| (1,2661) | 1:A:44:ILE:HG23 | 1:A:45:PHE:H | 16 | 0.04 |
| (1,2638) | 1:B:44:ILE:HG13 | 1:B:45:PHE:H | 6 | 0.04 |
| (1,2638) | 1:B:44:ILE:HG13 | 1:B:45:PHE:H | 8 | 0.04 |
| (1,2638) | 1:B:44:ILE:HG13 | 1:B:45:PHE:H | 18 | 0.04 |
| (1,2623) | 1:A:44:ILE:HG12 | 1:A:45:PHE:H | 15 | 0.04 |
| (1,2572) | 1:B:40:ALA:HA | 1:B:45:PHE:HA | 5 | 0.04 |
| (1,2572) | 1:B:40:ALA:HA | 1:B:45:PHE:HA | 11 | 0.04 |
| (1,2572) | 1:B:40:ALA:HA | 1:B:45:PHE:HA | 19 | 0.04 |
| (1,2571) | 1:A:40:ALA:HA | 1:A:45:PHE:HA | 14 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2571) | 1:A:40:ALA:HA | 1:A:45:PHE:HA | 15 | 0.04 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD21 | 4 | 0.04 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD22 | 4 | 0.04 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD23 | 4 | 0.04 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD21 | 10 | 0.04 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD22 | 10 | 0.04 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD23 | 10 | 0.04 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD21 | 19 | 0.04 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD22 | 19 | 0.04 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD23 | 19 | 0.04 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD21 | 11 | 0.04 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD22 | 11 | 0.04 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD23 | 11 | 0.04 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD21 | 12 | 0.04 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD22 | 12 | 0.04 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD23 | 12 | 0.04 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD21 | 13 | 0.04 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD22 | 13 | 0.04 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD23 | 13 | 0.04 |
| (1,2534) | 1:B:23:THR:HG1 | 1:B:38:LEU:HD21 | 19 | 0.04 |
| (1,2534) | 1:B:23:THR:HG1 | 1:B:38:LEU:HD22 | 19 | 0.04 |
| (1,2534) | 1:B:23:THR:HG1 | 1:B:38:LEU:HD23 | 19 | 0.04 |
| (1,2510) | 1:B:38:LEU:HD11 | 1:B:39:ASN:H | 6 | 0.04 |
| (1,2510) | 1:B:38:LEU:HD12 | 1:B:39:ASN:H | 6 | 0.04 |
| (1,2510) | 1:B:38:LEU:HD13 | 1:B:39:ASN:H | 6 | 0.04 |
| (1,2510) | 1:B:38:LEU:HD11 | 1:B:39:ASN:H | 10 | 0.04 |
| (1,2510) | 1:B:38:LEU:HD12 | 1:B:39:ASN:H | 10 | 0.04 |
| (1,2510) | 1:B:38:LEU:HD13 | 1:B:39:ASN:H | 10 | 0.04 |
| (1,2509) | 1:A:38:LEU:HD11 | 1:A:39:ASN:H | 15 | 0.04 |
| (1,2509) | 1:A:38:LEU:HD12 | 1:A:39:ASN:H | 15 | 0.04 |
| (1,2509) | 1:A:38:LEU:HD13 | 1:A:39:ASN:H | 15 | 0.04 |
| (1,2473) | 1:A:37:VAL:HG21 | 1:A:38:LEU:H | 3 | 0.04 |
| (1,2473) | 1:A:37:VAL:HG22 | 1:A:38:LEU:H | 3 | 0.04 |
| (1,2473) | 1:A:37:VAL:HG23 | 1:A:38:LEU:H | 3 | 0.04 |
| (1,2466) | 1:B:37:VAL:HG21 | 1:B:48:ASN:HD22 | 6 | 0.04 |
| (1,2466) | 1:B:37:VAL:HG22 | 1:B:48:ASN:HD22 | 6 | 0.04 |
| (1,2466) | 1:B:37:VAL:HG23 | 1:B:48:ASN:HD22 | 6 | 0.04 |
| (1,2466) | 1:B:37:VAL:HG21 | 1:B:48:ASN:HD22 | 20 | 0.04 |
| (1,2466) | 1:B:37:VAL:HG22 | 1:B:48:ASN:HD22 | 20 | 0.04 |
| (1,2466) | 1:B:37:VAL:HG23 | 1:B:48:ASN:HD22 | 20 | 0.04 |
| (1,2431) | 1:A:37:VAL:HG11 | 1:A:48:ASN:HB3 | 14 | 0.04 |
| (1,2431) | 1:A:37:VAL:HG12 | 1:A:48:ASN:HB3 | 14 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2431) | 1:A:37:VAL:HG13 | 1:A:48:ASN:HB3 | 14 | 0.04 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 19 | 0.04 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 19 | 0.04 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 19 | 0.04 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 13 | 0.04 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 13 | 0.04 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 13 | 0.04 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 15 | 0.04 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 15 | 0.04 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 15 | 0.04 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 20 | 0.04 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 20 | 0.04 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 20 | 0.04 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 2 | 0.04 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 2 | 0.04 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 2 | 0.04 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 13 | 0.04 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 13 | 0.04 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 13 | 0.04 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG21 | 9 | 0.04 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG22 | 9 | 0.04 |
| (1,2371) | 1:A:23:THR:HB | 1:A:36:ILE:HG23 | 9 | 0.04 |
| (1,2368) | 1:B:36:ILE:HG21 | 1:B:37:VAL:HB | 11 | 0.04 |
| (1,2368) | 1:B:36:ILE:HG22 | 1:B:37:VAL:HB | 11 | 0.04 |
| (1,2368) | 1:B:36:ILE:HG23 | 1:B:37:VAL:HB | 11 | 0.04 |
| (1,2368) | 1:B:36:ILE:HG21 | 1:B:37:VAL:HB | 14 | 0.04 |
| (1,2368) | 1:B:36:ILE:HG22 | 1:B:37:VAL:HB | 14 | 0.04 |
| (1,2368) | 1:B:36:ILE:HG23 | 1:B:37:VAL:HB | 14 | 0.04 |
| (1,2344) | 1:B:35:THR:HB | 1:B:50:MET:HB2 | 1 | 0.04 |
| (1,2343) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 17 | 0.04 |
| (1,2268) | 1:B:29:PHE:HD1 | 1:B:31:THR:HB | 5 | 0.04 |
| (1,2268) | 1:B:29:PHE:HD2 | 1:B:31:THR:HB | 5 | 0.04 |
| (1,2268) | 1:B:29:PHE:HD1 | 1:B:31:THR:HB | 6 | 0.04 |
| (1,2268) | 1:B:29:PHE:HD2 | 1:B:31:THR:HB | 6 | 0.04 |
| (1,2268) | 1:B:29:PHE:HD1 | 1:B:31:THR:HB | 7 | 0.04 |
| (1,2268) | 1:B:29:PHE:HD2 | 1:B:31:THR:HB | 7 | 0.04 |
| (1,2268) | 1:B:29:PHE:HD1 | 1:B:31:THR:HB | 8 | 0.04 |
| (1,2268) | 1:B:29:PHE:HD2 | 1:B:31:THR:HB | 8 | 0.04 |
| (1,2268) | 1:B:29:PHE:HD1 | 1:B:31:THR:HB | 20 | 0.04 |
| (1,2268) | 1:B:29:PHE:HD2 | 1:B:31:THR:HB | 20 | 0.04 |
| (1,2267) | 1:A:29:PHE:HD1 | 1:A:31:THR:HB | 2 | 0.04 |
| (1,2267) | 1:A:29:PHE:HD2 | 1:A:31:THR:HB | 2 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2267) | 1:A:29:PHE:HD1 | 1:A:31:THR:HB | 17 | 0.04 |
| (1,2267) | 1:A:29:PHE:HD2 | 1:A:31:THR:HB | 17 | 0.04 |
| (1,2267) | 1:A:29:PHE:HD1 | 1:A:31:THR:HB | 19 | 0.04 |
| (1,2267) | 1:A:29:PHE:HD2 | 1:A:31:THR:HB | 19 | 0.04 |
| (1,2262) | 1:B:25:VAL:HA | 1:B:28:LYS:HE2 | 9 | 0.04 |
| (1,2262) | 1:B:25:VAL:HA | 1:B:28:LYS:HE3 | 9 | 0.04 |
| (1,2233) | 1:A:23:THR:HG21 | 1:A:27:SER:HB2 | 4 | 0.04 |
| (1,2233) | 1:A:23:THR:HG22 | 1:A:27:SER:HB2 | 4 | 0.04 |
| (1,2233) | 1:A:23:THR:HG23 | 1:A:27:SER:HB2 | 4 | 0.04 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 9 | 0.04 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 9 | 0.04 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 9 | 0.04 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 7 | 0.04 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 7 | 0.04 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 7 | 0.04 |
| (1,2172) | 1:B:25:VAL:HG11 | 1:B:27:SER:H | 1 | 0.04 |
| (1,2172) | 1:B:25:VAL:HG12 | 1:B:27:SER:H | 1 | 0.04 |
| (1,2172) | 1:B:25:VAL:HG13 | 1:B:27:SER:H | 1 | 0.04 |
| (1,2172) | 1:B:25:VAL:HG11 | 1:B:27:SER:H | 7 | 0.04 |
| (1,2172) | 1:B:25:VAL:HG12 | 1:B:27:SER:H | 7 | 0.04 |
| (1,2172) | 1:B:25:VAL:HG13 | 1:B:27:SER:H | 7 | 0.04 |
| (1,2172) | 1:B:25:VAL:HG11 | 1:B:27:SER:H | 18 | 0.04 |
| (1,2172) | 1:B:25:VAL:HG12 | 1:B:27:SER:H | 18 | 0.04 |
| (1,2172) | 1:B:25:VAL:HG13 | 1:B:27:SER:H | 18 | 0.04 |
| (1,2171) | 1:A:25:VAL:HG11 | 1:A:27:SER:H | 14 | 0.04 |
| (1,2171) | 1:A:25:VAL:HG12 | 1:A:27:SER:H | 14 | 0.04 |
| (1,2171) | 1:A:25:VAL:HG13 | 1:A:27:SER:H | 14 | 0.04 |
| (1,2171) | 1:A:25:VAL:HG11 | 1:A:27:SER:H | 15 | 0.04 |
| (1,2171) | 1:A:25:VAL:HG12 | 1:A:27:SER:H | 15 | 0.04 |
| (1,2171) | 1:A:25:VAL:HG13 | 1:A:27:SER:H | 15 | 0.04 |
| (1,215) | 1:A:16:ASN:HA | 1:A:17:GLY:H | 3 | 0.04 |
| (1,215) | 1:A:16:ASN:HA | 1:A:17:GLY:H | 10 | 0.04 |
| (1,215) | 1:A:16:ASN:HA | 1:A:17:GLY:H | 14 | 0.04 |
| (1,215) | 1:A:16:ASN:HA | 1:A:17:GLY:H | 18 | 0.04 |
| (1,215) | 1:A:16:ASN:HA | 1:A:17:GLY:H | 19 | 0.04 |
| (1,215) | 1:A:16:ASN:HA | 1:A:17:GLY:H | 20 | 0.04 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 9 | 0.04 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 9 | 0.04 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 9 | 0.04 |
| (1,2102) | 1:B:22:ILE:HD11 | 1:B:23:THR:HA | 19 | 0.04 |
| (1,2102) | 1:B:22:ILE:HD12 | 1:B:23:THR:HA | 19 | 0.04 |
| (1,2102) | 1:B:22:ILE:HD13 | 1:B:23:THR:HA | 19 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 3 | 0.04 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 3 | 0.04 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 3 | 0.04 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 13 | 0.04 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 13 | 0.04 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 13 | 0.04 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 18 | 0.04 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 18 | 0.04 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 18 | 0.04 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 1 | 0.04 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 1 | 0.04 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 1 | 0.04 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 2 | 0.04 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 2 | 0.04 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 2 | 0.04 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 16 | 0.04 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 16 | 0.04 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 16 | 0.04 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG21 | 3 | 0.04 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG22 | 3 | 0.04 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG23 | 3 | 0.04 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG21 | 4 | 0.04 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG22 | 4 | 0.04 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG23 | 4 | 0.04 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG21 | 6 | 0.04 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG22 | 6 | 0.04 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG23 | 6 | 0.04 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG21 | 16 | 0.04 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG22 | 16 | 0.04 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG23 | 16 | 0.04 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG21 | 20 | 0.04 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG22 | 20 | 0.04 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG23 | 20 | 0.04 |
| (1,2016) | 1:A:21:GLN:HE21 | 1:A:22:ILE:HA | 15 | 0.04 |
| (1,1991) | 1:B:21:GLN:HG2 | 1:B:25:VAL:HG21 | 6 | 0.04 |
| (1,1991) | 1:B:21:GLN:HG2 | 1:B:25:VAL:HG22 | 6 | 0.04 |
| (1,1991) | 1:B:21:GLN:HG2 | 1:B:25:VAL:HG23 | 6 | 0.04 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 1 | 0.04 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 1 | 0.04 |
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 1 | 0.04 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 10 | 0.04 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 10 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 10 | 0.04 |
| (1,1878) | 1:A:25:VAL:HG21 | 1:A:65:LYS:HE2 | 12 | 0.04 |
| (1,1878) | 1:A:25:VAL:HG21 | 1:A:65:LYS:HE3 | 12 | 0.04 |
| (1,1878) | 1:A:25:VAL:HG22 | 1:A:65:LYS:HE2 | 12 | 0.04 |
| (1,1878) | 1:A:25:VAL:HG22 | 1:A:65:LYS:HE3 | 12 | 0.04 |
| (1,1878) | 1:A:25:VAL:HG23 | 1:A:65:LYS:HE2 | 12 | 0.04 |
| (1,1878) | 1:A:25:VAL:HG23 | 1:A:65:LYS:HE3 | 12 | 0.04 |
| (1,1877) | 1:B:41:LYS:HE2 | 1:B:44:ILE:HD11 | 9 | 0.04 |
| (1,1877) | 1:B:41:LYS:HE2 | 1:B:44:ILE:HD12 | 9 | 0.04 |
| (1,1877) | 1:B:41:LYS:HE2 | 1:B:44:ILE:HD13 | 9 | 0.04 |
| (1,1877) | 1:B:41:LYS:HE3 | 1:B:44:ILE:HD11 | 9 | 0.04 |
| (1,1877) | 1:B:41:LYS:HE3 | 1:B:44:ILE:HD12 | 9 | 0.04 |
| (1,1877) | 1:B:41:LYS:HE3 | 1:B:44:ILE:HD13 | 9 | 0.04 |
| (1,1874) | 1:A:11:VAL:HG21 | 1:A:41:LYS:HE2 | 1 | 0.04 |
| (1,1874) | 1:A:11:VAL:HG21 | 1:A:41:LYS:HE3 | 1 | 0.04 |
| (1,1874) | 1:A:11:VAL:HG22 | 1:A:41:LYS:HE2 | 1 | 0.04 |
| (1,1874) | 1:A:11:VAL:HG22 | 1:A:41:LYS:HE3 | 1 | 0.04 |
| (1,1874) | 1:A:11:VAL:HG23 | 1:A:41:LYS:HE2 | 1 | 0.04 |
| (1,1874) | 1:A:11:VAL:HG23 | 1:A:41:LYS:HE3 | 1 | 0.04 |
| (1,1863) | 1:B:13:GLU:HB2 | 1:B:15:LYS:HG2 | 4 | 0.04 |
| (1,1863) | 1:B:13:GLU:HB2 | 1:B:15:LYS:HG3 | 4 | 0.04 |
| (1,1861) | 1:B:15:LYS:HG2 | 1:B:18:MET:HE1 | 6 | 0.04 |
| (1,1861) | 1:B:15:LYS:HG2 | 1:B:18:MET:HE2 | 6 | 0.04 |
| (1,1861) | 1:B:15:LYS:HG2 | 1:B:18:MET:HE3 | 6 | 0.04 |
| (1,1861) | 1:B:15:LYS:HG3 | 1:B:18:MET:HE1 | 6 | 0.04 |
| (1,1861) | 1:B:15:LYS:HG3 | 1:B:18:MET:HE2 | 6 | 0.04 |
| (1,1861) | 1:B:15:LYS:HG3 | 1:B:18:MET:HE3 | 6 | 0.04 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG11 | 2 | 0.04 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG12 | 2 | 0.04 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG13 | 2 | 0.04 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG11 | 2 | 0.04 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG12 | 2 | 0.04 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG13 | 2 | 0.04 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG11 | 3 | 0.04 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG12 | 3 | 0.04 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG13 | 3 | 0.04 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG11 | 3 | 0.04 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG12 | 3 | 0.04 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG13 | 3 | 0.04 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG11 | 10 | 0.04 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG12 | 10 | 0.04 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG13 | 10 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG11 | 10 | 0.04 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG12 | 10 | 0.04 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG13 | 10 | 0.04 |
| (1,1803) | 1:B:13:GLU:HB3 | 1:B:71:GLY:HA3 | 14 | 0.04 |
| (1,1798) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HD2 | 10 | 0.04 |
| (1,1798) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HD3 | 10 | 0.04 |
| (1,1797) | 1:B:13:GLU:HB3 | 1:B:15:LYS:HG2 | 1 | 0.04 |
| (1,1797) | 1:B:13:GLU:HB3 | 1:B:15:LYS:HG3 | 1 | 0.04 |
| (1,176) | 1:B:13:GLU:HG2 | 1:B:15:LYS:H | 20 | 0.04 |
| (1,176) | 1:B:13:GLU:HG3 | 1:B:15:LYS:H | 20 | 0.04 |
| (1,1752) | 1:A:11:VAL:HG21 | 1:A:45:PHE:HE1 | 5 | 0.04 |
| (1,1752) | 1:A:11:VAL:HG22 | 1:A:45:PHE:HE1 | 5 | 0.04 |
| (1,1752) | 1:A:11:VAL:HG23 | 1:A:45:PHE:HE1 | 5 | 0.04 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 5 | 0.04 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 5 | 0.04 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 5 | 0.04 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 19 | 0.04 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 19 | 0.04 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 19 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG21 | 7 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG22 | 7 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG23 | 7 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG21 | 7 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG22 | 7 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG23 | 7 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG21 | 7 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG22 | 7 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG23 | 7 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG21 | 15 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG22 | 15 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG23 | 15 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG21 | 15 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG22 | 15 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG23 | 15 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG21 | 15 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG22 | 15 | 0.04 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG23 | 15 | 0.04 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD11 | 2 | 0.04 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD12 | 2 | 0.04 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD13 | 2 | 0.04 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD11 | 10 | 0.04 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD12 | 10 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD13 | 10 | 0.04 |
| (1,1631) | 1:B:9:ARG:HD2 | 1:B:11:VAL:HB | 1 | 0.04 |
| (1,1631) | 1:B:9:ARG:HD3 | 1:B:11:VAL:HB | 1 | 0.04 |
| (1,1629) | 1:A:9:ARG:HD2 | 1:A:76:GLU:HB2 | 5 | 0.04 |
| (1,1629) | 1:A:9:ARG:HD3 | 1:A:76:GLU:HB2 | 5 | 0.04 |
| (1,1626) | 1:B:9:ARG:HG3 | 1:B:10:ILE:H | 19 | 0.04 |
| (1,1606) | 1:B:8:ILE:HD11 | 1:B:77:ARG:HA | 3 | 0.04 |
| (1,1606) | 1:B:8:ILE:HD12 | 1:B:77:ARG:HA | 3 | 0.04 |
| (1,1606) | 1:B:8:ILE:HD13 | 1:B:77:ARG:HA | 3 | 0.04 |
| (1,1606) | 1:B:8:ILE:HD11 | 1:B:77:ARG:HA | 19 | 0.04 |
| (1,1606) | 1:B:8:ILE:HD12 | 1:B:77:ARG:HA | 19 | 0.04 |
| (1,1606) | 1:B:8:ILE:HD13 | 1:B:77:ARG:HA | 19 | 0.04 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 15 | 0.04 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 15 | 0.04 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 15 | 0.04 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 15 | 0.04 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 15 | 0.04 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 15 | 0.04 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 15 | 0.04 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 15 | 0.04 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 15 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD2 | 5 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD3 | 5 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD2 | 5 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD3 | 5 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD2 | 5 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD3 | 5 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD2 | 13 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD3 | 13 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD2 | 13 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD3 | 13 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD2 | 13 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD3 | 13 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD2 | 17 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD3 | 17 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD2 | 17 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD3 | 17 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD2 | 17 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD3 | 17 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD2 | 20 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD3 | 20 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD2 | 20 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD3 | 20 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD2 | 20 | 0.04 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD3 | 20 | 0.04 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 16 | 0.04 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 16 | 0.04 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 16 | 0.04 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 16 | 0.04 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 16 | 0.04 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 16 | 0.04 |
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 6 | 0.04 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 6 | 0.04 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 6 | 0.04 |
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 10 | 0.04 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 10 | 0.04 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 10 | 0.04 |
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 17 | 0.04 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 17 | 0.04 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 17 | 0.04 |
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 20 | 0.04 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 20 | 0.04 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 20 | 0.04 |
| (1,1527) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HA | 8 | 0.04 |
| (1,1527) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HA | 8 | 0.04 |
| (1,1527) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HA | 8 | 0.04 |
| (1,1527) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HA | 13 | 0.04 |
| (1,1527) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HA | 13 | 0.04 |
| (1,1527) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HA | 13 | 0.04 |
| (1,1456) | 1:B:3:ASP:HB2 | 1:B:53:VAL:H | 16 | 0.04 |
| (1,1420) | 1:B:40:ALA:H | 1:B:41:LYS:HD2 | 10 | 0.04 |
| (1,1420) | 1:B:40:ALA:H | 1:B:41:LYS:HD3 | 10 | 0.04 |
| (1,1347) | 1:A:77:ARG:H | 1:A:77:ARG:HD2 | 9 | 0.04 |
| (1,1347) | 1:A:77:ARG:H | 1:A:77:ARG:HD3 | 9 | 0.04 |
| (1,1253) | 1:A:69:VAL:HG21 | 1:A:72:VAL:H | 5 | 0.04 |
| (1,1253) | 1:A:69:VAL:HG22 | 1:A:72:VAL:H | 5 | 0.04 |
| (1,1253) | 1:A:69:VAL:HG23 | 1:A:72:VAL:H | 5 | 0.04 |
| (1,1222) | 1:B:69:VAL:H | 1:B:72:VAL:H | 3 | 0.04 |
| (1,1222) | 1:B:69:VAL:H | 1:B:72:VAL:H | 6 | 0.04 |
| (1,1222) | 1:B:69:VAL:H | 1:B:72:VAL:H | 7 | 0.04 |
| (1,1222) | 1:B:69:VAL:H | 1:B:72:VAL:H | 10 | 0.04 |
| (1,1222) | 1:B:69:VAL:H | 1:B:72:VAL:H | 12 | 0.04 |
| (1,1222) | 1:B:69:VAL:H | 1:B:72:VAL:H | 13 | 0.04 |
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 1 | 0.04 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 2 | 0.04 |
| (1,1184) | 1:B:68:LYS:H | 1:B:75:VAL:HG21 | 7 | 0.04 |
| (1,1184) | 1:B:68:LYS:H | 1:B:75:VAL:HG22 | 7 | 0.04 |
| (1,1184) | 1:B:68:LYS:H | 1:B:75:VAL:HG23 | 7 | 0.04 |
| (1,1176) | 1:B:67:ARG:HE | 1:B:75:VAL:HB | 13 | 0.04 |
| (1,1131) | 1:A:62:LEU:HD11 | 1:A:66:LEU:H | 10 | 0.04 |
| (1,1131) | 1:A:62:LEU:HD12 | 1:A:66:LEU:H | 10 | 0.04 |
| (1,1131) | 1:A:62:LEU:HD13 | 1:A:66:LEU:H | 10 | 0.04 |
| (1,1131) | 1:A:62:LEU:HD11 | 1:A:66:LEU:H | 14 | 0.04 |
| (1,1131) | 1:A:62:LEU:HD12 | 1:A:66:LEU:H | 14 | 0.04 |
| (1,1131) | 1:A:62:LEU:HD13 | 1:A:66:LEU:H | 14 | 0.04 |
| (1,1130) | 1:B:62:LEU:HD11 | 1:B:65:LYS:H | 9 | 0.04 |
| (1,1130) | 1:B:62:LEU:HD12 | 1:B:65:LYS:H | 9 | 0.04 |
| (1,1130) | 1:B:62:LEU:HD13 | 1:B:65:LYS:H | 9 | 0.04 |
| (1,1130) | 1:B:62:LEU:HD11 | 1:B:65:LYS:H | 11 | 0.04 |
| (1,1130) | 1:B:62:LEU:HD12 | 1:B:65:LYS:H | 11 | 0.04 |
| (1,1130) | 1:B:62:LEU:HD13 | 1:B:65:LYS:H | 11 | 0.04 |
| (1,1120) | 1:B:65:LYS:H | 1:B:68:LYS:HE2 | 18 | 0.04 |
| (1,1120) | 1:B:65:LYS:H | 1:B:68:LYS:HE3 | 18 | 0.04 |
| (1,1115) | 1:A:64:ASP:HB2 | 1:A:65:LYS:H | 1 | 0.04 |
| (1,979) | 1:B:58:LYS:H | 1:B:58:LYS:HG3 | 1 | 0.03 |
| (1,978) | 1:A:58:LYS:H | 1:A:58:LYS:HG3 | 17 | 0.03 |
| (1,925) | 1:B:3:ASP:HB3 | 1:B:53:VAL:H | 1 | 0.03 |
| (1,915) | 1:B:51:ILE:HG12 | 1:B:52:PHE:H | 3 | 0.03 |
| (1,915) | 1:B:51:ILE:HG12 | 1:B:52:PHE:H | 8 | 0.03 |
| (1,914) | 1:A:51:ILE:HG12 | 1:A:52:PHE:H | 9 | 0.03 |
| (1,914) | 1:A:51:ILE:HG12 | 1:A:52:PHE:H | 17 | 0.03 |
| (1,855) | 1:B:48:ASN:HD21 | 1:B:78:LEU:HD21 | 15 | 0.03 |
| (1,855) | 1:B:48:ASN:HD21 | 1:B:78:LEU:HD22 | 15 | 0.03 |
| (1,855) | 1:B:48:ASN:HD21 | 1:B:78:LEU:HD23 | 15 | 0.03 |
| (1,854) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD21 | 6 | 0.03 |
| (1,854) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD22 | 6 | 0.03 |
| (1,854) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD23 | 6 | 0.03 |
| (1,848) | 1:A:47:CYS:HG | 1:A:48:ASN:H | 20 | 0.03 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 14 | 0.03 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 7 | 0.03 |
| (1,838) | 1:A:45:PHE:HZ | 1:A:47:CYS:H | 11 | 0.03 |
| (1,777) | 1:B:43:GLY:H | 1:B:44:ILE:H | 19 | 0.03 |
| (1,742) | 1:A:41:LYS:HB2 | 1:A:42:ASP:H | 15 | 0.03 |
| (1,742) | 1:A:41:LYS:HB3 | 1:A:42:ASP:H | 15 | 0.03 |
| (1,741) | 1:B:41:LYS:HG2 | 1:B:42:ASP:H | 1 | 0.03 |
| (1,741) | 1:B:41:LYS:HG3 | 1:B:42:ASP:H | 1 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,735) | 1:B:41:LYS:H | 1:B:46:THR:H | 5 | 0.03 |
| (1,735) | 1:B:41:LYS:H | 1:B:46:THR:H | 6 | 0.03 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD1 | 3 | 0.03 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD2 | 3 | 0.03 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD1 | 19 | 0.03 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD2 | 19 | 0.03 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD1 | 14 | 0.03 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD2 | 14 | 0.03 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD1 | 18 | 0.03 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD2 | 18 | 0.03 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD1 | 19 | 0.03 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD2 | 19 | 0.03 |
| (1,684) | 1:A:39:ASN:H | 1:A:48:ASN:H | 18 | 0.03 |
| (1,631) | 1:B:35:THR:H | 1:B:83:HIS:HE1 | 3 | 0.03 |
| (1,631) | 1:B:35:THR:H | 1:B:83:HIS:HE1 | 19 | 0.03 |
| (1,586) | 1:A:32:ASN:HD22 | 1:B:16:ASN:HA | 3 | 0.03 |
| (1,579) | 1:A:32:ASN:HD21 | 1:A:33:ILE:HB | 13 | 0.03 |
| (1,579) | 1:A:32:ASN:HD21 | 1:A:33:ILE:HB | 18 | 0.03 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD11 | 2 | 0.03 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD12 | 2 | 0.03 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD13 | 2 | 0.03 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD11 | 9 | 0.03 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD12 | 9 | 0.03 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD13 | 9 | 0.03 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD11 | 17 | 0.03 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD12 | 17 | 0.03 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD13 | 17 | 0.03 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD11 | 1 | 0.03 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD12 | 1 | 0.03 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD13 | 1 | 0.03 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD11 | 4 | 0.03 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD12 | 4 | 0.03 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD13 | 4 | 0.03 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD11 | 9 | 0.03 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD12 | 9 | 0.03 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD13 | 9 | 0.03 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD11 | 14 | 0.03 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD12 | 14 | 0.03 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD13 | 14 | 0.03 |
| (1,562) | 1:B:29:PHE:HD1 | 1:B:31:THR:H | 3 | 0.03 |
| (1,562) | 1:B:29:PHE:HD2 | 1:B:31:THR:H | 3 | 0.03 |
| (1,558) | 1:B:30:ASP:HA | 1:B:31:THR:H | 15 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5260) | 1:B:82:GLU:H | 1:B:82:GLU:HG2 | 18 | 0.03 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 4 | 0.03 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 4 | 0.03 |
| (1,5258) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 4 | 0.03 |
| (1,5248) | 1:B:76:GLU:HB2 | 1:B:77:ARG:H | 11 | 0.03 |
| (1,5242) | 1:B:68:LYS:HA | 1:B:68:LYS:HG2 | 13 | 0.03 |
| (1,5241) | 1:B:68:LYS:H | 1:B:68:LYS:HD2 | 13 | 0.03 |
| (1,5223) | 1:B:65:LYS:H | 1:B:65:LYS:HD2 | 10 | 0.03 |
| (1,5222) | 1:B:65:LYS:H | 1:B:65:LYS:HG2 | 7 | 0.03 |
| (1,5185) | 1:B:56:THR:HG21 | 1:B:59:LEU:HB2 | 14 | 0.03 |
| (1,5185) | 1:B:56:THR:HG22 | 1:B:59:LEU:HB2 | 14 | 0.03 |
| (1,5185) | 1:B:56:THR:HG23 | 1:B:59:LEU:HB2 | 14 | 0.03 |
| (1,5153) | 1:B:48:ASN:HB2 | 1:B:49:LEU:H | 17 | 0.03 |
| (1,5145) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HG12 | 19 | 0.03 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG21 | 18 | 0.03 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG22 | 18 | 0.03 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG23 | 18 | 0.03 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG21 | 20 | 0.03 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG22 | 20 | 0.03 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG23 | 20 | 0.03 |
| (1,5114) | 1:B:35:THR:HB | 1:B:50:MET:HB2 | 6 | 0.03 |
| (1,5114) | 1:B:35:THR:HB | 1:B:50:MET:HB2 | 10 | 0.03 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD11 | 11 | 0.03 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD12 | 11 | 0.03 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD13 | 11 | 0.03 |
| (1,5056) | 1:B:26:ILE:HG12 | 1:B:27:SER:H | 3 | 0.03 |
| (1,5056) | 1:B:26:ILE:HG12 | 1:B:27:SER:H | 13 | 0.03 |
| (1,5056) | 1:B:26:ILE:HG12 | 1:B:27:SER:H | 14 | 0.03 |
| (1,5028) | 1:B:20:ASN:HB2 | 1:B:21:GLN:H | 7 | 0.03 |
| (1,5019) | 1:B:17:GLY:HA2 | 1:B:21:GLN:HE22 | 2 | 0.03 |
| (1,5005) | 1:B:15:LYS:HG2 | 1:B:16:ASN:HD21 | 6 | 0.03 |
| (1,5005) | 1:B:15:LYS:HG3 | 1:B:16:ASN:HD21 | 6 | 0.03 |
| (1,4999) | 1:B:15:LYS:H | 1:B:18:MET:HG2 | 10 | 0.03 |
| (1,4999) | 1:B:15:LYS:H | 1:B:18:MET:HG2 | 19 | 0.03 |
| (1,4990) | 1:B:14:ASP:H | 1:B:14:ASP:HB2 | 6 | 0.03 |
| (1,4981) | 1:B:9:ARG:H | 1:B:76:GLU:HB2 | 15 | 0.03 |
| (1,4968) | 1:B:8:ILE:H | 1:B:8:ILE:HG12 | 20 | 0.03 |
| (1,4956) | 1:B:4:PHE:H | 1:B:54:LYS:HB2 | 7 | 0.03 |
| (1,4954) | 1:B:3:ASP:HB2 | 1:B:54:LYS:HA | 17 | 0.03 |
| (1,4946) | 1:A:82:GLU:H | 1:A:82:GLU:HG2 | 15 | 0.03 |
| (1,4945) | 1:A:81:LEU:H | 1:A:82:GLU:HG2 | 13 | 0.03 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD21 | 13 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD22 | 13 | 0.03 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD23 | 13 | 0.03 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD21 | 20 | 0.03 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD22 | 20 | 0.03 |
| (1,4944) | 1:A:80:ASN:HB2 | 1:A:81:LEU:HD23 | 20 | 0.03 |
| (1,4912) | 1:A:65:LYS:H | 1:A:65:LYS:HD2 | 4 | 0.03 |
| (1,4902) | 1:A:62:LEU:H | 1:A:65:LYS:HD2 | 19 | 0.03 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB2 | 14 | 0.03 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB3 | 14 | 0.03 |
| (1,4866) | 1:A:54:LYS:HB2 | 1:A:54:LYS:HE2 | 17 | 0.03 |
| (1,4866) | 1:A:54:LYS:HB2 | 1:A:54:LYS:HE3 | 17 | 0.03 |
| (1,4862) | 1:A:53:VAL:HG21 | 1:A:54:LYS:HB2 | 3 | 0.03 |
| (1,4862) | 1:A:53:VAL:HG22 | 1:A:54:LYS:HB2 | 3 | 0.03 |
| (1,4862) | 1:A:53:VAL:HG23 | 1:A:54:LYS:HB2 | 3 | 0.03 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD11 | 8 | 0.03 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD12 | 8 | 0.03 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD13 | 8 | 0.03 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 10 | 0.03 |
| (1,4813) | 1:A:36:ILE:HG12 | 1:A:37:VAL:H | 1 | 0.03 |
| (1,4812) | 1:A:36:ILE:HG21 | 1:A:48:ASN:HB2 | 19 | 0.03 |
| (1,4812) | 1:A:36:ILE:HG22 | 1:A:48:ASN:HB2 | 19 | 0.03 |
| (1,4812) | 1:A:36:ILE:HG23 | 1:A:48:ASN:HB2 | 19 | 0.03 |
| (1,4809) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 11 | 0.03 |
| (1,4800) | 1:A:34:ARG:HB2 | 1:A:35:THR:H | 11 | 0.03 |
| (1,4792) | 1:A:32:ASN:HB2 | 1:A:33:ILE:HG13 | 20 | 0.03 |
| (1,4787) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HD2 | 19 | 0.03 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD11 | 10 | 0.03 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD12 | 10 | 0.03 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD13 | 10 | 0.03 |
| (1,4783) | 1:A:29:PHE:HB2 | 1:A:51:ILE:HD11 | 14 | 0.03 |
| (1,4783) | 1:A:29:PHE:HB2 | 1:A:51:ILE:HD12 | 14 | 0.03 |
| (1,4783) | 1:A:29:PHE:HB2 | 1:A:51:ILE:HD13 | 14 | 0.03 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 1 | 0.03 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 20 | 0.03 |
| (1,4733) | 1:A:23:THR:HG21 | 1:A:27:SER:HB2 | 10 | 0.03 |
| (1,4733) | 1:A:23:THR:HG22 | 1:A:27:SER:HB2 | 10 | 0.03 |
| (1,4733) | 1:A:23:THR:HG23 | 1:A:27:SER:HB2 | 10 | 0.03 |
| (1,4716) | 1:A:18:MET:HG2 | 1:A:45:PHE:HZ | 19 | 0.03 |
| (1,4690) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD21 | 10 | 0.03 |
| (1,4690) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD21 | 10 | 0.03 |
| (1,4689) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HB2 | 7 | 0.03 |
| (1,4689) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HB2 | 7 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4667) | 1:A:14:ASP:HA | 1:A:15:LYS:HB2 | 16 | 0.03 |
| (1,4645) | 1:A:8:ILE:H | 1:A:8:ILE:HG12 | 10 | 0.03 |
| (1,4633) | 1:A:4:PHE:H | 1:A:54:LYS:HB2 | 11 | 0.03 |
| (1,4620) | 1:B:82:GLU:HA | 1:B:83:HIS:HD2 | 13 | 0.03 |
| (1,4609) | 1:A:81:LEU:HB3 | 1:A:83:HIS:HD2 | 17 | 0.03 |
| (1,4608) | 1:B:5:LEU:HG | 1:B:83:HIS:HD2 | 3 | 0.03 |
| (1,4607) | 1:A:5:LEU:HG | 1:A:83:HIS:HD2 | 5 | 0.03 |
| (1,4607) | 1:A:5:LEU:HG | 1:A:83:HIS:HD2 | 10 | 0.03 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 2 | 0.03 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 3 | 0.03 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 9 | 0.03 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 15 | 0.03 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 18 | 0.03 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 20 | 0.03 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 1 | 0.03 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 12 | 0.03 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 15 | 0.03 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG21 | 12 | 0.03 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG22 | 12 | 0.03 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG23 | 12 | 0.03 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG21 | 7 | 0.03 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG22 | 7 | 0.03 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG23 | 7 | 0.03 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG21 | 9 | 0.03 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG22 | 9 | 0.03 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG23 | 9 | 0.03 |
| (1,4574) | 1:B:44:ILE:HG12 | 1:B:73:PHE:HE1 | 10 | 0.03 |
| (1,4574) | 1:B:44:ILE:HG12 | 1:B:73:PHE:HE1 | 16 | 0.03 |
| (1,4562) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HE2 | 20 | 0.03 |
| (1,4562) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HE3 | 20 | 0.03 |
| (1,4538) | 1:B:52:PHE:HD1 | 1:B:53:VAL:H | 10 | 0.03 |
| (1,4538) | 1:B:52:PHE:HD2 | 1:B:53:VAL:H | 10 | 0.03 |
| (1,4538) | 1:B:52:PHE:HD1 | 1:B:53:VAL:H | 16 | 0.03 |
| (1,4538) | 1:B:52:PHE:HD2 | 1:B:53:VAL:H | 16 | 0.03 |
| (1,4538) | 1:B:52:PHE:HD1 | 1:B:53:VAL:H | 18 | 0.03 |
| (1,4538) | 1:B:52:PHE:HD2 | 1:B:53:VAL:H | 18 | 0.03 |
| (1,4538) | 1:B:52:PHE:HD1 | 1:B:53:VAL:H | 20 | 0.03 |
| (1,4538) | 1:B:52:PHE:HD2 | 1:B:53:VAL:H | 20 | 0.03 |
| (1,4526) | 1:B:5:LEU:HA | 1:B:52:PHE:HD1 | 15 | 0.03 |
| (1,4526) | 1:B:5:LEU:HA | 1:B:52:PHE:HD2 | 15 | 0.03 |
| (1,4513) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HD1 | 5 | 0.03 |
| (1,4513) | 1:A:5:LEU:HD11 | 1:A:52:PHE:HD2 | 5 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4513) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HD1 | 5 | 0.03 |
| (1,4513) | 1:A:5:LEU:HD12 | 1:A:52:PHE:HD2 | 5 | 0.03 |
| (1,4513) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HD1 | 5 | 0.03 |
| (1,4513) | 1:A:5:LEU:HD13 | 1:A:52:PHE:HD2 | 5 | 0.03 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 1 | 0.03 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 8 | 0.03 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 16 | 0.03 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 17 | 0.03 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 20 | 0.03 |
| (1,4478) | 1:B:19:THR:HG21 | 1:B:45:PHE:HE1 | 20 | 0.03 |
| (1,4478) | 1:B:19:THR:HG22 | 1:B:45:PHE:HE1 | 20 | 0.03 |
| (1,4478) | 1:B:19:THR:HG23 | 1:B:45:PHE:HE1 | 20 | 0.03 |
| (1,4475) | 1:A:22:ILE:HD11 | 1:A:45:PHE:HE1 | 2 | 0.03 |
| (1,4475) | 1:A:22:ILE:HD12 | 1:A:45:PHE:HE1 | 2 | 0.03 |
| (1,4475) | 1:A:22:ILE:HD13 | 1:A:45:PHE:HE1 | 2 | 0.03 |
| (1,4444) | 1:A:45:PHE:HD1 | 1:A:47:CYS:HG | 2 | 0.03 |
| (1,4444) | 1:A:45:PHE:HD2 | 1:A:47:CYS:HG | 2 | 0.03 |
| (1,4413) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 7 | 0.03 |
| (1,4413) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 7 | 0.03 |
| (1,4413) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 8 | 0.03 |
| (1,4413) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 8 | 0.03 |
| (1,4412) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 9 | 0.03 |
| (1,4412) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 9 | 0.03 |
| (1,4412) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 19 | 0.03 |
| (1,4412) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 19 | 0.03 |
| (1,4393) | 1:B:4:PHE:HZ | 1:B:6:ALA:HA | 9 | 0.03 |
| (1,4393) | 1:B:4:PHE:HZ | 1:B:6:ALA:HA | 15 | 0.03 |
| (1,4392) | 1:A:4:PHE:HZ | 1:A:6:ALA:HA | 3 | 0.03 |
| (1,4392) | 1:A:4:PHE:HZ | 1:A:6:ALA:HA | 4 | 0.03 |
| (1,4392) | 1:A:4:PHE:HZ | 1:A:6:ALA:HA | 5 | 0.03 |
| (1,4392) | 1:A:4:PHE:HZ | 1:A:6:ALA:HA | 11 | 0.03 |
| (1,4392) | 1:A:4:PHE:HZ | 1:A:6:ALA:HA | 12 | 0.03 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG11 | 19 | 0.03 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG12 | 19 | 0.03 |
| (1,4382) | 1:A:4:PHE:HZ | 1:A:53:VAL:HG13 | 19 | 0.03 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD21 | 6 | 0.03 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD22 | 6 | 0.03 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD23 | 6 | 0.03 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD21 | 11 | 0.03 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD22 | 11 | 0.03 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD23 | 11 | 0.03 |
| (1,4353) | 1:B:4:PHE:H | 1:B:4:PHE:HD1 | 7 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4353) | 1:B:4:PHE:H | 1:B:4:PHE:HD2 | 7 | 0.03 |
| (1,4353) | 1:B:4:PHE:H | 1:B:4:PHE:HD1 | 17 | 0.03 |
| (1,4353) | 1:B:4:PHE:H | 1:B:4:PHE:HD2 | 17 | 0.03 |
| (1,4350) | 1:A:4:PHE:HD1 | 1:A:5:LEU:H | 9 | 0.03 |
| (1,4350) | 1:A:4:PHE:HD2 | 1:A:5:LEU:H | 9 | 0.03 |
| (1,4350) | 1:A:4:PHE:HD1 | 1:A:5:LEU:H | 20 | 0.03 |
| (1,4350) | 1:A:4:PHE:HD2 | 1:A:5:LEU:H | 20 | 0.03 |
| (1,4339) | 1:B:4:PHE:HD1 | 1:B:59:LEU:HD21 | 11 | 0.03 |
| (1,4339) | 1:B:4:PHE:HD1 | 1:B:59:LEU:HD22 | 11 | 0.03 |
| (1,4339) | 1:B:4:PHE:HD1 | 1:B:59:LEU:HD23 | 11 | 0.03 |
| (1,4339) | 1:B:4:PHE:HD2 | 1:B:59:LEU:HD21 | 11 | 0.03 |
| (1,4339) | 1:B:4:PHE:HD2 | 1:B:59:LEU:HD22 | 11 | 0.03 |
| (1,4339) | 1:B:4:PHE:HD2 | 1:B:59:LEU:HD23 | 11 | 0.03 |
| (1,4335) | 1:B:83:HIS:HA | 1:B:83:HIS:HD2 | 14 | 0.03 |
| (1,4333) | 1:B:83:HIS:HA | 1:B:83:HIS:HB3 | 16 | 0.03 |
| (1,4325) | 1:B:80:ASN:HA | 1:B:81:LEU:HG | 2 | 0.03 |
| (1,4325) | 1:B:80:ASN:HA | 1:B:81:LEU:HG | 6 | 0.03 |
| (1,4324) | 1:A:80:ASN:HA | 1:A:81:LEU:HG | 1 | 0.03 |
| (1,4324) | 1:A:80:ASN:HA | 1:A:81:LEU:HG | 13 | 0.03 |
| (1,4319) | 1:B:77:ARG:HG3 | 1:B:79:SER:HA | 20 | 0.03 |
| (1,4318) | 1:A:77:ARG:HG3 | 1:A:79:SER:HA | 18 | 0.03 |
| (1,4317) | 1:B:79:SER:HA | 1:B:81:LEU:HG | 8 | 0.03 |
| (1,4317) | 1:B:79:SER:HA | 1:B:81:LEU:HG | 18 | 0.03 |
| (1,4316) | 1:A:79:SER:HA | 1:A:81:LEU:HG | 19 | 0.03 |
| (1,4314) | 1:A:79:SER:HA | 1:A:81:LEU:HD21 | 12 | 0.03 |
| (1,4314) | 1:A:79:SER:HA | 1:A:81:LEU:HD22 | 12 | 0.03 |
| (1,4314) | 1:A:79:SER:HA | 1:A:81:LEU:HD23 | 12 | 0.03 |
| (1,4292) | 1:A:73:PHE:HA | 1:A:75:VAL:HG21 | 11 | 0.03 |
| (1,4292) | 1:A:73:PHE:HA | 1:A:75:VAL:HG22 | 11 | 0.03 |
| (1,4292) | 1:A:73:PHE:HA | 1:A:75:VAL:HG23 | 11 | 0.03 |
| (1,4259) | 1:B:41:LYS:HG2 | 1:B:42:ASP:HA | 3 | 0.03 |
| (1,4259) | 1:B:41:LYS:HG3 | 1:B:42:ASP:HA | 3 | 0.03 |
| (1,4259) | 1:B:41:LYS:HG2 | 1:B:42:ASP:HA | 4 | 0.03 |
| (1,4259) | 1:B:41:LYS:HG3 | 1:B:42:ASP:HA | 4 | 0.03 |
| (1,4259) | 1:B:41:LYS:HG2 | 1:B:42:ASP:HA | 16 | 0.03 |
| (1,4259) | 1:B:41:LYS:HG3 | 1:B:42:ASP:HA | 16 | 0.03 |
| (1,4255) | 1:B:41:LYS:HA | 1:B:41:LYS:HD2 | 2 | 0.03 |
| (1,4255) | 1:B:41:LYS:HA | 1:B:41:LYS:HD3 | 2 | 0.03 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG2 | 5 | 0.03 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG3 | 5 | 0.03 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG2 | 17 | 0.03 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG3 | 17 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG2 | 18 | 0.03 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG3 | 18 | 0.03 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 3 | 0.03 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 3 | 0.03 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 6 | 0.03 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 6 | 0.03 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 8 | 0.03 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 8 | 0.03 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 11 | 0.03 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 11 | 0.03 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 13 | 0.03 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 13 | 0.03 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 17 | 0.03 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 17 | 0.03 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 18 | 0.03 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 18 | 0.03 |
| (1,4243) | 1:B:15:LYS:HA | 1:B:17:GLY:H | 18 | 0.03 |
| (1,4243) | 1:B:15:LYS:HA | 1:B:17:GLY:H | 19 | 0.03 |
| (1,4242) | 1:A:15:LYS:HA | 1:A:17:GLY:H | 15 | 0.03 |
| (1,4217) | 1:B:8:ILE:HA | 1:B:78:LEU:HB2 | 17 | 0.03 |
| (1,4192) | 1:A:5:LEU:HB2 | 1:A:83:HIS:HB3 | 13 | 0.03 |
| (1,4192) | 1:A:5:LEU:HB2 | 1:A:83:HIS:HB3 | 16 | 0.03 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD11 | 4 | 0.03 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD12 | 4 | 0.03 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD13 | 4 | 0.03 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD11 | 4 | 0.03 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD12 | 4 | 0.03 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD13 | 4 | 0.03 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD11 | 4 | 0.03 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD12 | 4 | 0.03 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD13 | 4 | 0.03 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 2 | 0.03 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 2 | 0.03 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 2 | 0.03 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 19 | 0.03 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 19 | 0.03 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 19 | 0.03 |
| (1,4147) | 1:B:61:THR:HG21 | 1:B:65:LYS:HB3 | 2 | 0.03 |
| (1,4147) | 1:B:61:THR:HG22 | 1:B:65:LYS:HB3 | 2 | 0.03 |
| (1,4147) | 1:B:61:THR:HG23 | 1:B:65:LYS:HB3 | 2 | 0.03 |
| (1,4147) | 1:B:61:THR:HG21 | 1:B:65:LYS:HB3 | 18 | 0.03 |
| (1,4147) | 1:B:61:THR:HG22 | 1:B:65:LYS:HB3 | 18 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4147) | 1:B:61:THR:HG23 | 1:B:65:LYS:HB3 | 18 | 0.03 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD11 | 8 | 0.03 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD12 | 8 | 0.03 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD13 | 8 | 0.03 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD11 | 12 | 0.03 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD12 | 12 | 0.03 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD13 | 12 | 0.03 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD11 | 16 | 0.03 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD12 | 16 | 0.03 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD13 | 16 | 0.03 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD11 | 19 | 0.03 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD12 | 19 | 0.03 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD13 | 19 | 0.03 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD11 | 3 | 0.03 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD12 | 3 | 0.03 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD13 | 3 | 0.03 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD11 | 15 | 0.03 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD12 | 15 | 0.03 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD13 | 15 | 0.03 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 3 | 0.03 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 10 | 0.03 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 11 | 0.03 |
| (1,4115) | 1:A:18:MET:HA | 1:A:21:GLN:HB2 | 13 | 0.03 |
| (1,4115) | 1:A:18:MET:HA | 1:A:21:GLN:HB2 | 18 | 0.03 |
| (1,4110) | 1:B:18:MET:HE1 | 1:B:72:VAL:HG21 | 6 | 0.03 |
| (1,4110) | 1:B:18:MET:HE1 | 1:B:72:VAL:HG22 | 6 | 0.03 |
| (1,4110) | 1:B:18:MET:HE1 | 1:B:72:VAL:HG23 | 6 | 0.03 |
| (1,4110) | 1:B:18:MET:HE2 | 1:B:72:VAL:HG21 | 6 | 0.03 |
| (1,4110) | 1:B:18:MET:HE2 | 1:B:72:VAL:HG22 | 6 | 0.03 |
| (1,4110) | 1:B:18:MET:HE2 | 1:B:72:VAL:HG23 | 6 | 0.03 |
| (1,4110) | 1:B:18:MET:HE3 | 1:B:72:VAL:HG21 | 6 | 0.03 |
| (1,4110) | 1:B:18:MET:HE3 | 1:B:72:VAL:HG22 | 6 | 0.03 |
| (1,4110) | 1:B:18:MET:HE3 | 1:B:72:VAL:HG23 | 6 | 0.03 |
| (1,4110) | 1:B:18:MET:HE1 | 1:B:72:VAL:HG21 | 15 | 0.03 |
| (1,4110) | 1:B:18:MET:HE1 | 1:B:72:VAL:HG22 | 15 | 0.03 |
| (1,4110) | 1:B:18:MET:HE1 | 1:B:72:VAL:HG23 | 15 | 0.03 |
| (1,4110) | 1:B:18:MET:HE2 | 1:B:72:VAL:HG21 | 15 | 0.03 |
| (1,4110) | 1:B:18:MET:HE2 | 1:B:72:VAL:HG22 | 15 | 0.03 |
| (1,4110) | 1:B:18:MET:HE2 | 1:B:72:VAL:HG23 | 15 | 0.03 |
| (1,4110) | 1:B:18:MET:HE3 | 1:B:72:VAL:HG21 | 15 | 0.03 |
| (1,4110) | 1:B:18:MET:HE3 | 1:B:72:VAL:HG22 | 15 | 0.03 |
| (1,4110) | 1:B:18:MET:HE3 | 1:B:72:VAL:HG23 | 15 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4075) | 1:B:82:GLU:HA | 1:B:83:HIS:HB2 | 20 | 0.03 |
| (1,4074) | 1:A:82:GLU:HA | 1:A:83:HIS:HB2 | 5 | 0.03 |
| (1,4074) | 1:A:82:GLU:HA | 1:A:83:HIS:HB2 | 20 | 0.03 |
| (1,4073) | 1:B:8:ILE:H | 1:B:81:LEU:HD21 | 6 | 0.03 |
| (1,4073) | 1:B:8:ILE:H | 1:B:81:LEU:HD22 | 6 | 0.03 |
| (1,4073) | 1:B:8:ILE:H | 1:B:81:LEU:HD23 | 6 | 0.03 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD21 | 15 | 0.03 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD22 | 15 | 0.03 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD23 | 15 | 0.03 |
| (1,4061) | 1:B:7:GLY:HA2 | 1:B:81:LEU:HD21 | 16 | 0.03 |
| (1,4061) | 1:B:7:GLY:HA2 | 1:B:81:LEU:HD22 | 16 | 0.03 |
| (1,4061) | 1:B:7:GLY:HA2 | 1:B:81:LEU:HD23 | 16 | 0.03 |
| (1,4037) | 1:B:50:MET:HG2 | 1:B:81:LEU:HD11 | 8 | 0.03 |
| (1,4037) | 1:B:50:MET:HG2 | 1:B:81:LEU:HD12 | 8 | 0.03 |
| (1,4037) | 1:B:50:MET:HG2 | 1:B:81:LEU:HD13 | 8 | 0.03 |
| (1,4022) | 1:A:80:ASN:HB3 | 1:A:81:LEU:HD21 | 9 | 0.03 |
| (1,4022) | 1:A:80:ASN:HB3 | 1:A:81:LEU:HD22 | 9 | 0.03 |
| (1,4022) | 1:A:80:ASN:HB3 | 1:A:81:LEU:HD23 | 9 | 0.03 |
| (1,4019) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 12 | 0.03 |
| (1,4019) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 12 | 0.03 |
| (1,4019) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 12 | 0.03 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD21 | 11 | 0.03 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD22 | 11 | 0.03 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD23 | 11 | 0.03 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD21 | 11 | 0.03 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD22 | 11 | 0.03 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD23 | 11 | 0.03 |
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD21 | 2 | 0.03 |
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD22 | 2 | 0.03 |
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD23 | 2 | 0.03 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD21 | 2 | 0.03 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD22 | 2 | 0.03 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD23 | 2 | 0.03 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD11 | 7 | 0.03 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD12 | 7 | 0.03 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD13 | 7 | 0.03 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD11 | 8 | 0.03 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD12 | 8 | 0.03 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD13 | 8 | 0.03 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD11 | 2 | 0.03 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD12 | 2 | 0.03 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD13 | 2 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD11 | 19 | 0.03 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD12 | 19 | 0.03 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD13 | 19 | 0.03 |
| (1,3987) | 1:B:48:ASN:HD21 | 1:B:78:LEU:HD11 | 19 | 0.03 |
| (1,3987) | 1:B:48:ASN:HD21 | 1:B:78:LEU:HD12 | 19 | 0.03 |
| (1,3987) | 1:B:48:ASN:HD21 | 1:B:78:LEU:HD13 | 19 | 0.03 |
| (1,3986) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD11 | 13 | 0.03 |
| (1,3986) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD12 | 13 | 0.03 |
| (1,3986) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD13 | 13 | 0.03 |
| (1,397) | 1:B:22:ILE:H | 1:B:23:THR:HG1 | 16 | 0.03 |
| (1,3967) | 1:B:50:MET:HE1 | 1:B:78:LEU:HD11 | 5 | 0.03 |
| (1,3967) | 1:B:50:MET:HE1 | 1:B:78:LEU:HD12 | 5 | 0.03 |
| (1,3967) | 1:B:50:MET:HE1 | 1:B:78:LEU:HD13 | 5 | 0.03 |
| (1,3967) | 1:B:50:MET:HE2 | 1:B:78:LEU:HD11 | 5 | 0.03 |
| (1,3967) | 1:B:50:MET:HE2 | 1:B:78:LEU:HD12 | 5 | 0.03 |
| (1,3967) | 1:B:50:MET:HE2 | 1:B:78:LEU:HD13 | 5 | 0.03 |
| (1,3967) | 1:B:50:MET:HE3 | 1:B:78:LEU:HD11 | 5 | 0.03 |
| (1,3967) | 1:B:50:MET:HE3 | 1:B:78:LEU:HD12 | 5 | 0.03 |
| (1,3967) | 1:B:50:MET:HE3 | 1:B:78:LEU:HD13 | 5 | 0.03 |
| (1,3966) | 1:A:50:MET:HE1 | 1:A:78:LEU:HD11 | 13 | 0.03 |
| (1,3966) | 1:A:50:MET:HE1 | 1:A:78:LEU:HD12 | 13 | 0.03 |
| (1,3966) | 1:A:50:MET:HE1 | 1:A:78:LEU:HD13 | 13 | 0.03 |
| (1,3966) | 1:A:50:MET:HE2 | 1:A:78:LEU:HD11 | 13 | 0.03 |
| (1,3966) | 1:A:50:MET:HE2 | 1:A:78:LEU:HD12 | 13 | 0.03 |
| (1,3966) | 1:A:50:MET:HE2 | 1:A:78:LEU:HD13 | 13 | 0.03 |
| (1,3966) | 1:A:50:MET:HE3 | 1:A:78:LEU:HD11 | 13 | 0.03 |
| (1,3966) | 1:A:50:MET:HE3 | 1:A:78:LEU:HD12 | 13 | 0.03 |
| (1,3966) | 1:A:50:MET:HE3 | 1:A:78:LEU:HD13 | 13 | 0.03 |
| (1,396) | 1:A:22:ILE:H | 1:A:23:THR:HG1 | 11 | 0.03 |
| (1,396) | 1:A:22:ILE:H | 1:A:23:THR:HG1 | 15 | 0.03 |
| (1,396) | 1:A:22:ILE:H | 1:A:23:THR:HG1 | 16 | 0.03 |
| (1,3953) | 1:B:78:LEU:HB2 | 1:B:80:ASN:H | 9 | 0.03 |
| (1,3936) | 1:A:7:GLY:HA2 | 1:A:78:LEU:HB3 | 1 | 0.03 |
| (1,3936) | 1:A:7:GLY:HA2 | 1:A:78:LEU:HB3 | 14 | 0.03 |
| (1,3927) | 1:B:4:PHE:HZ | 1:B:77:ARG:HD2 | 17 | 0.03 |
| (1,3927) | 1:B:4:PHE:HZ | 1:B:77:ARG:HD3 | 17 | 0.03 |
| (1,3917) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HD2 | 17 | 0.03 |
| (1,3917) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HD3 | 17 | 0.03 |
| (1,3917) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HD2 | 17 | 0.03 |
| (1,3917) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HD3 | 17 | 0.03 |
| (1,3917) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HD2 | 17 | 0.03 |
| (1,3917) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HD3 | 17 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3916) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HD2 | 13 | 0.03 |
| (1,3916) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HD3 | 13 | 0.03 |
| (1,3916) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HD2 | 13 | 0.03 |
| (1,3916) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HD3 | 13 | 0.03 |
| (1,3916) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HD2 | 13 | 0.03 |
| (1,3916) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HD3 | 13 | 0.03 |
| (1,3916) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HD2 | 19 | 0.03 |
| (1,3916) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HD3 | 19 | 0.03 |
| (1,3916) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HD2 | 19 | 0.03 |
| (1,3916) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HD3 | 19 | 0.03 |
| (1,3916) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HD2 | 19 | 0.03 |
| (1,3916) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HD3 | 19 | 0.03 |
| (1,3897) | 1:B:74:THR:HA | 1:B:76:GLU:HG2 | 18 | 0.03 |
| (1,3897) | 1:B:74:THR:HA | 1:B:76:GLU:HG3 | 18 | 0.03 |
| (1,3897) | 1:B:74:THR:HA | 1:B:76:GLU:HG2 | 20 | 0.03 |
| (1,3897) | 1:B:74:THR:HA | 1:B:76:GLU:HG3 | 20 | 0.03 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 13 | 0.03 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 13 | 0.03 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 13 | 0.03 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 3 | 0.03 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 3 | 0.03 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 3 | 0.03 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG21 | 9 | 0.03 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG22 | 9 | 0.03 |
| (1,3863) | 1:A:11:VAL:H | 1:A:74:THR:HG23 | 9 | 0.03 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG21 | 7 | 0.03 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG22 | 7 | 0.03 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG23 | 7 | 0.03 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG21 | 7 | 0.03 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG22 | 7 | 0.03 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG23 | 7 | 0.03 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG21 | 11 | 0.03 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG22 | 11 | 0.03 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG23 | 11 | 0.03 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG21 | 11 | 0.03 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG22 | 11 | 0.03 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG23 | 11 | 0.03 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG21 | 19 | 0.03 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG22 | 19 | 0.03 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG23 | 19 | 0.03 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG21 | 19 | 0.03 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG22 | 19 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG23 | 19 | 0.03 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG21 | 17 | 0.03 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG22 | 17 | 0.03 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG23 | 17 | 0.03 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG21 | 4 | 0.03 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG22 | 4 | 0.03 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG23 | 4 | 0.03 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG21 | 9 | 0.03 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG22 | 9 | 0.03 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG23 | 9 | 0.03 |
| (1,3848) | 1:B:74:THR:HB | 1:B:75:VAL:H | 6 | 0.03 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG11 | 7 | 0.03 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG12 | 7 | 0.03 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG13 | 7 | 0.03 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG11 | 8 | 0.03 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG12 | 8 | 0.03 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG13 | 8 | 0.03 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG11 | 9 | 0.03 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG12 | 9 | 0.03 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG13 | 9 | 0.03 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG11 | 20 | 0.03 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG12 | 20 | 0.03 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG13 | 20 | 0.03 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG11 | 10 | 0.03 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG12 | 10 | 0.03 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG13 | 10 | 0.03 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG11 | 12 | 0.03 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG12 | 12 | 0.03 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG13 | 12 | 0.03 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG11 | 15 | 0.03 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG12 | 15 | 0.03 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG13 | 15 | 0.03 |
| (1,3755) | 1:A:69:VAL:H | 1:A:70:GLN:HB2 | 19 | 0.03 |
| (1,3755) | 1:A:69:VAL:H | 1:A:70:GLN:HB3 | 19 | 0.03 |
| (1,3755) | 1:A:69:VAL:H | 1:A:70:GLN:HB2 | 20 | 0.03 |
| (1,3755) | 1:A:69:VAL:H | 1:A:70:GLN:HB3 | 20 | 0.03 |
| (1,3736) | 1:B:66:LEU:HA | 1:B:69:VAL:HB | 9 | 0.03 |
| (1,3735) | 1:A:66:LEU:HA | 1:A:69:VAL:HB | 17 | 0.03 |
| (1,3734) | 1:B:20:ASN:HA | 1:B:22:ILE:HB | 17 | 0.03 |
| (1,3734) | 1:B:20:ASN:HA | 1:B:22:ILE:HB | 18 | 0.03 |
| (1,3703) | 1:A:67:ARG:H | 1:A:68:LYS:HE2 | 14 | 0.03 |
| (1,3703) | 1:A:67:ARG:H | 1:A:68:LYS:HE3 | 14 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,3702) | 1:B:15:LYS:HE2 | 1:B:18:MET:H | 15 | 0.03 |
| (1,3702) | 1:B:15:LYS:HE3 | 1:B:18:MET:H | 15 | 0.03 |
| (1,3701) | 1:A:15:LYS:HE2 | 1:A:18:MET:H | 10 | 0.03 |
| (1,3701) | 1:A:15:LYS:HE3 | 1:A:18:MET:H | 10 | 0.03 |
| (1,3700) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD21 | 16 | 0.03 |
| (1,3700) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD21 | 16 | 0.03 |
| (1,3699) | 1:A:15:LYS:HE2 | 1:A:16:ASN:HD21 | 5 | 0.03 |
| (1,3699) | 1:A:15:LYS:HE3 | 1:A:16:ASN:HD21 | 5 | 0.03 |
| (1,3666) | 1:A:68:LYS:HA | 1:A:68:LYS:HG3 | 3 | 0.03 |
| (1,358) | 1:A:21:GLN:HE22 | 1:A:69:VAL:HG11 | 10 | 0.03 |
| (1,358) | 1:A:21:GLN:HE22 | 1:A:69:VAL:HG12 | 10 | 0.03 |
| (1,358) | 1:A:21:GLN:HE22 | 1:A:69:VAL:HG13 | 10 | 0.03 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 11 | 0.03 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 11 | 0.03 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 11 | 0.03 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 5 | 0.03 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 5 | 0.03 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 5 | 0.03 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 14 | 0.03 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 14 | 0.03 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 14 | 0.03 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB2 | 2 | 0.03 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB3 | 2 | 0.03 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB2 | 8 | 0.03 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB3 | 8 | 0.03 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB2 | 11 | 0.03 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB3 | 11 | 0.03 |
| (1,3537) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HB2 | 11 | 0.03 |
| (1,3537) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HB2 | 16 | 0.03 |
| (1,3528) | 1:B:63:MET:HE1 | 1:B:77:ARG:H | 3 | 0.03 |
| (1,3528) | 1:B:63:MET:HE2 | 1:B:77:ARG:H | 3 | 0.03 |
| (1,3528) | 1:B:63:MET:HE3 | 1:B:77:ARG:H | 3 | 0.03 |
| (1,3528) | 1:B:63:MET:HE1 | 1:B:77:ARG:H | 7 | 0.03 |
| (1,3528) | 1:B:63:MET:HE2 | 1:B:77:ARG:H | 7 | 0.03 |
| (1,3528) | 1:B:63:MET:HE3 | 1:B:77:ARG:H | 7 | 0.03 |
| (1,3528) | 1:B:63:MET:HE1 | 1:B:77:ARG:H | 10 | 0.03 |
| (1,3528) | 1:B:63:MET:HE2 | 1:B:77:ARG:H | 10 | 0.03 |
| (1,3528) | 1:B:63:MET:HE3 | 1:B:77:ARG:H | 10 | 0.03 |
| (1,3528) | 1:B:63:MET:HE1 | 1:B:77:ARG:H | 13 | 0.03 |
| (1,3528) | 1:B:63:MET:HE2 | 1:B:77:ARG:H | 13 | 0.03 |
| (1,3528) | 1:B:63:MET:HE3 | 1:B:77:ARG:H | 13 | 0.03 |
| (1,3528) | 1:B:63:MET:HE1 | 1:B:77:ARG:H | 17 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3528) | 1:B:63:MET:HE2 | 1:B:77:ARG:H | 17 | 0.03 |
| (1,3528) | 1:B:63:MET:HE3 | 1:B:77:ARG:H | 17 | 0.03 |
| (1,3527) | 1:A:63:MET:HE1 | 1:A:77:ARG:H | 8 | 0.03 |
| (1,3527) | 1:A:63:MET:HE2 | 1:A:77:ARG:H | 8 | 0.03 |
| (1,3527) | 1:A:63:MET:HE3 | 1:A:77:ARG:H | 8 | 0.03 |
| (1,3527) | 1:A:63:MET:HE1 | 1:A:77:ARG:H | 16 | 0.03 |
| (1,3527) | 1:A:63:MET:HE2 | 1:A:77:ARG:H | 16 | 0.03 |
| (1,3527) | 1:A:63:MET:HE3 | 1:A:77:ARG:H | 16 | 0.03 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 11 | 0.03 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 11 | 0.03 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 11 | 0.03 |
| (1,3519) | 1:A:63:MET:HE1 | 1:A:76:GLU:HA | 2 | 0.03 |
| (1,3519) | 1:A:63:MET:HE2 | 1:A:76:GLU:HA | 2 | 0.03 |
| (1,3519) | 1:A:63:MET:HE3 | 1:A:76:GLU:HA | 2 | 0.03 |
| (1,3519) | 1:A:63:MET:HE1 | 1:A:76:GLU:HA | 10 | 0.03 |
| (1,3519) | 1:A:63:MET:HE2 | 1:A:76:GLU:HA | 10 | 0.03 |
| (1,3519) | 1:A:63:MET:HE3 | 1:A:76:GLU:HA | 10 | 0.03 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE1 | 18 | 0.03 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE2 | 18 | 0.03 |
| (1,3513) | 1:A:61:THR:HA | 1:A:63:MET:HE3 | 18 | 0.03 |
| (1,3420) | 1:B:29:PHE:HE1 | 1:B:62:LEU:HB2 | 19 | 0.03 |
| (1,3386) | 1:A:61:THR:HG21 | 1:A:65:LYS:HE2 | 10 | 0.03 |
| (1,3386) | 1:A:61:THR:HG21 | 1:A:65:LYS:HE3 | 10 | 0.03 |
| (1,3386) | 1:A:61:THR:HG22 | 1:A:65:LYS:HE2 | 10 | 0.03 |
| (1,3386) | 1:A:61:THR:HG22 | 1:A:65:LYS:HE3 | 10 | 0.03 |
| (1,3386) | 1:A:61:THR:HG23 | 1:A:65:LYS:HE2 | 10 | 0.03 |
| (1,3386) | 1:A:61:THR:HG23 | 1:A:65:LYS:HE3 | 10 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD21 | 19 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD22 | 19 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD23 | 19 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD21 | 19 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD22 | 19 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD23 | 19 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD21 | 19 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD22 | 19 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD23 | 19 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD21 | 20 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD22 | 20 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD23 | 20 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD21 | 20 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD22 | 20 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD23 | 20 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD21 | 20 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD22 | 20 | 0.03 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD23 | 20 | 0.03 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD11 | 18 | 0.03 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD12 | 18 | 0.03 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD13 | 18 | 0.03 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD11 | 18 | 0.03 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD12 | 18 | 0.03 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD13 | 18 | 0.03 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD11 | 18 | 0.03 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD12 | 18 | 0.03 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD13 | 18 | 0.03 |
| (1,3284) | 1:A:58:LYS:H | 1:A:58:LYS:HD2 | 7 | 0.03 |
| (1,3284) | 1:A:58:LYS:H | 1:A:58:LYS:HD3 | 7 | 0.03 |
| (1,3272) | 1:A:58:LYS:HD2 | 1:A:62:LEU:HB2 | 16 | 0.03 |
| (1,3272) | 1:A:58:LYS:HD3 | 1:A:62:LEU:HB2 | 16 | 0.03 |
| (1,3249) | 1:B:31:THR:HG21 | 1:B:58:LYS:HG3 | 5 | 0.03 |
| (1,3249) | 1:B:31:THR:HG22 | 1:B:58:LYS:HG3 | 5 | 0.03 |
| (1,3249) | 1:B:31:THR:HG23 | 1:B:58:LYS:HG3 | 5 | 0.03 |
| (1,3249) | 1:B:31:THR:HG21 | 1:B:58:LYS:HG3 | 19 | 0.03 |
| (1,3249) | 1:B:31:THR:HG22 | 1:B:58:LYS:HG3 | 19 | 0.03 |
| (1,3249) | 1:B:31:THR:HG23 | 1:B:58:LYS:HG3 | 19 | 0.03 |
| (1,3248) | 1:A:31:THR:HG21 | 1:A:58:LYS:HG3 | 6 | 0.03 |
| (1,3248) | 1:A:31:THR:HG22 | 1:A:58:LYS:HG3 | 6 | 0.03 |
| (1,3248) | 1:A:31:THR:HG23 | 1:A:58:LYS:HG3 | 6 | 0.03 |
| (1,3230) | 1:A:57:ASP:HB2 | 1:A:58:LYS:HG3 | 13 | 0.03 |
| (1,3230) | 1:A:57:ASP:HB3 | 1:A:58:LYS:HG3 | 13 | 0.03 |
| (1,3220) | 1:A:4:PHE:HD1 | 1:A:56:THR:HG21 | 17 | 0.03 |
| (1,3220) | 1:A:4:PHE:HD1 | 1:A:56:THR:HG22 | 17 | 0.03 |
| (1,3220) | 1:A:4:PHE:HD1 | 1:A:56:THR:HG23 | 17 | 0.03 |
| (1,3220) | 1:A:4:PHE:HD2 | 1:A:56:THR:HG21 | 17 | 0.03 |
| (1,3220) | 1:A:4:PHE:HD2 | 1:A:56:THR:HG22 | 17 | 0.03 |
| (1,3220) | 1:A:4:PHE:HD2 | 1:A:56:THR:HG23 | 17 | 0.03 |
| (1,3196) | 1:A:54:LYS:H | 1:A:54:LYS:HE2 | 7 | 0.03 |
| (1,3196) | 1:A:54:LYS:H | 1:A:54:LYS:HE3 | 7 | 0.03 |
| (1,3189) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HD21 | 14 | 0.03 |
| (1,3189) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HD21 | 14 | 0.03 |
| (1,3188) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD21 | 20 | 0.03 |
| (1,3188) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD21 | 20 | 0.03 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD2 | 9 | 0.03 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD3 | 9 | 0.03 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD2 | 16 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD3 | 16 | 0.03 |
| (1,3182) | 1:A:54:LYS:HA | 1:A:54:LYS:HD2 | 2 | 0.03 |
| (1,3182) | 1:A:54:LYS:HA | 1:A:54:LYS:HD3 | 2 | 0.03 |
| (1,3182) | 1:A:54:LYS:HA | 1:A:54:LYS:HD2 | 3 | 0.03 |
| (1,3182) | 1:A:54:LYS:HA | 1:A:54:LYS:HD3 | 3 | 0.03 |
| (1,3182) | 1:A:54:LYS:HA | 1:A:54:LYS:HD2 | 5 | 0.03 |
| (1,3182) | 1:A:54:LYS:HA | 1:A:54:LYS:HD3 | 5 | 0.03 |
| (1,311) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HG12 | 13 | 0.03 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG11 | 16 | 0.03 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG12 | 16 | 0.03 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG13 | 16 | 0.03 |
| (1,3097) | 1:B:53:VAL:HG11 | 1:B:55:ASN:H | 20 | 0.03 |
| (1,3097) | 1:B:53:VAL:HG12 | 1:B:55:ASN:H | 20 | 0.03 |
| (1,3097) | 1:B:53:VAL:HG13 | 1:B:55:ASN:H | 20 | 0.03 |
| (1,3094) | 1:A:53:VAL:HG11 | 1:A:58:LYS:HZ1 | 6 | 0.03 |
| (1,3094) | 1:A:53:VAL:HG12 | 1:A:58:LYS:HZ1 | 6 | 0.03 |
| (1,3094) | 1:A:53:VAL:HG13 | 1:A:58:LYS:HZ1 | 6 | 0.03 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 2 | 0.03 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 2 | 0.03 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 2 | 0.03 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 2 | 0.03 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 2 | 0.03 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 2 | 0.03 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG11 | 3 | 0.03 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG12 | 3 | 0.03 |
| (1,3081) | 1:B:4:PHE:HB2 | 1:B:53:VAL:HG13 | 3 | 0.03 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG11 | 3 | 0.03 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG12 | 3 | 0.03 |
| (1,3081) | 1:B:4:PHE:HB3 | 1:B:53:VAL:HG13 | 3 | 0.03 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 5 | 0.03 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 5 | 0.03 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 5 | 0.03 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 5 | 0.03 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 5 | 0.03 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 5 | 0.03 |
| (1,3063) | 1:B:53:VAL:HG11 | 1:B:62:LEU:HD21 | 4 | 0.03 |
| (1,3063) | 1:B:53:VAL:HG11 | 1:B:62:LEU:HD22 | 4 | 0.03 |
| (1,3063) | 1:B:53:VAL:HG11 | 1:B:62:LEU:HD23 | 4 | 0.03 |
| (1,3063) | 1:B:53:VAL:HG12 | 1:B:62:LEU:HD21 | 4 | 0.03 |
| (1,3063) | 1:B:53:VAL:HG12 | 1:B:62:LEU:HD22 | 4 | 0.03 |
| (1,3063) | 1:B:53:VAL:HG12 | 1:B:62:LEU:HD23 | 4 | 0.03 |
| (1,3063) | 1:B:53:VAL:HG13 | 1:B:62:LEU:HD21 | 4 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3063) | 1:B:53:VAL:HG13 | 1:B:62:LEU:HD22 | 4 | 0.03 |
| (1,3063) | 1:B:53:VAL:HG13 | 1:B:62:LEU:HD23 | 4 | 0.03 |
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD11 | 17 | 0.03 |
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD12 | 17 | 0.03 |
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD13 | 17 | 0.03 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD11 | 6 | 0.03 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD12 | 6 | 0.03 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD13 | 6 | 0.03 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD11 | 6 | 0.03 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD12 | 6 | 0.03 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD13 | 6 | 0.03 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD11 | 8 | 0.03 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD12 | 8 | 0.03 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD13 | 8 | 0.03 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD11 | 8 | 0.03 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD12 | 8 | 0.03 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD13 | 8 | 0.03 |
| (1,3013) | 1:B:51:ILE:HD11 | 1:B:62:LEU:HD21 | 17 | 0.03 |
| (1,3013) | 1:B:51:ILE:HD11 | 1:B:62:LEU:HD22 | 17 | 0.03 |
| (1,3013) | 1:B:51:ILE:HD11 | 1:B:62:LEU:HD23 | 17 | 0.03 |
| (1,3013) | 1:B:51:ILE:HD12 | 1:B:62:LEU:HD21 | 17 | 0.03 |
| (1,3013) | 1:B:51:ILE:HD12 | 1:B:62:LEU:HD22 | 17 | 0.03 |
| (1,3013) | 1:B:51:ILE:HD12 | 1:B:62:LEU:HD23 | 17 | 0.03 |
| (1,3013) | 1:B:51:ILE:HD13 | 1:B:62:LEU:HD21 | 17 | 0.03 |
| (1,3013) | 1:B:51:ILE:HD13 | 1:B:62:LEU:HD22 | 17 | 0.03 |
| (1,3013) | 1:B:51:ILE:HD13 | 1:B:62:LEU:HD23 | 17 | 0.03 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG21 | 5 | 0.03 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG22 | 5 | 0.03 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG23 | 5 | 0.03 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG21 | 18 | 0.03 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG22 | 18 | 0.03 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG23 | 18 | 0.03 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG21 | 7 | 0.03 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG22 | 7 | 0.03 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG23 | 7 | 0.03 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG21 | 12 | 0.03 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG22 | 12 | 0.03 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG23 | 12 | 0.03 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD11 | 7 | 0.03 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD12 | 7 | 0.03 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD13 | 7 | 0.03 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD11 | 7 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD12 | 7 | 0.03 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD13 | 7 | 0.03 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD11 | 7 | 0.03 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD12 | 7 | 0.03 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD13 | 7 | 0.03 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD11 | 13 | 0.03 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD12 | 13 | 0.03 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD13 | 13 | 0.03 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD11 | 13 | 0.03 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD12 | 13 | 0.03 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD13 | 13 | 0.03 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD11 | 13 | 0.03 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD12 | 13 | 0.03 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD13 | 13 | 0.03 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 1 | 0.03 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 1 | 0.03 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 1 | 0.03 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 4 | 0.03 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 4 | 0.03 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 4 | 0.03 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 7 | 0.03 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 7 | 0.03 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 7 | 0.03 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 14 | 0.03 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 14 | 0.03 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 14 | 0.03 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 19 | 0.03 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 19 | 0.03 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 19 | 0.03 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 8 | 0.03 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 8 | 0.03 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 8 | 0.03 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 15 | 0.03 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 15 | 0.03 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 15 | 0.03 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 20 | 0.03 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 20 | 0.03 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 20 | 0.03 |
| (1,2879) | 1:B:8:ILE:H | 1:B:50:MET:HG3 | 3 | 0.03 |
| (1,2879) | 1:B:8:ILE:H | 1:B:50:MET:HG3 | 9 | 0.03 |
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 10 | 0.03 |
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 12 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 16 | 0.03 |
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 20 | 0.03 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 8 | 0.03 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 15 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD21 | 2 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD22 | 2 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD23 | 2 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD21 | 2 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD22 | 2 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD23 | 2 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD21 | 2 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD22 | 2 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD23 | 2 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD21 | 14 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD22 | 14 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD23 | 14 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD21 | 14 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD22 | 14 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD23 | 14 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD21 | 14 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD22 | 14 | 0.03 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD23 | 14 | 0.03 |
| (1,2754) | 1:B:23:THR:HG1 | 1:B:47:CYS:HB3 | 7 | 0.03 |
| (1,2753) | 1:A:23:THR:HG1 | 1:A:47:CYS:HB3 | 14 | 0.03 |
| (1,2753) | 1:A:23:THR:HG1 | 1:A:47:CYS:HB3 | 20 | 0.03 |
| (1,2726) | 1:B:46:THR:HG21 | 1:B:47:CYS:H | 19 | 0.03 |
| (1,2726) | 1:B:46:THR:HG22 | 1:B:47:CYS:H | 19 | 0.03 |
| (1,2726) | 1:B:46:THR:HG23 | 1:B:47:CYS:H | 19 | 0.03 |
| (1,2725) | 1:A:46:THR:HG21 | 1:A:47:CYS:H | 13 | 0.03 |
| (1,2725) | 1:A:46:THR:HG22 | 1:A:47:CYS:H | 13 | 0.03 |
| (1,2725) | 1:A:46:THR:HG23 | 1:A:47:CYS:H | 13 | 0.03 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG21 | 8 | 0.03 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG22 | 8 | 0.03 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG23 | 8 | 0.03 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 10 | 0.03 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 10 | 0.03 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 10 | 0.03 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 14 | 0.03 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 14 | 0.03 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 14 | 0.03 |
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD11 | 4 | 0.03 |
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD12 | 4 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD13 | 4 | 0.03 |
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD11 | 8 | 0.03 |
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD12 | 8 | 0.03 |
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD13 | 8 | 0.03 |
| (1,2677) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HZ | 4 | 0.03 |
| (1,2677) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HZ | 4 | 0.03 |
| (1,2677) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HZ | 4 | 0.03 |
| (1,2672) | 1:B:13:GLU:HA | 1:B:44:ILE:HD11 | 1 | 0.03 |
| (1,2672) | 1:B:13:GLU:HA | 1:B:44:ILE:HD12 | 1 | 0.03 |
| (1,2672) | 1:B:13:GLU:HA | 1:B:44:ILE:HD13 | 1 | 0.03 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD11 | 1 | 0.03 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD12 | 1 | 0.03 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD13 | 1 | 0.03 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD11 | 14 | 0.03 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD12 | 14 | 0.03 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD13 | 14 | 0.03 |
| (1,2670) | 1:B:44:ILE:HD11 | 1:B:46:THR:HB | 3 | 0.03 |
| (1,2670) | 1:B:44:ILE:HD12 | 1:B:46:THR:HB | 3 | 0.03 |
| (1,2670) | 1:B:44:ILE:HD13 | 1:B:46:THR:HB | 3 | 0.03 |
| (1,2669) | 1:A:44:ILE:HD11 | 1:A:46:THR:HB | 3 | 0.03 |
| (1,2669) | 1:A:44:ILE:HD12 | 1:A:46:THR:HB | 3 | 0.03 |
| (1,2669) | 1:A:44:ILE:HD13 | 1:A:46:THR:HB | 3 | 0.03 |
| (1,2669) | 1:A:44:ILE:HD11 | 1:A:46:THR:HB | 8 | 0.03 |
| (1,2669) | 1:A:44:ILE:HD12 | 1:A:46:THR:HB | 8 | 0.03 |
| (1,2669) | 1:A:44:ILE:HD13 | 1:A:46:THR:HB | 8 | 0.03 |
| (1,2662) | 1:B:44:ILE:HG21 | 1:B:45:PHE:H | 7 | 0.03 |
| (1,2662) | 1:B:44:ILE:HG22 | 1:B:45:PHE:H | 7 | 0.03 |
| (1,2662) | 1:B:44:ILE:HG23 | 1:B:45:PHE:H | 7 | 0.03 |
| (1,2661) | 1:A:44:ILE:HG21 | 1:A:45:PHE:H | 2 | 0.03 |
| (1,2661) | 1:A:44:ILE:HG22 | 1:A:45:PHE:H | 2 | 0.03 |
| (1,2661) | 1:A:44:ILE:HG23 | 1:A:45:PHE:H | 2 | 0.03 |
| (1,2657) | 1:A:14:ASP:H | 1:A:44:ILE:HG21 | 7 | 0.03 |
| (1,2657) | 1:A:14:ASP:H | 1:A:44:ILE:HG22 | 7 | 0.03 |
| (1,2657) | 1:A:14:ASP:H | 1:A:44:ILE:HG23 | 7 | 0.03 |
| (1,2611) | 1:A:13:GLU:HA | 1:A:44:ILE:HB | 7 | 0.03 |
| (1,2572) | 1:B:40:ALA:HA | 1:B:45:PHE:HA | 3 | 0.03 |
| (1,2571) | 1:A:40:ALA:HA | 1:A:45:PHE:HA | 20 | 0.03 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD21 | 5 | 0.03 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD22 | 5 | 0.03 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD23 | 5 | 0.03 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD21 | 9 | 0.03 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD22 | 9 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD23 | 9 | 0.03 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD21 | 15 | 0.03 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD22 | 15 | 0.03 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD23 | 15 | 0.03 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD21 | 2 | 0.03 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD22 | 2 | 0.03 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD23 | 2 | 0.03 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD21 | 8 | 0.03 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD22 | 8 | 0.03 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD23 | 8 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD21 | 1:B:35:THR:HG21 | 5 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD21 | 1:B:35:THR:HG22 | 5 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD21 | 1:B:35:THR:HG23 | 5 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD22 | 1:B:35:THR:HG21 | 5 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD22 | 1:B:35:THR:HG22 | 5 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD22 | 1:B:35:THR:HG23 | 5 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD23 | 1:B:35:THR:HG21 | 5 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD23 | 1:B:35:THR:HG22 | 5 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD23 | 1:B:35:THR:HG23 | 5 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD21 | 1:B:35:THR:HG21 | 19 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD21 | 1:B:35:THR:HG22 | 19 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD21 | 1:B:35:THR:HG23 | 19 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD22 | 1:B:35:THR:HG21 | 19 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD22 | 1:B:35:THR:HG22 | 19 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD22 | 1:B:35:THR:HG23 | 19 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD23 | 1:B:35:THR:HG21 | 19 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD23 | 1:B:35:THR:HG22 | 19 | 0.03 |
| (1,2518) | 1:A:38:LEU:HD23 | 1:B:35:THR:HG23 | 19 | 0.03 |
| (1,2510) | 1:B:38:LEU:HD11 | 1:B:39:ASN:H | 5 | 0.03 |
| (1,2510) | 1:B:38:LEU:HD12 | 1:B:39:ASN:H | 5 | 0.03 |
| (1,2510) | 1:B:38:LEU:HD13 | 1:B:39:ASN:H | 5 | 0.03 |
| (1,2510) | 1:B:38:LEU:HD11 | 1:B:39:ASN:H | 8 | 0.03 |
| (1,2510) | 1:B:38:LEU:HD12 | 1:B:39:ASN:H | 8 | 0.03 |
| (1,2510) | 1:B:38:LEU:HD13 | 1:B:39:ASN:H | 8 | 0.03 |
| (1,2510) | 1:B:38:LEU:HD11 | 1:B:39:ASN:H | 9 | 0.03 |
| (1,2510) | 1:B:38:LEU:HD12 | 1:B:39:ASN:H | 9 | 0.03 |
| (1,2510) | 1:B:38:LEU:HD13 | 1:B:39:ASN:H | 9 | 0.03 |
| (1,2509) | 1:A:38:LEU:HD11 | 1:A:39:ASN:H | 10 | 0.03 |
| (1,2509) | 1:A:38:LEU:HD12 | 1:A:39:ASN:H | 10 | 0.03 |
| (1,2509) | 1:A:38:LEU:HD13 | 1:A:39:ASN:H | 10 | 0.03 |
| (1,2486) | 1:B:38:LEU:HD11 | 1:B:47:CYS:HG | 6 | 0.03 |
| (1,2486) | 1:B:38:LEU:HD12 | 1:B:47:CYS:HG | 6 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2486) | 1:B:38:LEU:HD13 | 1:B:47:CYS:HG | 6 | 0.03 |
| (1,2486) | 1:B:38:LEU:HD11 | 1:B:47:CYS:HG | 8 | 0.03 |
| (1,2486) | 1:B:38:LEU:HD12 | 1:B:47:CYS:HG | 8 | 0.03 |
| (1,2486) | 1:B:38:LEU:HD13 | 1:B:47:CYS:HG | 8 | 0.03 |
| (1,2474) | 1:B:37:VAL:HG21 | 1:B:38:LEU:H | 7 | 0.03 |
| (1,2474) | 1:B:37:VAL:HG22 | 1:B:38:LEU:H | 7 | 0.03 |
| (1,2474) | 1:B:37:VAL:HG23 | 1:B:38:LEU:H | 7 | 0.03 |
| (1,2473) | 1:A:37:VAL:HG21 | 1:A:38:LEU:H | 7 | 0.03 |
| (1,2473) | 1:A:37:VAL:HG22 | 1:A:38:LEU:H | 7 | 0.03 |
| (1,2473) | 1:A:37:VAL:HG23 | 1:A:38:LEU:H | 7 | 0.03 |
| (1,2465) | 1:A:37:VAL:HG21 | 1:A:48:ASN:HD22 | 3 | 0.03 |
| (1,2465) | 1:A:37:VAL:HG22 | 1:A:48:ASN:HD22 | 3 | 0.03 |
| (1,2465) | 1:A:37:VAL:HG23 | 1:A:48:ASN:HD22 | 3 | 0.03 |
| (1,245) | 1:B:15:LYS:HG2 | 1:B:19:THR:H | 2 | 0.03 |
| (1,245) | 1:B:15:LYS:HG3 | 1:B:19:THR:H | 2 | 0.03 |
| (1,245) | 1:B:15:LYS:HG2 | 1:B:19:THR:H | 8 | 0.03 |
| (1,245) | 1:B:15:LYS:HG3 | 1:B:19:THR:H | 8 | 0.03 |
| (1,244) | 1:A:15:LYS:HG2 | 1:A:19:THR:H | 1 | 0.03 |
| (1,244) | 1:A:15:LYS:HG3 | 1:A:19:THR:H | 1 | 0.03 |
| (1,244) | 1:A:15:LYS:HG2 | 1:A:19:THR:H | 20 | 0.03 |
| (1,244) | 1:A:15:LYS:HG3 | 1:A:19:THR:H | 20 | 0.03 |
| (1,2432) | 1:B:37:VAL:HG11 | 1:B:48:ASN:HB3 | 8 | 0.03 |
| (1,2432) | 1:B:37:VAL:HG12 | 1:B:48:ASN:HB3 | 8 | 0.03 |
| (1,2432) | 1:B:37:VAL:HG13 | 1:B:48:ASN:HB3 | 8 | 0.03 |
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD11 | 1 | 0.03 |
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD12 | 1 | 0.03 |
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD13 | 1 | 0.03 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 4 | 0.03 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 4 | 0.03 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 4 | 0.03 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 8 | 0.03 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 8 | 0.03 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 8 | 0.03 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 14 | 0.03 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 14 | 0.03 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 14 | 0.03 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 16 | 0.03 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 16 | 0.03 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 16 | 0.03 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 18 | 0.03 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 18 | 0.03 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 18 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD11 | 19 | 0.03 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD12 | 19 | 0.03 |
| (1,240) | 1:A:19:THR:H | 1:A:38:LEU:HD13 | 19 | 0.03 |
| (1,2389) | 1:A:36:ILE:HG21 | 1:A:48:ASN:H | 7 | 0.03 |
| (1,2389) | 1:A:36:ILE:HG22 | 1:A:48:ASN:H | 7 | 0.03 |
| (1,2389) | 1:A:36:ILE:HG23 | 1:A:48:ASN:H | 7 | 0.03 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG21 | 5 | 0.03 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG22 | 5 | 0.03 |
| (1,2372) | 1:B:23:THR:HB | 1:B:36:ILE:HG23 | 5 | 0.03 |
| (1,2368) | 1:B:36:ILE:HG21 | 1:B:37:VAL:HB | 2 | 0.03 |
| (1,2368) | 1:B:36:ILE:HG22 | 1:B:37:VAL:HB | 2 | 0.03 |
| (1,2368) | 1:B:36:ILE:HG23 | 1:B:37:VAL:HB | 2 | 0.03 |
| (1,2367) | 1:A:36:ILE:HG21 | 1:A:37:VAL:HB | 5 | 0.03 |
| (1,2367) | 1:A:36:ILE:HG22 | 1:A:37:VAL:HB | 5 | 0.03 |
| (1,2367) | 1:A:36:ILE:HG23 | 1:A:37:VAL:HB | 5 | 0.03 |
| (1,2344) | 1:B:35:THR:HB | 1:B:50:MET:HB2 | 6 | 0.03 |
| (1,2344) | 1:B:35:THR:HB | 1:B:50:MET:HB2 | 10 | 0.03 |
| (1,2343) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 11 | 0.03 |
| (1,2334) | 1:B:33:ILE:HD11 | 1:B:34:ARG:H | 15 | 0.03 |
| (1,2334) | 1:B:33:ILE:HD12 | 1:B:34:ARG:H | 15 | 0.03 |
| (1,2334) | 1:B:33:ILE:HD13 | 1:B:34:ARG:H | 15 | 0.03 |
| (1,2333) | 1:A:33:ILE:HD11 | 1:A:34:ARG:H | 11 | 0.03 |
| (1,2333) | 1:A:33:ILE:HD12 | 1:A:34:ARG:H | 11 | 0.03 |
| (1,2333) | 1:A:33:ILE:HD13 | 1:A:34:ARG:H | 11 | 0.03 |
| (1,2329) | 1:A:20:ASN:HD21 | 1:B:33:ILE:HD11 | 13 | 0.03 |
| (1,2329) | 1:A:20:ASN:HD21 | 1:B:33:ILE:HD12 | 13 | 0.03 |
| (1,2329) | 1:A:20:ASN:HD21 | 1:B:33:ILE:HD13 | 13 | 0.03 |
| (1,2274) | 1:B:31:THR:HG21 | 1:B:51:ILE:HD11 | 19 | 0.03 |
| (1,2274) | 1:B:31:THR:HG21 | 1:B:51:ILE:HD12 | 19 | 0.03 |
| (1,2274) | 1:B:31:THR:HG21 | 1:B:51:ILE:HD13 | 19 | 0.03 |
| (1,2274) | 1:B:31:THR:HG22 | 1:B:51:ILE:HD11 | 19 | 0.03 |
| (1,2274) | 1:B:31:THR:HG22 | 1:B:51:ILE:HD12 | 19 | 0.03 |
| (1,2274) | 1:B:31:THR:HG22 | 1:B:51:ILE:HD13 | 19 | 0.03 |
| (1,2274) | 1:B:31:THR:HG23 | 1:B:51:ILE:HD11 | 19 | 0.03 |
| (1,2274) | 1:B:31:THR:HG23 | 1:B:51:ILE:HD12 | 19 | 0.03 |
| (1,2274) | 1:B:31:THR:HG23 | 1:B:51:ILE:HD13 | 19 | 0.03 |
| (1,227) | 1:B:18:MET:H | 1:B:18:MET:HG3 | 3 | 0.03 |
| (1,2268) | 1:B:29:PHE:HD1 | 1:B:31:THR:HB | 15 | 0.03 |
| (1,2268) | 1:B:29:PHE:HD2 | 1:B:31:THR:HB | 15 | 0.03 |
| (1,2267) | 1:A:29:PHE:HD1 | 1:A:31:THR:HB | 9 | 0.03 |
| (1,2267) | 1:A:29:PHE:HD2 | 1:A:31:THR:HB | 9 | 0.03 |
| (1,2267) | 1:A:29:PHE:HD1 | 1:A:31:THR:HB | 11 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2267) | 1:A:29:PHE:HD2 | 1:A:31:THR:HB | 11 | 0.03 |
| (1,2267) | 1:A:29:PHE:HD1 | 1:A:31:THR:HB | 18 | 0.03 |
| (1,2267) | 1:A:29:PHE:HD2 | 1:A:31:THR:HB | 18 | 0.03 |
| (1,2262) | 1:B:25:VAL:HA | 1:B:28:LYS:HE2 | 2 | 0.03 |
| (1,2262) | 1:B:25:VAL:HA | 1:B:28:LYS:HE3 | 2 | 0.03 |
| (1,2261) | 1:A:25:VAL:HA | 1:A:28:LYS:HE2 | 8 | 0.03 |
| (1,2261) | 1:A:25:VAL:HA | 1:A:28:LYS:HE3 | 8 | 0.03 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 8 | 0.03 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 8 | 0.03 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 8 | 0.03 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 14 | 0.03 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 14 | 0.03 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 14 | 0.03 |
| (1,2185) | 1:A:25:VAL:HG21 | 1:A:29:PHE:HD1 | 13 | 0.03 |
| (1,2185) | 1:A:25:VAL:HG21 | 1:A:29:PHE:HD2 | 13 | 0.03 |
| (1,2185) | 1:A:25:VAL:HG22 | 1:A:29:PHE:HD1 | 13 | 0.03 |
| (1,2185) | 1:A:25:VAL:HG22 | 1:A:29:PHE:HD2 | 13 | 0.03 |
| (1,2185) | 1:A:25:VAL:HG23 | 1:A:29:PHE:HD1 | 13 | 0.03 |
| (1,2185) | 1:A:25:VAL:HG23 | 1:A:29:PHE:HD2 | 13 | 0.03 |
| (1,2172) | 1:B:25:VAL:HG11 | 1:B:27:SER:H | 3 | 0.03 |
| (1,2172) | 1:B:25:VAL:HG12 | 1:B:27:SER:H | 3 | 0.03 |
| (1,2172) | 1:B:25:VAL:HG13 | 1:B:27:SER:H | 3 | 0.03 |
| (1,2172) | 1:B:25:VAL:HG11 | 1:B:27:SER:H | 19 | 0.03 |
| (1,2172) | 1:B:25:VAL:HG12 | 1:B:27:SER:H | 19 | 0.03 |
| (1,2172) | 1:B:25:VAL:HG13 | 1:B:27:SER:H | 19 | 0.03 |
| (1,2171) | 1:A:25:VAL:HG11 | 1:A:27:SER:H | 10 | 0.03 |
| (1,2171) | 1:A:25:VAL:HG12 | 1:A:27:SER:H | 10 | 0.03 |
| (1,2171) | 1:A:25:VAL:HG13 | 1:A:27:SER:H | 10 | 0.03 |
| (1,2171) | 1:A:25:VAL:HG11 | 1:A:27:SER:H | 19 | 0.03 |
| (1,2171) | 1:A:25:VAL:HG12 | 1:A:27:SER:H | 19 | 0.03 |
| (1,2171) | 1:A:25:VAL:HG13 | 1:A:27:SER:H | 19 | 0.03 |
| (1,216) | 1:B:16:ASN:HA | 1:B:17:GLY:H | 3 | 0.03 |
| (1,216) | 1:B:16:ASN:HA | 1:B:17:GLY:H | 9 | 0.03 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 9 | 0.03 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 9 | 0.03 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 9 | 0.03 |
| (1,2101) | 1:A:22:ILE:HD11 | 1:A:23:THR:HA | 13 | 0.03 |
| (1,2101) | 1:A:22:ILE:HD12 | 1:A:23:THR:HA | 13 | 0.03 |
| (1,2101) | 1:A:22:ILE:HD13 | 1:A:23:THR:HA | 13 | 0.03 |
| (1,2091) | 1:A:22:ILE:HD11 | 1:A:69:VAL:HG21 | 20 | 0.03 |
| (1,2091) | 1:A:22:ILE:HD11 | 1:A:69:VAL:HG22 | 20 | 0.03 |
| (1,2091) | 1:A:22:ILE:HD11 | 1:A:69:VAL:HG23 | 20 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2091) | 1:A:22:ILE:HD12 | 1:A:69:VAL:HG21 | 20 | 0.03 |
| (1,2091) | 1:A:22:ILE:HD12 | 1:A:69:VAL:HG22 | 20 | 0.03 |
| (1,2091) | 1:A:22:ILE:HD12 | 1:A:69:VAL:HG23 | 20 | 0.03 |
| (1,2091) | 1:A:22:ILE:HD13 | 1:A:69:VAL:HG21 | 20 | 0.03 |
| (1,2091) | 1:A:22:ILE:HD13 | 1:A:69:VAL:HG22 | 20 | 0.03 |
| (1,2091) | 1:A:22:ILE:HD13 | 1:A:69:VAL:HG23 | 20 | 0.03 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 5 | 0.03 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 5 | 0.03 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 5 | 0.03 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 10 | 0.03 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 10 | 0.03 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 10 | 0.03 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 11 | 0.03 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 11 | 0.03 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 11 | 0.03 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 7 | 0.03 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 7 | 0.03 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 7 | 0.03 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 10 | 0.03 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 10 | 0.03 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 10 | 0.03 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 11 | 0.03 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 11 | 0.03 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 11 | 0.03 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG21 | 8 | 0.03 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG22 | 8 | 0.03 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG23 | 8 | 0.03 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG21 | 11 | 0.03 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG22 | 11 | 0.03 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG23 | 11 | 0.03 |
| (1,2054) | 1:A:20:ASN:H | 1:A:22:ILE:HG13 | 12 | 0.03 |
| (1,2020) | 1:A:19:THR:HG21 | 1:A:22:ILE:HB | 13 | 0.03 |
| (1,2020) | 1:A:19:THR:HG22 | 1:A:22:ILE:HB | 13 | 0.03 |
| (1,2020) | 1:A:19:THR:HG23 | 1:A:22:ILE:HB | 13 | 0.03 |
| (1,2009) | 1:B:21:GLN:HG3 | 1:B:25:VAL:H | 2 | 0.03 |
| (1,2008) | 1:A:21:GLN:HG3 | 1:A:25:VAL:H | 6 | 0.03 |
| (1,1977) | 1:B:21:GLN:HB3 | 1:B:69:VAL:HG11 | 14 | 0.03 |
| (1,1977) | 1:B:21:GLN:HB3 | 1:B:69:VAL:HG12 | 14 | 0.03 |
| (1,1977) | 1:B:21:GLN:HB3 | 1:B:69:VAL:HG13 | 14 | 0.03 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 8 | 0.03 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 8 | 0.03 |
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 8 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 9 | 0.03 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 9 | 0.03 |
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 9 | 0.03 |
| (1,1907) | 1:A:18:MET:HA | 1:A:21:GLN:HG2 | 4 | 0.03 |
| (1,1875) | 1:B:11:VAL:HG21 | 1:B:41:LYS:HE2 | 4 | 0.03 |
| (1,1875) | 1:B:11:VAL:HG21 | 1:B:41:LYS:HE3 | 4 | 0.03 |
| (1,1875) | 1:B:11:VAL:HG22 | 1:B:41:LYS:HE2 | 4 | 0.03 |
| (1,1875) | 1:B:11:VAL:HG22 | 1:B:41:LYS:HE3 | 4 | 0.03 |
| (1,1875) | 1:B:11:VAL:HG23 | 1:B:41:LYS:HE2 | 4 | 0.03 |
| (1,1875) | 1:B:11:VAL:HG23 | 1:B:41:LYS:HE3 | 4 | 0.03 |
| (1,1873) | 1:B:15:LYS:HD2 | 1:B:71:GLY:HA3 | 4 | 0.03 |
| (1,1873) | 1:B:15:LYS:HD3 | 1:B:71:GLY:HA3 | 4 | 0.03 |
| (1,187) | 1:A:15:LYS:H | 1:A:44:ILE:HA | 19 | 0.03 |
| (1,1861) | 1:B:15:LYS:HG2 | 1:B:18:MET:HE1 | 1 | 0.03 |
| (1,1861) | 1:B:15:LYS:HG2 | 1:B:18:MET:HE2 | 1 | 0.03 |
| (1,1861) | 1:B:15:LYS:HG2 | 1:B:18:MET:HE3 | 1 | 0.03 |
| (1,1861) | 1:B:15:LYS:HG3 | 1:B:18:MET:HE1 | 1 | 0.03 |
| (1,1861) | 1:B:15:LYS:HG3 | 1:B:18:MET:HE2 | 1 | 0.03 |
| (1,1861) | 1:B:15:LYS:HG3 | 1:B:18:MET:HE3 | 1 | 0.03 |
| (1,1861) | 1:B:15:LYS:HG2 | 1:B:18:MET:HE1 | 9 | 0.03 |
| (1,1861) | 1:B:15:LYS:HG2 | 1:B:18:MET:HE2 | 9 | 0.03 |
| (1,1861) | 1:B:15:LYS:HG2 | 1:B:18:MET:HE3 | 9 | 0.03 |
| (1,1861) | 1:B:15:LYS:HG3 | 1:B:18:MET:HE1 | 9 | 0.03 |
| (1,1861) | 1:B:15:LYS:HG3 | 1:B:18:MET:HE2 | 9 | 0.03 |
| (1,1861) | 1:B:15:LYS:HG3 | 1:B:18:MET:HE3 | 9 | 0.03 |
| (1,1857) | 1:B:15:LYS:HB3 | 1:B:16:ASN:HB2 | 2 | 0.03 |
| (1,1847) | 1:B:14:ASP:HB3 | 1:B:43:GLY:HA3 | 19 | 0.03 |
| (1,1839) | 1:B:13:GLU:HG2 | 1:B:44:ILE:HA | 11 | 0.03 |
| (1,1839) | 1:B:13:GLU:HG3 | 1:B:44:ILE:HA | 11 | 0.03 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG11 | 17 | 0.03 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG12 | 17 | 0.03 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG13 | 17 | 0.03 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG11 | 17 | 0.03 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG12 | 17 | 0.03 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG13 | 17 | 0.03 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG11 | 15 | 0.03 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG12 | 15 | 0.03 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG13 | 15 | 0.03 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG11 | 15 | 0.03 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG12 | 15 | 0.03 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG13 | 15 | 0.03 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG11 | 18 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG12 | 18 | 0.03 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG13 | 18 | 0.03 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG11 | 18 | 0.03 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG12 | 18 | 0.03 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG13 | 18 | 0.03 |
| (1,181) | 1:A:15:LYS:H | 1:A:18:MET:HG2 | 20 | 0.03 |
| (1,1762) | 1:A:11:VAL:HG11 | 1:A:73:PHE:HB2 | 19 | 0.03 |
| (1,1762) | 1:A:11:VAL:HG12 | 1:A:73:PHE:HB2 | 19 | 0.03 |
| (1,1762) | 1:A:11:VAL:HG13 | 1:A:73:PHE:HB2 | 19 | 0.03 |
| (1,1762) | 1:A:11:VAL:HG11 | 1:A:73:PHE:HB2 | 20 | 0.03 |
| (1,1762) | 1:A:11:VAL:HG12 | 1:A:73:PHE:HB2 | 20 | 0.03 |
| (1,1762) | 1:A:11:VAL:HG13 | 1:A:73:PHE:HB2 | 20 | 0.03 |
| (1,175) | 1:A:13:GLU:HG2 | 1:A:15:LYS:H | 6 | 0.03 |
| (1,175) | 1:A:13:GLU:HG3 | 1:A:15:LYS:H | 6 | 0.03 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 2 | 0.03 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 2 | 0.03 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 2 | 0.03 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 15 | 0.03 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 15 | 0.03 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 15 | 0.03 |
| (1,1744) | 1:A:11:VAL:HG21 | 1:A:46:THR:HB | 5 | 0.03 |
| (1,1744) | 1:A:11:VAL:HG22 | 1:A:46:THR:HB | 5 | 0.03 |
| (1,1744) | 1:A:11:VAL:HG23 | 1:A:46:THR:HB | 5 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG21 | 13 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG22 | 13 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG23 | 13 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG21 | 13 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG22 | 13 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG23 | 13 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG21 | 13 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG22 | 13 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG23 | 13 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG21 | 16 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG22 | 16 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG23 | 16 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG21 | 16 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG22 | 16 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG23 | 16 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG21 | 16 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG22 | 16 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG23 | 16 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG21 | 17 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG22 | 17 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG23 | 17 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG21 | 17 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG22 | 17 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG23 | 17 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG21 | 17 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG22 | 17 | 0.03 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG23 | 17 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG21 | 6 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG22 | 6 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG23 | 6 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG21 | 6 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG22 | 6 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG23 | 6 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG21 | 6 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG22 | 6 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG23 | 6 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG21 | 7 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG22 | 7 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG23 | 7 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG21 | 7 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG22 | 7 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG23 | 7 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG21 | 7 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG22 | 7 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG23 | 7 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG21 | 9 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG22 | 9 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG23 | 9 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG21 | 9 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG22 | 9 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG23 | 9 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG21 | 9 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG22 | 9 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG23 | 9 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG21 | 11 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG22 | 11 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG23 | 11 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG21 | 11 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG22 | 11 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG23 | 11 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG21 | 11 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG22 | 11 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG23 | 11 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG21 | 20 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG22 | 20 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG23 | 20 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG21 | 20 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG22 | 20 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG23 | 20 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG21 | 20 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG22 | 20 | 0.03 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG23 | 20 | 0.03 |
| (1,1720) | 1:A:10:ILE:HD11 | 1:A:11:VAL:H | 4 | 0.03 |
| (1,1720) | 1:A:10:ILE:HD12 | 1:A:11:VAL:H | 4 | 0.03 |
| (1,1720) | 1:A:10:ILE:HD13 | 1:A:11:VAL:H | 4 | 0.03 |
| (1,171) | 1:A:15:LYS:H | 1:A:18:MET:HE1 | 5 | 0.03 |
| (1,171) | 1:A:15:LYS:H | 1:A:18:MET:HE2 | 5 | 0.03 |
| (1,171) | 1:A:15:LYS:H | 1:A:18:MET:HE3 | 5 | 0.03 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD11 | 7 | 0.03 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD12 | 7 | 0.03 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD13 | 7 | 0.03 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD11 | 10 | 0.03 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD12 | 10 | 0.03 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD13 | 10 | 0.03 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD11 | 12 | 0.03 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD12 | 12 | 0.03 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD13 | 12 | 0.03 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD11 | 14 | 0.03 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD12 | 14 | 0.03 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD13 | 14 | 0.03 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD11 | 3 | 0.03 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD12 | 3 | 0.03 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD13 | 3 | 0.03 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD11 | 18 | 0.03 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD12 | 18 | 0.03 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD13 | 18 | 0.03 |
| (1,1631) | 1:B:9:ARG:HD2 | 1:B:11:VAL:HB | 14 | 0.03 |
| (1,1631) | 1:B:9:ARG:HD3 | 1:B:11:VAL:HB | 14 | 0.03 |
| (1,1630) | 1:A:9:ARG:HD2 | 1:A:11:VAL:HB | 12 | 0.03 |
| (1,1630) | 1:A:9:ARG:HD3 | 1:A:11:VAL:HB | 12 | 0.03 |
| (1,1630) | 1:A:9:ARG:HD2 | 1:A:11:VAL:HB | 19 | 0.03 |
| (1,1630) | 1:A:9:ARG:HD3 | 1:A:11:VAL:HB | 19 | 0.03 |
| (1,1626) | 1:B:9:ARG:HG3 | 1:B:10:ILE:H | 6 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1612) | 1:B:24:GLY:H | 1:B:26:ILE:HD11 | 9 | 0.03 |
| (1,1612) | 1:B:24:GLY:H | 1:B:26:ILE:HD12 | 9 | 0.03 |
| (1,1612) | 1:B:24:GLY:H | 1:B:26:ILE:HD13 | 9 | 0.03 |
| (1,1605) | 1:A:8:ILE:HD11 | 1:A:77:ARG:HA | 7 | 0.03 |
| (1,1605) | 1:A:8:ILE:HD12 | 1:A:77:ARG:HA | 7 | 0.03 |
| (1,1605) | 1:A:8:ILE:HD13 | 1:A:77:ARG:HA | 7 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 1 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 1 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 1 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 1 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 1 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 1 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 1 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 1 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 1 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 5 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 5 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 5 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 5 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 5 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 5 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 5 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 5 | 0.03 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 5 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 3 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 3 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 3 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 3 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 3 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 3 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 3 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 3 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 3 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 5 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 5 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 5 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 5 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 5 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 5 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 5 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 5 | 0.03 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 5 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD2 | 6 | 0.03 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD3 | 6 | 0.03 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD2 | 6 | 0.03 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD3 | 6 | 0.03 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD2 | 6 | 0.03 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD3 | 6 | 0.03 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD2 | 14 | 0.03 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD3 | 14 | 0.03 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD2 | 14 | 0.03 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD3 | 14 | 0.03 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD2 | 14 | 0.03 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD3 | 14 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 3 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 3 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 3 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 3 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 3 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 3 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 6 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 6 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 6 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 6 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 6 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 6 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 9 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 9 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 9 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 9 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 9 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 9 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 12 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 12 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 12 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 12 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 12 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 12 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 17 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 17 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 17 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 17 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 17 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 17 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 19 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 19 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 19 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 19 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 19 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 19 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 20 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 20 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 20 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 20 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 20 | 0.03 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 20 | 0.03 |
| (1,1570) | 1:B:8:ILE:HG21 | 1:B:63:MET:HG3 | 8 | 0.03 |
| (1,1570) | 1:B:8:ILE:HG22 | 1:B:63:MET:HG3 | 8 | 0.03 |
| (1,1570) | 1:B:8:ILE:HG23 | 1:B:63:MET:HG3 | 8 | 0.03 |
| (1,1570) | 1:B:8:ILE:HG21 | 1:B:63:MET:HG3 | 16 | 0.03 |
| (1,1570) | 1:B:8:ILE:HG22 | 1:B:63:MET:HG3 | 16 | 0.03 |
| (1,1570) | 1:B:8:ILE:HG23 | 1:B:63:MET:HG3 | 16 | 0.03 |
| (1,1541) | 1:A:6:ALA:HB1 | 1:A:7:GLY:HA3 | 16 | 0.03 |
| (1,1541) | 1:A:6:ALA:HB2 | 1:A:7:GLY:HA3 | 16 | 0.03 |
| (1,1541) | 1:A:6:ALA:HB3 | 1:A:7:GLY:HA3 | 16 | 0.03 |
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 3 | 0.03 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 3 | 0.03 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 3 | 0.03 |
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 11 | 0.03 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 11 | 0.03 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 11 | 0.03 |
| (1,1456) | 1:B:3:ASP:HB2 | 1:B:53:VAL:H | 18 | 0.03 |
| (1,1420) | 1:B:40:ALA:H | 1:B:41:LYS:HD2 | 1 | 0.03 |
| (1,1420) | 1:B:40:ALA:H | 1:B:41:LYS:HD3 | 1 | 0.03 |
| (1,1420) | 1:B:40:ALA:H | 1:B:41:LYS:HD2 | 4 | 0.03 |
| (1,1420) | 1:B:40:ALA:H | 1:B:41:LYS:HD3 | 4 | 0.03 |
| (1,1398) | 1:B:82:GLU:H | 1:B:82:GLU:HG2 | 18 | 0.03 |
| (1,1370) | 1:B:78:LEU:HD21 | 1:B:79:SER:H | 7 | 0.03 |
| (1,1370) | 1:B:78:LEU:HD22 | 1:B:79:SER:H | 7 | 0.03 |
| (1,1370) | 1:B:78:LEU:HD23 | 1:B:79:SER:H | 7 | 0.03 |
| (1,1339) | 1:A:76:GLU:HB2 | 1:A:77:ARG:H | 10 | 0.03 |
| (1,1277) | 1:A:74:THR:H | 1:A:75:VAL:HG21 | 10 | 0.03 |
| (1,1277) | 1:A:74:THR:H | 1:A:75:VAL:HG22 | 10 | 0.03 |
| (1,1277) | 1:A:74:THR:H | 1:A:75:VAL:HG23 | 10 | 0.03 |
| (1,1254) | 1:B:69:VAL:HG21 | 1:B:72:VAL:H | 3 | 0.03 |
| (1,1254) | 1:B:69:VAL:HG22 | 1:B:72:VAL:H | 3 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1254) | 1:B:69:VAL:HG23 | 1:B:72:VAL:H | 3 | 0.03 |
| (1,1242) | 1:B:69:VAL:HG11 | 1:B:71:GLY:H | 11 | 0.03 |
| (1,1242) | 1:B:69:VAL:HG12 | 1:B:71:GLY:H | 11 | 0.03 |
| (1,1242) | 1:B:69:VAL:HG13 | 1:B:71:GLY:H | 11 | 0.03 |
| (1,1241) | 1:A:69:VAL:HG11 | 1:A:71:GLY:H | 14 | 0.03 |
| (1,1241) | 1:A:69:VAL:HG12 | 1:A:71:GLY:H | 14 | 0.03 |
| (1,1241) | 1:A:69:VAL:HG13 | 1:A:71:GLY:H | 14 | 0.03 |
| (1,1222) | 1:B:69:VAL:H | 1:B:72:VAL:H | 4 | 0.03 |
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 5 | 0.03 |
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 9 | 0.03 |
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 17 | 0.03 |
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 18 | 0.03 |
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 20 | 0.03 |
| (1,1175) | 1:A:67:ARG:HE | 1:A:75:VAL:HB | 3 | 0.03 |
| (1,1132) | 1:B:62:LEU:HD11 | 1:B:66:LEU:H | 4 | 0.03 |
| (1,1132) | 1:B:62:LEU:HD12 | 1:B:66:LEU:H | 4 | 0.03 |
| (1,1132) | 1:B:62:LEU:HD13 | 1:B:66:LEU:H | 4 | 0.03 |
| (1,1132) | 1:B:62:LEU:HD11 | 1:B:66:LEU:H | 12 | 0.03 |
| (1,1132) | 1:B:62:LEU:HD12 | 1:B:66:LEU:H | 12 | 0.03 |
| (1,1132) | 1:B:62:LEU:HD13 | 1:B:66:LEU:H | 12 | 0.03 |
| (1,1132) | 1:B:62:LEU:HD11 | 1:B:66:LEU:H | 20 | 0.03 |
| (1,1132) | 1:B:62:LEU:HD12 | 1:B:66:LEU:H | 20 | 0.03 |
| (1,1132) | 1:B:62:LEU:HD13 | 1:B:66:LEU:H | 20 | 0.03 |
| (1,1131) | 1:A:62:LEU:HD11 | 1:A:66:LEU:H | 2 | 0.03 |
| (1,1131) | 1:A:62:LEU:HD12 | 1:A:66:LEU:H | 2 | 0.03 |
| (1,1131) | 1:A:62:LEU:HD13 | 1:A:66:LEU:H | 2 | 0.03 |
| (1,1131) | 1:A:62:LEU:HD11 | 1:A:66:LEU:H | 3 | 0.03 |
| (1,1131) | 1:A:62:LEU:HD12 | 1:A:66:LEU:H | 3 | 0.03 |
| (1,1131) | 1:A:62:LEU:HD13 | 1:A:66:LEU:H | 3 | 0.03 |
| (1,1130) | 1:B:62:LEU:HD11 | 1:B:65:LYS:H | 6 | 0.03 |
| (1,1130) | 1:B:62:LEU:HD12 | 1:B:65:LYS:H | 6 | 0.03 |
| (1,1130) | 1:B:62:LEU:HD13 | 1:B:65:LYS:H | 6 | 0.03 |
| (1,1130) | 1:B:62:LEU:HD11 | 1:B:65:LYS:H | 7 | 0.03 |
| (1,1130) | 1:B:62:LEU:HD12 | 1:B:65:LYS:H | 7 | 0.03 |
| (1,1130) | 1:B:62:LEU:HD13 | 1:B:65:LYS:H | 7 | 0.03 |
| (1,1130) | 1:B:62:LEU:HD11 | 1:B:65:LYS:H | 10 | 0.03 |
| (1,1130) | 1:B:62:LEU:HD12 | 1:B:65:LYS:H | 10 | 0.03 |
| (1,1130) | 1:B:62:LEU:HD13 | 1:B:65:LYS:H | 10 | 0.03 |
| (1,1130) | 1:B:62:LEU:HD11 | 1:B:65:LYS:H | 14 | 0.03 |
| (1,1130) | 1:B:62:LEU:HD12 | 1:B:65:LYS:H | 14 | 0.03 |
| (1,1130) | 1:B:62:LEU:HD13 | 1:B:65:LYS:H | 14 | 0.03 |
| (1,1129) | 1:A:62:LEU:HD11 | 1:A:65:LYS:H | 2 | 0.03 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1129) | 1:A:62:LEU:HD12 | 1:A:65:LYS:H | 2 | 0.03 |
| (1,1129) | 1:A:62:LEU:HD13 | 1:A:65:LYS:H | 2 | 0.03 |
| (1,1129) | 1:A:62:LEU:HD11 | 1:A:65:LYS:H | 6 | 0.03 |
| (1,1129) | 1:A:62:LEU:HD12 | 1:A:65:LYS:H | 6 | 0.03 |
| (1,1129) | 1:A:62:LEU:HD13 | 1:A:65:LYS:H | 6 | 0.03 |
| (1,979) | 1:B:58:LYS:H | 1:B:58:LYS:HG3 | 4 | 0.02 |
| (1,979) | 1:B:58:LYS:H | 1:B:58:LYS:HG3 | 6 | 0.02 |
| (1,979) | 1:B:58:LYS:H | 1:B:58:LYS:HG3 | 10 | 0.02 |
| (1,979) | 1:B:58:LYS:H | 1:B:58:LYS:HG3 | 19 | 0.02 |
| (1,978) | 1:A:58:LYS:H | 1:A:58:LYS:HG3 | 7 | 0.02 |
| (1,978) | 1:A:58:LYS:H | 1:A:58:LYS:HG3 | 16 | 0.02 |
| (1,974) | 1:A:53:VAL:HG21 | 1:A:58:LYS:H | 13 | 0.02 |
| (1,974) | 1:A:53:VAL:HG22 | 1:A:58:LYS:H | 13 | 0.02 |
| (1,974) | 1:A:53:VAL:HG23 | 1:A:58:LYS:H | 13 | 0.02 |
| (1,959) | 1:B:57:ASP:H | 1:B:58:LYS:HG3 | 11 | 0.02 |
| (1,957) | 1:B:54:LYS:HE2 | 1:B:55:ASN:HD22 | 15 | 0.02 |
| (1,957) | 1:B:54:LYS:HE3 | 1:B:55:ASN:HD22 | 15 | 0.02 |
| (1,925) | 1:B:3:ASP:HB3 | 1:B:53:VAL:H | 17 | 0.02 |
| (1,924) | 1:A:3:ASP:HB3 | 1:A:53:VAL:H | 7 | 0.02 |
| (1,924) | 1:A:3:ASP:HB3 | 1:A:53:VAL:H | 16 | 0.02 |
| (1,915) | 1:B:51:ILE:HG12 | 1:B:52:PHE:H | 1 | 0.02 |
| (1,915) | 1:B:51:ILE:HG12 | 1:B:52:PHE:H | 5 | 0.02 |
| (1,915) | 1:B:51:ILE:HG12 | 1:B:52:PHE:H | 10 | 0.02 |
| (1,915) | 1:B:51:ILE:HG12 | 1:B:52:PHE:H | 13 | 0.02 |
| (1,915) | 1:B:51:ILE:HG12 | 1:B:52:PHE:H | 17 | 0.02 |
| (1,914) | 1:A:51:ILE:HG12 | 1:A:52:PHE:H | 16 | 0.02 |
| (1,86) | 1:A:9:ARG:HE | 1:A:10:ILE:H | 19 | 0.02 |
| (1,855) | 1:B:48:ASN:HD21 | 1:B:78:LEU:HD21 | 8 | 0.02 |
| (1,855) | 1:B:48:ASN:HD21 | 1:B:78:LEU:HD22 | 8 | 0.02 |
| (1,855) | 1:B:48:ASN:HD21 | 1:B:78:LEU:HD23 | 8 | 0.02 |
| (1,854) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD21 | 14 | 0.02 |
| (1,854) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD22 | 14 | 0.02 |
| (1,854) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD23 | 14 | 0.02 |
| (1,85) | 1:B:9:ARG:HE | 1:B:11:VAL:HG21 | 5 | 0.02 |
| (1,85) | 1:B:9:ARG:HE | 1:B:11:VAL:HG22 | 5 | 0.02 |
| (1,85) | 1:B:9:ARG:HE | 1:B:11:VAL:HG23 | 5 | 0.02 |
| (1,849) | 1:B:47:CYS:HG | 1:B:48:ASN:H | 18 | 0.02 |
| (1,848) | 1:A:47:CYS:HG | 1:A:48:ASN:H | 3 | 0.02 |
| (1,848) | 1:A:47:CYS:HG | 1:A:48:ASN:H | 4 | 0.02 |
| (1,848) | 1:A:47:CYS:HG | 1:A:48:ASN:H | 6 | 0.02 |
| (1,848) | 1:A:47:CYS:HG | 1:A:48:ASN:H | 10 | 0.02 |
| (1,848) | 1:A:47:CYS:HG | 1:A:48:ASN:H | 12 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,848) | 1:A:47:CYS:HG | 1:A:48:ASN:H | 14 | 0.02 |
| (1,787) | 1:B:44:ILE:HB | 1:B:45:PHE:H | 8 | 0.02 |
| (1,777) | 1:B:43:GLY:H | 1:B:44:ILE:H | 10 | 0.02 |
| (1,760) | 1:A:44:ILE:H | 1:A:44:ILE:HG21 | 15 | 0.02 |
| (1,760) | 1:A:44:ILE:H | 1:A:44:ILE:HG22 | 15 | 0.02 |
| (1,760) | 1:A:44:ILE:H | 1:A:44:ILE:HG23 | 15 | 0.02 |
| (1,735) | 1:B:41:LYS:H | 1:B:46:THR:H | 14 | 0.02 |
| (1,735) | 1:B:41:LYS:H | 1:B:46:THR:H | 16 | 0.02 |
| (1,734) | 1:A:41:LYS:H | 1:A:46:THR:H | 10 | 0.02 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD1 | 5 | 0.02 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD2 | 5 | 0.02 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD1 | 11 | 0.02 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD2 | 11 | 0.02 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD1 | 13 | 0.02 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD2 | 13 | 0.02 |
| (1,630) | 1:A:35:THR:H | 1:A:83:HIS:HE1 | 15 | 0.02 |
| (1,581) | 1:B:32:ASN:HA | 1:B:32:ASN:HD21 | 19 | 0.02 |
| (1,579) | 1:A:32:ASN:HD21 | 1:A:33:ILE:HB | 7 | 0.02 |
| (1,579) | 1:A:32:ASN:HD21 | 1:A:33:ILE:HB | 20 | 0.02 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD11 | 10 | 0.02 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD12 | 10 | 0.02 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD13 | 10 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD11 | 2 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD12 | 2 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD13 | 2 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD11 | 5 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD12 | 5 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD13 | 5 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD11 | 7 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD12 | 7 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD13 | 7 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD11 | 8 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD12 | 8 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD13 | 8 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD11 | 12 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD12 | 12 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD13 | 12 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD11 | 19 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD12 | 19 | 0.02 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD13 | 19 | 0.02 |
| (1,562) | 1:B:29:PHE:HD1 | 1:B:31:THR:H | 5 | 0.02 |
| (1,562) | 1:B:29:PHE:HD2 | 1:B:31:THR:H | 5 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,561) | 1:A:29:PHE:HD1 | 1:A:31:THR:H | 15 | 0.02 |
| (1,561) | 1:A:29:PHE:HD2 | 1:A:31:THR:H | 15 | 0.02 |
| (1,561) | 1:A:29:PHE:HD1 | 1:A:31:THR:H | 19 | 0.02 |
| (1,561) | 1:A:29:PHE:HD2 | 1:A:31:THR:H | 19 | 0.02 |
| (1,5260) | 1:B:82:GLU:H | 1:B:82:GLU:HG2 | 5 | 0.02 |
| (1,5242) | 1:B:68:LYS:HA | 1:B:68:LYS:HG2 | 3 | 0.02 |
| (1,5239) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG21 | 3 | 0.02 |
| (1,5239) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG22 | 3 | 0.02 |
| (1,5239) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG23 | 3 | 0.02 |
| (1,5239) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG21 | 6 | 0.02 |
| (1,5239) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG22 | 6 | 0.02 |
| (1,5239) | 1:B:67:ARG:HG2 | 1:B:75:VAL:HG23 | 6 | 0.02 |
| (1,5222) | 1:B:65:LYS:H | 1:B:65:LYS:HG2 | 15 | 0.02 |
| (1,5220) | 1:B:64:ASP:HB3 | 1:B:65:LYS:HG2 | 10 | 0.02 |
| (1,5218) | 1:B:64:ASP:HA | 1:B:67:ARG:HG2 | 11 | 0.02 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD11 | 2 | 0.02 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD12 | 2 | 0.02 |
| (1,5194) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD13 | 2 | 0.02 |
| (1,5192) | 1:B:58:LYS:HE2 | 1:B:59:LEU:HA | 7 | 0.02 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB2 | 15 | 0.02 |
| (1,5180) | 1:B:55:ASN:HD21 | 1:B:57:ASP:HB3 | 15 | 0.02 |
| (1,5175) | 1:B:54:LYS:HD2 | 1:B:55:ASN:HD21 | 1 | 0.02 |
| (1,5175) | 1:B:54:LYS:HD3 | 1:B:55:ASN:HD21 | 1 | 0.02 |
| (1,5167) | 1:B:53:VAL:HG21 | 1:B:58:LYS:HB2 | 5 | 0.02 |
| (1,5167) | 1:B:53:VAL:HG22 | 1:B:58:LYS:HB2 | 5 | 0.02 |
| (1,5167) | 1:B:53:VAL:HG23 | 1:B:58:LYS:HB2 | 5 | 0.02 |
| (1,5165) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HB2 | 18 | 0.02 |
| (1,5165) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HB2 | 18 | 0.02 |
| (1,5165) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HB2 | 18 | 0.02 |
| (1,5164) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HE2 | 18 | 0.02 |
| (1,5164) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HE2 | 18 | 0.02 |
| (1,5164) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HE2 | 18 | 0.02 |
| (1,5162) | 1:B:53:VAL:HA | 1:B:54:LYS:HB2 | 1 | 0.02 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD11 | 2 | 0.02 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD12 | 2 | 0.02 |
| (1,5154) | 1:B:48:ASN:HB2 | 1:B:78:LEU:HD13 | 2 | 0.02 |
| (1,5141) | 1:B:41:LYS:H | 1:B:45:PHE:HB2 | 14 | 0.02 |
| (1,5126) | 1:B:37:VAL:HG11 | 1:B:48:ASN:HD21 | 2 | 0.02 |
| (1,5126) | 1:B:37:VAL:HG12 | 1:B:48:ASN:HD21 | 2 | 0.02 |
| (1,5126) | 1:B:37:VAL:HG13 | 1:B:48:ASN:HD21 | 2 | 0.02 |
| (1,5126) | 1:B:37:VAL:HG11 | 1:B:48:ASN:HD21 | 4 | 0.02 |
| (1,5126) | 1:B:37:VAL:HG12 | 1:B:48:ASN:HD21 | 4 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5126) | 1:B:37:VAL:HG13 | 1:B:48:ASN:HD21 | 4 | 0.02 |
| (1,5117) | 1:B:36:ILE:HG12 | 1:B:37:VAL:H | 2 | 0.02 |
| (1,5114) | 1:B:35:THR:HB | 1:B:50:MET:HB2 | 12 | 0.02 |
| (1,5114) | 1:B:35:THR:HB | 1:B:50:MET:HB2 | 20 | 0.02 |
| (1,5092) | 1:B:32:ASN:HA | 1:B:32:ASN:HD21 | 19 | 0.02 |
| (1,5086) | 1:B:29:PHE:HE1 | 1:B:65:LYS:HD2 | 1 | 0.02 |
| (1,5072) | 1:B:28:LYS:HB2 | 1:B:28:LYS:HD2 | 2 | 0.02 |
| (1,5034) | 1:B:23:THR:HG21 | 1:B:27:SER:HB2 | 2 | 0.02 |
| (1,5034) | 1:B:23:THR:HG22 | 1:B:27:SER:HB2 | 2 | 0.02 |
| (1,5034) | 1:B:23:THR:HG23 | 1:B:27:SER:HB2 | 2 | 0.02 |
| (1,5034) | 1:B:23:THR:HG21 | 1:B:27:SER:HB2 | 18 | 0.02 |
| (1,5034) | 1:B:23:THR:HG22 | 1:B:27:SER:HB2 | 18 | 0.02 |
| (1,5034) | 1:B:23:THR:HG23 | 1:B:27:SER:HB2 | 18 | 0.02 |
| (1,5028) | 1:B:20:ASN:HB2 | 1:B:21:GLN:H | 4 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 3 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 3 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 3 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 5 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 5 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 5 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 7 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 7 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 7 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 8 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 8 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 8 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 9 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 9 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 9 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 10 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 10 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 10 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 12 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 12 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 12 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 13 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 13 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 13 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 16 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 16 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 16 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 17 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 17 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 17 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 19 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 19 | 0.02 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 19 | 0.02 |
| (1,4990) | 1:B:14:ASP:H | 1:B:14:ASP:HB2 | 8 | 0.02 |
| (1,4981) | 1:B:9:ARG:H | 1:B:76:GLU:HB2 | 1 | 0.02 |
| (1,4981) | 1:B:9:ARG:H | 1:B:76:GLU:HB2 | 18 | 0.02 |
| (1,497) | 1:A:23:THR:HG21 | 1:A:28:LYS:H | 17 | 0.02 |
| (1,497) | 1:A:23:THR:HG22 | 1:A:28:LYS:H | 17 | 0.02 |
| (1,497) | 1:A:23:THR:HG23 | 1:A:28:LYS:H | 17 | 0.02 |
| (1,4956) | 1:B:4:PHE:H | 1:B:54:LYS:HB2 | 15 | 0.02 |
| (1,4952) | 1:B:3:ASP:HB2 | 1:B:52:PHE:HB2 | 6 | 0.02 |
| (1,4933) | 1:A:69:VAL:HG11 | 1:A:70:GLN:HE21 | 17 | 0.02 |
| (1,4933) | 1:A:69:VAL:HG12 | 1:A:70:GLN:HE21 | 17 | 0.02 |
| (1,4933) | 1:A:69:VAL:HG13 | 1:A:70:GLN:HE21 | 17 | 0.02 |
| (1,4930) | 1:A:68:LYS:HA | 1:A:68:LYS:HG2 | 15 | 0.02 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG11 | 13 | 0.02 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG12 | 13 | 0.02 |
| (1,4924) | 1:A:67:ARG:HG2 | 1:A:72:VAL:HG13 | 13 | 0.02 |
| (1,4912) | 1:A:65:LYS:H | 1:A:65:LYS:HD2 | 8 | 0.02 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB2 | 7 | 0.02 |
| (1,4877) | 1:A:55:ASN:HD21 | 1:A:57:ASP:HB3 | 7 | 0.02 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD11 | 11 | 0.02 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD12 | 11 | 0.02 |
| (1,4851) | 1:A:48:ASN:HB2 | 1:A:78:LEU:HD13 | 11 | 0.02 |
| (1,4850) | 1:A:48:ASN:HB2 | 1:A:49:LEU:H | 6 | 0.02 |
| (1,4841) | 1:A:42:ASP:HB2 | 1:A:44:ILE:H | 1 | 0.02 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE2 | 15 | 0.02 |
| (1,4833) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HE3 | 15 | 0.02 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB2 | 14 | 0.02 |
| (1,4831) | 1:A:39:ASN:HD21 | 1:A:41:LYS:HB3 | 14 | 0.02 |
| (1,4813) | 1:A:36:ILE:HG12 | 1:A:37:VAL:H | 8 | 0.02 |
| (1,4809) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 16 | 0.02 |
| (1,4787) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HD2 | 18 | 0.02 |
| (1,4778) | 1:A:28:LYS:HG2 | 1:A:29:PHE:H | 17 | 0.02 |
| (1,4766) | 1:A:27:SER:HB2 | 1:B:24:GLY:H | 17 | 0.02 |
| (1,4762) | 1:A:27:SER:HB2 | 1:A:28:LYS:H | 18 | 0.02 |
| (1,476) | 1:A:27:SER:H | 1:A:33:ILE:HG12 | 5 | 0.02 |
| (1,476) | 1:A:27:SER:H | 1:A:33:ILE:HG12 | 13 | 0.02 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 2 | 0.02 |
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 10 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4757) | 1:A:26:ILE:HG12 | 1:A:27:SER:H | 19 | 0.02 |
| (1,4734) | 1:A:23:THR:HG21 | 1:B:27:SER:HB2 | 9 | 0.02 |
| (1,4734) | 1:A:23:THR:HG22 | 1:B:27:SER:HB2 | 9 | 0.02 |
| (1,4734) | 1:A:23:THR:HG23 | 1:B:27:SER:HB2 | 9 | 0.02 |
| (1,4724) | 1:A:20:ASN:HB2 | 1:A:21:GLN:HE21 | 4 | 0.02 |
| (1,4723) | 1:A:20:ASN:HB2 | 1:A:21:GLN:H | 13 | 0.02 |
| (1,4713) | 1:A:18:MET:HG2 | 1:A:19:THR:H | 2 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE1 | 1 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE2 | 1 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE3 | 1 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE1 | 3 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE2 | 3 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE3 | 3 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE1 | 6 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE2 | 6 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE3 | 6 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE1 | 9 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE2 | 9 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE3 | 9 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE1 | 11 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE2 | 11 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE3 | 11 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE1 | 12 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE2 | 12 | 0.02 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE3 | 12 | 0.02 |
| (1,4667) | 1:A:14:ASP:HA | 1:A:15:LYS:HB2 | 4 | 0.02 |
| (1,4666) | 1:A:14:ASP:H | 1:A:14:ASP:HB2 | 7 | 0.02 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 3 | 0.02 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 3 | 0.02 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 3 | 0.02 |
| (1,4613) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HD2 | 9 | 0.02 |
| (1,4610) | 1:B:81:LEU:HB3 | 1:B:83:HIS:HD2 | 4 | 0.02 |
| (1,4609) | 1:A:81:LEU:HB3 | 1:A:83:HIS:HD2 | 4 | 0.02 |
| (1,4608) | 1:B:5:LEU:HG | 1:B:83:HIS:HD2 | 7 | 0.02 |
| (1,4608) | 1:B:5:LEU:HG | 1:B:83:HIS:HD2 | 17 | 0.02 |
| (1,4608) | 1:B:5:LEU:HG | 1:B:83:HIS:HD2 | 20 | 0.02 |
| (1,4607) | 1:A:5:LEU:HG | 1:A:83:HIS:HD2 | 1 | 0.02 |
| (1,4607) | 1:A:5:LEU:HG | 1:A:83:HIS:HD2 | 6 | 0.02 |
| (1,4607) | 1:A:5:LEU:HG | 1:A:83:HIS:HD2 | 7 | 0.02 |
| (1,4591) | 1:A:13:GLU:H | 1:A:73:PHE:HZ | 13 | 0.02 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 7 | 0.02 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 19 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 10 | 0.02 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 13 | 0.02 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG21 | 1 | 0.02 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG22 | 1 | 0.02 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG23 | 1 | 0.02 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG21 | 10 | 0.02 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG22 | 10 | 0.02 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG23 | 10 | 0.02 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG21 | 13 | 0.02 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG22 | 13 | 0.02 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG23 | 13 | 0.02 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG21 | 2 | 0.02 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG22 | 2 | 0.02 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG23 | 2 | 0.02 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG21 | 8 | 0.02 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG22 | 8 | 0.02 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG23 | 8 | 0.02 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG21 | 11 | 0.02 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG22 | 11 | 0.02 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG23 | 11 | 0.02 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG21 | 12 | 0.02 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG22 | 12 | 0.02 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG23 | 12 | 0.02 |
| (1,4561) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HE2 | 5 | 0.02 |
| (1,4561) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HE3 | 5 | 0.02 |
| (1,4561) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HE2 | 12 | 0.02 |
| (1,4561) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HE3 | 12 | 0.02 |
| (1,4538) | 1:B:52:PHE:HD1 | 1:B:53:VAL:H | 1 | 0.02 |
| (1,4538) | 1:B:52:PHE:HD2 | 1:B:53:VAL:H | 1 | 0.02 |
| (1,4538) | 1:B:52:PHE:HD1 | 1:B:53:VAL:H | 6 | 0.02 |
| (1,4538) | 1:B:52:PHE:HD2 | 1:B:53:VAL:H | 6 | 0.02 |
| (1,4537) | 1:A:52:PHE:HD1 | 1:A:53:VAL:H | 6 | 0.02 |
| (1,4537) | 1:A:52:PHE:HD2 | 1:A:53:VAL:H | 6 | 0.02 |
| (1,4537) | 1:A:52:PHE:HD1 | 1:A:53:VAL:H | 9 | 0.02 |
| (1,4537) | 1:A:52:PHE:HD2 | 1:A:53:VAL:H | 9 | 0.02 |
| (1,4537) | 1:A:52:PHE:HD1 | 1:A:53:VAL:H | 10 | 0.02 |
| (1,4537) | 1:A:52:PHE:HD2 | 1:A:53:VAL:H | 10 | 0.02 |
| (1,4526) | 1:B:5:LEU:HA | 1:B:52:PHE:HD1 | 12 | 0.02 |
| (1,4526) | 1:B:5:LEU:HA | 1:B:52:PHE:HD2 | 12 | 0.02 |
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD1 | 9 | 0.02 |
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD2 | 9 | 0.02 |
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD1 | 10 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD2 | 10 | 0.02 |
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD1 | 14 | 0.02 |
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD2 | 14 | 0.02 |
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD1 | 18 | 0.02 |
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD2 | 18 | 0.02 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 4 | 0.02 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 7 | 0.02 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 12 | 0.02 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 19 | 0.02 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 2 | 0.02 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 3 | 0.02 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 4 | 0.02 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 5 | 0.02 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 6 | 0.02 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 7 | 0.02 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 8 | 0.02 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 12 | 0.02 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 14 | 0.02 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 15 | 0.02 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 18 | 0.02 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 20 | 0.02 |
| (1,4496) | 1:B:12:GLY:H | 1:B:45:PHE:HE1 | 18 | 0.02 |
| (1,4494) | 1:B:12:GLY:HA2 | 1:B:45:PHE:HE1 | 4 | 0.02 |
| (1,4478) | 1:B:19:THR:HG21 | 1:B:45:PHE:HE1 | 18 | 0.02 |
| (1,4478) | 1:B:19:THR:HG22 | 1:B:45:PHE:HE1 | 18 | 0.02 |
| (1,4478) | 1:B:19:THR:HG23 | 1:B:45:PHE:HE1 | 18 | 0.02 |
| (1,4475) | 1:A:22:ILE:HD11 | 1:A:45:PHE:HE1 | 7 | 0.02 |
| (1,4475) | 1:A:22:ILE:HD12 | 1:A:45:PHE:HE1 | 7 | 0.02 |
| (1,4475) | 1:A:22:ILE:HD13 | 1:A:45:PHE:HE1 | 7 | 0.02 |
| (1,4456) | 1:B:14:ASP:HA | 1:B:45:PHE:HD1 | 9 | 0.02 |
| (1,4456) | 1:B:14:ASP:HA | 1:B:45:PHE:HD2 | 9 | 0.02 |
| (1,4451) | 1:B:18:MET:HE1 | 1:B:45:PHE:HD1 | 16 | 0.02 |
| (1,4451) | 1:B:18:MET:HE1 | 1:B:45:PHE:HD2 | 16 | 0.02 |
| (1,4451) | 1:B:18:MET:HE2 | 1:B:45:PHE:HD1 | 16 | 0.02 |
| (1,4451) | 1:B:18:MET:HE2 | 1:B:45:PHE:HD2 | 16 | 0.02 |
| (1,4451) | 1:B:18:MET:HE3 | 1:B:45:PHE:HD1 | 16 | 0.02 |
| (1,4451) | 1:B:18:MET:HE3 | 1:B:45:PHE:HD2 | 16 | 0.02 |
| (1,4444) | 1:A:45:PHE:HD1 | 1:A:47:CYS:HG | 16 | 0.02 |
| (1,4444) | 1:A:45:PHE:HD2 | 1:A:47:CYS:HG | 16 | 0.02 |
| (1,4425) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HZ | 3 | 0.02 |
| (1,4425) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HZ | 3 | 0.02 |
| (1,4425) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HZ | 3 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4425) | 1:B:26:ILE:HG21 | 1:B:29:PHE:HZ | 4 | 0.02 |
| (1,4425) | 1:B:26:ILE:HG22 | 1:B:29:PHE:HZ | 4 | 0.02 |
| (1,4425) | 1:B:26:ILE:HG23 | 1:B:29:PHE:HZ | 4 | 0.02 |
| (1,4419) | 1:B:29:PHE:H | 1:B:29:PHE:HD1 | 1 | 0.02 |
| (1,4419) | 1:B:29:PHE:H | 1:B:29:PHE:HD2 | 1 | 0.02 |
| (1,4417) | 1:B:29:PHE:HA | 1:B:29:PHE:HD1 | 12 | 0.02 |
| (1,4417) | 1:B:29:PHE:HA | 1:B:29:PHE:HD2 | 12 | 0.02 |
| (1,4416) | 1:A:29:PHE:HA | 1:A:29:PHE:HD1 | 3 | 0.02 |
| (1,4416) | 1:A:29:PHE:HA | 1:A:29:PHE:HD2 | 3 | 0.02 |
| (1,4413) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 20 | 0.02 |
| (1,4413) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 20 | 0.02 |
| (1,4412) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 1 | 0.02 |
| (1,4412) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 1 | 0.02 |
| (1,4412) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 13 | 0.02 |
| (1,4412) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 13 | 0.02 |
| (1,4412) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 18 | 0.02 |
| (1,4412) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 18 | 0.02 |
| (1,4393) | 1:B:4:PHE:HZ | 1:B:6:ALA:HA | 1 | 0.02 |
| (1,4393) | 1:B:4:PHE:HZ | 1:B:6:ALA:HA | 5 | 0.02 |
| (1,4393) | 1:B:4:PHE:HZ | 1:B:6:ALA:HA | 7 | 0.02 |
| (1,4393) | 1:B:4:PHE:HZ | 1:B:6:ALA:HA | 19 | 0.02 |
| (1,4393) | 1:B:4:PHE:HZ | 1:B:6:ALA:HA | 20 | 0.02 |
| (1,4392) | 1:A:4:PHE:HZ | 1:A:6:ALA:HA | 7 | 0.02 |
| (1,4392) | 1:A:4:PHE:HZ | 1:A:6:ALA:HA | 10 | 0.02 |
| (1,4392) | 1:A:4:PHE:HZ | 1:A:6:ALA:HA | 16 | 0.02 |
| (1,4366) | 1:A:29:PHE:HE1 | 1:A:62:LEU:HA | 9 | 0.02 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD21 | 1 | 0.02 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD22 | 1 | 0.02 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD23 | 1 | 0.02 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD21 | 4 | 0.02 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD22 | 4 | 0.02 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD23 | 4 | 0.02 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD21 | 17 | 0.02 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD22 | 17 | 0.02 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD23 | 17 | 0.02 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD21 | 3 | 0.02 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD22 | 3 | 0.02 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD23 | 3 | 0.02 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD21 | 6 | 0.02 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD22 | 6 | 0.02 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD23 | 6 | 0.02 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD21 | 10 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD22 | 10 | 0.02 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD23 | 10 | 0.02 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD21 | 11 | 0.02 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD22 | 11 | 0.02 |
| (1,4356) | 1:A:4:PHE:HE1 | 1:A:59:LEU:HD23 | 11 | 0.02 |
| (1,4351) | 1:B:4:PHE:HD1 | 1:B:5:LEU:H | 1 | 0.02 |
| (1,4351) | 1:B:4:PHE:HD2 | 1:B:5:LEU:H | 1 | 0.02 |
| (1,4351) | 1:B:4:PHE:HD1 | 1:B:5:LEU:H | 16 | 0.02 |
| (1,4351) | 1:B:4:PHE:HD2 | 1:B:5:LEU:H | 16 | 0.02 |
| (1,4351) | 1:B:4:PHE:HD1 | 1:B:5:LEU:H | 18 | 0.02 |
| (1,4351) | 1:B:4:PHE:HD2 | 1:B:5:LEU:H | 18 | 0.02 |
| (1,4350) | 1:A:4:PHE:HD1 | 1:A:5:LEU:H | 1 | 0.02 |
| (1,4350) | 1:A:4:PHE:HD2 | 1:A:5:LEU:H | 1 | 0.02 |
| (1,4350) | 1:A:4:PHE:HD1 | 1:A:5:LEU:H | 3 | 0.02 |
| (1,4350) | 1:A:4:PHE:HD2 | 1:A:5:LEU:H | 3 | 0.02 |
| (1,4350) | 1:A:4:PHE:HD1 | 1:A:5:LEU:H | 7 | 0.02 |
| (1,4350) | 1:A:4:PHE:HD2 | 1:A:5:LEU:H | 7 | 0.02 |
| (1,4350) | 1:A:4:PHE:HD1 | 1:A:5:LEU:H | 12 | 0.02 |
| (1,4350) | 1:A:4:PHE:HD2 | 1:A:5:LEU:H | 12 | 0.02 |
| (1,4350) | 1:A:4:PHE:HD1 | 1:A:5:LEU:H | 17 | 0.02 |
| (1,4350) | 1:A:4:PHE:HD2 | 1:A:5:LEU:H | 17 | 0.02 |
| (1,4344) | 1:A:4:PHE:HD1 | 1:A:54:LYS:HA | 5 | 0.02 |
| (1,4344) | 1:A:4:PHE:HD2 | 1:A:54:LYS:HA | 5 | 0.02 |
| (1,4339) | 1:B:4:PHE:HD1 | 1:B:59:LEU:HD21 | 15 | 0.02 |
| (1,4339) | 1:B:4:PHE:HD1 | 1:B:59:LEU:HD22 | 15 | 0.02 |
| (1,4339) | 1:B:4:PHE:HD1 | 1:B:59:LEU:HD23 | 15 | 0.02 |
| (1,4339) | 1:B:4:PHE:HD2 | 1:B:59:LEU:HD21 | 15 | 0.02 |
| (1,4339) | 1:B:4:PHE:HD2 | 1:B:59:LEU:HD22 | 15 | 0.02 |
| (1,4339) | 1:B:4:PHE:HD2 | 1:B:59:LEU:HD23 | 15 | 0.02 |
| (1,4339) | 1:B:4:PHE:HD1 | 1:B:59:LEU:HD21 | 18 | 0.02 |
| (1,4339) | 1:B:4:PHE:HD1 | 1:B:59:LEU:HD22 | 18 | 0.02 |
| (1,4339) | 1:B:4:PHE:HD1 | 1:B:59:LEU:HD23 | 18 | 0.02 |
| (1,4339) | 1:B:4:PHE:HD2 | 1:B:59:LEU:HD21 | 18 | 0.02 |
| (1,4339) | 1:B:4:PHE:HD2 | 1:B:59:LEU:HD22 | 18 | 0.02 |
| (1,4339) | 1:B:4:PHE:HD2 | 1:B:59:LEU:HD23 | 18 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD21 | 3 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD22 | 3 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD23 | 3 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD21 | 3 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD22 | 3 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD23 | 3 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD21 | 4 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD22 | 4 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD23 | 4 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD21 | 4 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD22 | 4 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD23 | 4 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD21 | 6 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD22 | 6 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD23 | 6 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD21 | 6 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD22 | 6 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD23 | 6 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD21 | 10 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD22 | 10 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD23 | 10 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD21 | 10 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD22 | 10 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD23 | 10 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD21 | 11 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD22 | 11 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD1 | 1:A:59:LEU:HD23 | 11 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD21 | 11 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD22 | 11 | 0.02 |
| (1,4338) | 1:A:4:PHE:HD2 | 1:A:59:LEU:HD23 | 11 | 0.02 |
| (1,4335) | 1:B:83:HIS:HA | 1:B:83:HIS:HD2 | 10 | 0.02 |
| (1,4334) | 1:A:83:HIS:HA | 1:A:83:HIS:HD2 | 5 | 0.02 |
| (1,4325) | 1:B:80:ASN:HA | 1:B:81:LEU:HG | 8 | 0.02 |
| (1,4325) | 1:B:80:ASN:HA | 1:B:81:LEU:HG | 10 | 0.02 |
| (1,4325) | 1:B:80:ASN:HA | 1:B:81:LEU:HG | 16 | 0.02 |
| (1,4324) | 1:A:80:ASN:HA | 1:A:81:LEU:HG | 7 | 0.02 |
| (1,4324) | 1:A:80:ASN:HA | 1:A:81:LEU:HG | 20 | 0.02 |
| (1,4321) | 1:B:77:ARG:HG2 | 1:B:79:SER:HA | 8 | 0.02 |
| (1,432) | 1:A:24:GLY:H | 1:A:27:SER:HG | 6 | 0.02 |
| (1,4318) | 1:A:77:ARG:HG3 | 1:A:79:SER:HA | 4 | 0.02 |
| (1,4318) | 1:A:77:ARG:HG3 | 1:A:79:SER:HA | 6 | 0.02 |
| (1,4315) | 1:B:79:SER:HA | 1:B:81:LEU:HD21 | 20 | 0.02 |
| (1,4315) | 1:B:79:SER:HA | 1:B:81:LEU:HD22 | 20 | 0.02 |
| (1,4315) | 1:B:79:SER:HA | 1:B:81:LEU:HD23 | 20 | 0.02 |
| (1,4297) | 1:B:73:PHE:HA | 1:B:73:PHE:HD1 | 3 | 0.02 |
| (1,4297) | 1:B:73:PHE:HA | 1:B:73:PHE:HD2 | 3 | 0.02 |
| (1,4296) | 1:A:73:PHE:HA | 1:A:73:PHE:HD1 | 4 | 0.02 |
| (1,4296) | 1:A:73:PHE:HA | 1:A:73:PHE:HD2 | 4 | 0.02 |
| (1,4296) | 1:A:73:PHE:HA | 1:A:73:PHE:HD1 | 6 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4296) | 1:A:73:PHE:HA | 1:A:73:PHE:HD2 | 6 | 0.02 |
| (1,4296) | 1:A:73:PHE:HA | 1:A:73:PHE:HD1 | 13 | 0.02 |
| (1,4296) | 1:A:73:PHE:HA | 1:A:73:PHE:HD2 | 13 | 0.02 |
| (1,4296) | 1:A:73:PHE:HA | 1:A:73:PHE:HD1 | 16 | 0.02 |
| (1,4296) | 1:A:73:PHE:HA | 1:A:73:PHE:HD2 | 16 | 0.02 |
| (1,4296) | 1:A:73:PHE:HA | 1:A:73:PHE:HD1 | 20 | 0.02 |
| (1,4296) | 1:A:73:PHE:HA | 1:A:73:PHE:HD2 | 20 | 0.02 |
| (1,4259) | 1:B:41:LYS:HG2 | 1:B:42:ASP:HA | 9 | 0.02 |
| (1,4259) | 1:B:41:LYS:HG3 | 1:B:42:ASP:HA | 9 | 0.02 |
| (1,4258) | 1:A:41:LYS:HG2 | 1:A:42:ASP:HA | 11 | 0.02 |
| (1,4258) | 1:A:41:LYS:HG3 | 1:A:42:ASP:HA | 11 | 0.02 |
| (1,4258) | 1:A:41:LYS:HG2 | 1:A:42:ASP:HA | 20 | 0.02 |
| (1,4258) | 1:A:41:LYS:HG3 | 1:A:42:ASP:HA | 20 | 0.02 |
| (1,4255) | 1:B:41:LYS:HA | 1:B:41:LYS:HD2 | 9 | 0.02 |
| (1,4255) | 1:B:41:LYS:HA | 1:B:41:LYS:HD3 | 9 | 0.02 |
| (1,4255) | 1:B:41:LYS:HA | 1:B:41:LYS:HD2 | 12 | 0.02 |
| (1,4255) | 1:B:41:LYS:HA | 1:B:41:LYS:HD3 | 12 | 0.02 |
| (1,4254) | 1:A:41:LYS:HA | 1:A:41:LYS:HD2 | 9 | 0.02 |
| (1,4254) | 1:A:41:LYS:HA | 1:A:41:LYS:HD3 | 9 | 0.02 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG2 | 6 | 0.02 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG3 | 6 | 0.02 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG2 | 15 | 0.02 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG3 | 15 | 0.02 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 7 | 0.02 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 7 | 0.02 |
| (1,4243) | 1:B:15:LYS:HA | 1:B:17:GLY:H | 3 | 0.02 |
| (1,4242) | 1:A:15:LYS:HA | 1:A:17:GLY:H | 8 | 0.02 |
| (1,4217) | 1:B:8:ILE:HA | 1:B:78:LEU:HB2 | 4 | 0.02 |
| (1,4217) | 1:B:8:ILE:HA | 1:B:78:LEU:HB2 | 6 | 0.02 |
| (1,4217) | 1:B:8:ILE:HA | 1:B:78:LEU:HB2 | 7 | 0.02 |
| (1,4217) | 1:B:8:ILE:HA | 1:B:78:LEU:HB2 | 16 | 0.02 |
| (1,4217) | 1:B:8:ILE:HA | 1:B:78:LEU:HB2 | 20 | 0.02 |
| (1,4216) | 1:A:8:ILE:HA | 1:A:78:LEU:HB2 | 2 | 0.02 |
| (1,4216) | 1:A:8:ILE:HA | 1:A:78:LEU:HB2 | 7 | 0.02 |
| (1,4216) | 1:A:8:ILE:HA | 1:A:78:LEU:HB2 | 9 | 0.02 |
| (1,4216) | 1:A:8:ILE:HA | 1:A:78:LEU:HB2 | 10 | 0.02 |
| (1,4216) | 1:A:8:ILE:HA | 1:A:78:LEU:HB2 | 12 | 0.02 |
| (1,4216) | 1:A:8:ILE:HA | 1:A:78:LEU:HB2 | 17 | 0.02 |
| (1,4216) | 1:A:8:ILE:HA | 1:A:78:LEU:HB2 | 19 | 0.02 |
| (1,4198) | 1:A:82:GLU:H | 1:A:83:HIS:HB3 | 5 | 0.02 |
| (1,4198) | 1:A:82:GLU:H | 1:A:83:HIS:HB3 | 16 | 0.02 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD11 | 10 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD12 | 10 | 0.02 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD13 | 10 | 0.02 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD11 | 10 | 0.02 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD12 | 10 | 0.02 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD13 | 10 | 0.02 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD11 | 10 | 0.02 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD12 | 10 | 0.02 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD13 | 10 | 0.02 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD11 | 18 | 0.02 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD12 | 18 | 0.02 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD13 | 18 | 0.02 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD11 | 18 | 0.02 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD12 | 18 | 0.02 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD13 | 18 | 0.02 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD11 | 18 | 0.02 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD12 | 18 | 0.02 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD13 | 18 | 0.02 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD11 | 3 | 0.02 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD12 | 3 | 0.02 |
| (1,4188) | 1:A:5:LEU:HD11 | 1:A:81:LEU:HD13 | 3 | 0.02 |
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD11 | 3 | 0.02 |
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD12 | 3 | 0.02 |
| (1,4188) | 1:A:5:LEU:HD12 | 1:A:81:LEU:HD13 | 3 | 0.02 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD11 | 3 | 0.02 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD12 | 3 | 0.02 |
| (1,4188) | 1:A:5:LEU:HD13 | 1:A:81:LEU:HD13 | 3 | 0.02 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG21 | 17 | 0.02 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG22 | 17 | 0.02 |
| (1,4173) | 1:B:73:PHE:HB3 | 1:B:75:VAL:HG23 | 17 | 0.02 |
| (1,4169) | 1:B:44:ILE:HG21 | 1:B:73:PHE:HB3 | 17 | 0.02 |
| (1,4169) | 1:B:44:ILE:HG22 | 1:B:73:PHE:HB3 | 17 | 0.02 |
| (1,4169) | 1:B:44:ILE:HG23 | 1:B:73:PHE:HB3 | 17 | 0.02 |
| (1,4168) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HB3 | 20 | 0.02 |
| (1,4168) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HB3 | 20 | 0.02 |
| (1,4168) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HB3 | 20 | 0.02 |
| (1,4147) | 1:B:61:THR:HG21 | 1:B:65:LYS:HB3 | 6 | 0.02 |
| (1,4147) | 1:B:61:THR:HG22 | 1:B:65:LYS:HB3 | 6 | 0.02 |
| (1,4147) | 1:B:61:THR:HG23 | 1:B:65:LYS:HB3 | 6 | 0.02 |
| (1,4147) | 1:B:61:THR:HG21 | 1:B:65:LYS:HB3 | 16 | 0.02 |
| (1,4147) | 1:B:61:THR:HG22 | 1:B:65:LYS:HB3 | 16 | 0.02 |
| (1,4147) | 1:B:61:THR:HG23 | 1:B:65:LYS:HB3 | 16 | 0.02 |
| (1,4123) | 1:B:23:THR:H | 1:B:26:ILE:HD11 | 4 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4123) | 1:B:23:THR:H | 1:B:26:ILE:HD12 | 4 | 0.02 |
| (1,4123) | 1:B:23:THR:H | 1:B:26:ILE:HD13 | 4 | 0.02 |
| (1,4115) | 1:A:18:MET:HA | 1:A:21:GLN:HB2 | 10 | 0.02 |
| (1,4115) | 1:A:18:MET:HA | 1:A:21:GLN:HB2 | 17 | 0.02 |
| (1,4087) | 1:B:82:GLU:H | 1:B:82:GLU:HG3 | 10 | 0.02 |
| (1,4080) | 1:A:82:GLU:HG2 | 1:A:83:HIS:HA | 9 | 0.02 |
| (1,4075) | 1:B:82:GLU:HA | 1:B:83:HIS:HB2 | 11 | 0.02 |
| (1,4073) | 1:B:8:ILE:H | 1:B:81:LEU:HD21 | 3 | 0.02 |
| (1,4073) | 1:B:8:ILE:H | 1:B:81:LEU:HD22 | 3 | 0.02 |
| (1,4073) | 1:B:8:ILE:H | 1:B:81:LEU:HD23 | 3 | 0.02 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD21 | 8 | 0.02 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD22 | 8 | 0.02 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD23 | 8 | 0.02 |
| (1,4059) | 1:B:50:MET:HG3 | 1:B:81:LEU:HD21 | 8 | 0.02 |
| (1,4059) | 1:B:50:MET:HG3 | 1:B:81:LEU:HD22 | 8 | 0.02 |
| (1,4059) | 1:B:50:MET:HG3 | 1:B:81:LEU:HD23 | 8 | 0.02 |
| (1,4039) | 1:B:50:MET:HG3 | 1:B:81:LEU:HD11 | 17 | 0.02 |
| (1,4039) | 1:B:50:MET:HG3 | 1:B:81:LEU:HD12 | 17 | 0.02 |
| (1,4039) | 1:B:50:MET:HG3 | 1:B:81:LEU:HD13 | 17 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD21 | 5 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD22 | 5 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD23 | 5 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD21 | 5 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD22 | 5 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD23 | 5 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD21 | 6 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD22 | 6 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD23 | 6 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD21 | 6 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD22 | 6 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD23 | 6 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD21 | 19 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD22 | 19 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD23 | 19 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD21 | 19 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD22 | 19 | 0.02 |
| (1,4001) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD23 | 19 | 0.02 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD21 | 4 | 0.02 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD22 | 4 | 0.02 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD23 | 4 | 0.02 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD21 | 4 | 0.02 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD22 | 4 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD23 | 4 | 0.02 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD21 | 13 | 0.02 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD22 | 13 | 0.02 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD23 | 13 | 0.02 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD21 | 13 | 0.02 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD22 | 13 | 0.02 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD23 | 13 | 0.02 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD21 | 16 | 0.02 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD22 | 16 | 0.02 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD23 | 16 | 0.02 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD21 | 16 | 0.02 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD22 | 16 | 0.02 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD23 | 16 | 0.02 |
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD21 | 12 | 0.02 |
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD22 | 12 | 0.02 |
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD23 | 12 | 0.02 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD21 | 12 | 0.02 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD22 | 12 | 0.02 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD23 | 12 | 0.02 |
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD21 | 17 | 0.02 |
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD22 | 17 | 0.02 |
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD23 | 17 | 0.02 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD21 | 17 | 0.02 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD22 | 17 | 0.02 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD23 | 17 | 0.02 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD11 | 6 | 0.02 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD12 | 6 | 0.02 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD13 | 6 | 0.02 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD11 | 9 | 0.02 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD12 | 9 | 0.02 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD13 | 9 | 0.02 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD11 | 12 | 0.02 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD12 | 12 | 0.02 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD13 | 12 | 0.02 |
| (1,3986) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD11 | 12 | 0.02 |
| (1,3986) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD12 | 12 | 0.02 |
| (1,3986) | 1:A:48:ASN:HD21 | 1:A:78:LEU:HD13 | 12 | 0.02 |
| (1,3975) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HD11 | 15 | 0.02 |
| (1,3975) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HD12 | 15 | 0.02 |
| (1,3975) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HD13 | 15 | 0.02 |
| (1,397) | 1:B:22:ILE:H | 1:B:23:THR:HG1 | 2 | 0.02 |
| (1,397) | 1:B:22:ILE:H | 1:B:23:THR:HG1 | 4 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,397) | 1:B:22:ILE:H | 1:B:23:THR:HG1 | 5 | 0.02 |
| (1,397) | 1:B:22:ILE:H | 1:B:23:THR:HG1 | 6 | 0.02 |
| (1,397) | 1:B:22:ILE:H | 1:B:23:THR:HG1 | 12 | 0.02 |
| (1,397) | 1:B:22:ILE:H | 1:B:23:THR:HG1 | 13 | 0.02 |
| (1,397) | 1:B:22:ILE:H | 1:B:23:THR:HG1 | 19 | 0.02 |
| (1,396) | 1:A:22:ILE:H | 1:A:23:THR:HG1 | 2 | 0.02 |
| (1,396) | 1:A:22:ILE:H | 1:A:23:THR:HG1 | 18 | 0.02 |
| (1,3953) | 1:B:78:LEU:HB2 | 1:B:80:ASN:H | 12 | 0.02 |
| (1,3952) | 1:A:78:LEU:HB2 | 1:A:80:ASN:H | 1 | 0.02 |
| (1,3952) | 1:A:78:LEU:HB2 | 1:A:80:ASN:H | 5 | 0.02 |
| (1,3945) | 1:B:9:ARG:H | 1:B:78:LEU:HB3 | 10 | 0.02 |
| (1,3931) | 1:B:77:ARG:HD2 | 1:B:78:LEU:H | 19 | 0.02 |
| (1,3931) | 1:B:77:ARG:HD3 | 1:B:78:LEU:H | 19 | 0.02 |
| (1,3927) | 1:B:4:PHE:HZ | 1:B:77:ARG:HD2 | 18 | 0.02 |
| (1,3927) | 1:B:4:PHE:HZ | 1:B:77:ARG:HD3 | 18 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HD2 | 7 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HD3 | 7 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HD2 | 7 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HD3 | 7 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HD2 | 7 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HD3 | 7 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HD2 | 8 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HD3 | 8 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HD2 | 8 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HD3 | 8 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HD2 | 8 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HD3 | 8 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HD2 | 19 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB1 | 1:B:77:ARG:HD3 | 19 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HD2 | 19 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB2 | 1:B:77:ARG:HD3 | 19 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HD2 | 19 | 0.02 |
| (1,3921) | 1:B:6:ALA:HB3 | 1:B:77:ARG:HD3 | 19 | 0.02 |
| (1,3920) | 1:A:6:ALA:HB1 | 1:A:77:ARG:HD2 | 18 | 0.02 |
| (1,3920) | 1:A:6:ALA:HB1 | 1:A:77:ARG:HD3 | 18 | 0.02 |
| (1,3920) | 1:A:6:ALA:HB2 | 1:A:77:ARG:HD2 | 18 | 0.02 |
| (1,3920) | 1:A:6:ALA:HB2 | 1:A:77:ARG:HD3 | 18 | 0.02 |
| (1,3920) | 1:A:6:ALA:HB3 | 1:A:77:ARG:HD2 | 18 | 0.02 |
| (1,3920) | 1:A:6:ALA:HB3 | 1:A:77:ARG:HD3 | 18 | 0.02 |
| (1,3918) | 1:A:59:LEU:HD21 | 1:A:77:ARG:HD2 | 10 | 0.02 |
| (1,3918) | 1:A:59:LEU:HD21 | 1:A:77:ARG:HD3 | 10 | 0.02 |
| (1,3918) | 1:A:59:LEU:HD22 | 1:A:77:ARG:HD2 | 10 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3918) | 1:A:59:LEU:HD22 | 1:A:77:ARG:HD3 | 10 | 0.02 |
| (1,3918) | 1:A:59:LEU:HD23 | 1:A:77:ARG:HD2 | 10 | 0.02 |
| (1,3918) | 1:A:59:LEU:HD23 | 1:A:77:ARG:HD3 | 10 | 0.02 |
| (1,3917) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HD2 | 7 | 0.02 |
| (1,3917) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HD3 | 7 | 0.02 |
| (1,3917) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HD2 | 7 | 0.02 |
| (1,3917) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HD3 | 7 | 0.02 |
| (1,3917) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HD2 | 7 | 0.02 |
| (1,3917) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HD3 | 7 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HD2 | 6 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HD3 | 6 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HD2 | 6 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HD3 | 6 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HD2 | 6 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HD3 | 6 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HD2 | 12 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HD3 | 12 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HD2 | 12 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HD3 | 12 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HD2 | 12 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HD3 | 12 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HD2 | 16 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HD3 | 16 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HD2 | 16 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HD3 | 16 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HD2 | 16 | 0.02 |
| (1,3916) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HD3 | 16 | 0.02 |
| (1,3897) | 1:B:74:THR:HA | 1:B:76:GLU:HG2 | 15 | 0.02 |
| (1,3897) | 1:B:74:THR:HA | 1:B:76:GLU:HG3 | 15 | 0.02 |
| (1,3895) | 1:B:9:ARG:HB2 | 1:B:76:GLU:HG2 | 1 | 0.02 |
| (1,3895) | 1:B:9:ARG:HB2 | 1:B:76:GLU:HG3 | 1 | 0.02 |
| (1,3895) | 1:B:9:ARG:HB3 | 1:B:76:GLU:HG2 | 1 | 0.02 |
| (1,3895) | 1:B:9:ARG:HB3 | 1:B:76:GLU:HG3 | 1 | 0.02 |
| (1,3895) | 1:B:9:ARG:HB2 | 1:B:76:GLU:HG2 | 15 | 0.02 |
| (1,3895) | 1:B:9:ARG:HB2 | 1:B:76:GLU:HG3 | 15 | 0.02 |
| (1,3895) | 1:B:9:ARG:HB3 | 1:B:76:GLU:HG2 | 15 | 0.02 |
| (1,3895) | 1:B:9:ARG:HB3 | 1:B:76:GLU:HG3 | 15 | 0.02 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 8 | 0.02 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 8 | 0.02 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 8 | 0.02 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG21 | 17 | 0.02 |
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG22 | 17 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3864) | 1:B:11:VAL:H | 1:B:74:THR:HG23 | 17 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG21 | 6 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG22 | 6 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG23 | 6 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG21 | 6 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG22 | 6 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG23 | 6 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG21 | 9 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG22 | 9 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG23 | 9 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG21 | 9 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG22 | 9 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG23 | 9 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG21 | 11 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG22 | 11 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG23 | 11 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG21 | 11 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG22 | 11 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG23 | 11 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG21 | 18 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG22 | 18 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG23 | 18 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG21 | 18 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG22 | 18 | 0.02 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG23 | 18 | 0.02 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG21 | 20 | 0.02 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG22 | 20 | 0.02 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG23 | 20 | 0.02 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG21 | 20 | 0.02 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG22 | 20 | 0.02 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG23 | 20 | 0.02 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG21 | 12 | 0.02 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG22 | 12 | 0.02 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG23 | 12 | 0.02 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG21 | 1 | 0.02 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG22 | 1 | 0.02 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG23 | 1 | 0.02 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG21 | 6 | 0.02 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG22 | 6 | 0.02 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG23 | 6 | 0.02 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG21 | 13 | 0.02 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG22 | 13 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG23 | 13 | 0.02 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG21 | 17 | 0.02 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG22 | 17 | 0.02 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG23 | 17 | 0.02 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG21 | 19 | 0.02 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG22 | 19 | 0.02 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG23 | 19 | 0.02 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG21 | 20 | 0.02 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG22 | 20 | 0.02 |
| (1,3851) | 1:A:73:PHE:HB3 | 1:A:74:THR:HG23 | 20 | 0.02 |
| (1,3846) | 1:B:10:ILE:HA | 1:B:74:THR:HB | 2 | 0.02 |
| (1,3846) | 1:B:10:ILE:HA | 1:B:74:THR:HB | 17 | 0.02 |
| (1,3813) | 1:A:66:LEU:HA | 1:A:72:VAL:HG21 | 7 | 0.02 |
| (1,3813) | 1:A:66:LEU:HA | 1:A:72:VAL:HG22 | 7 | 0.02 |
| (1,3813) | 1:A:66:LEU:HA | 1:A:72:VAL:HG23 | 7 | 0.02 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG11 | 12 | 0.02 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG12 | 12 | 0.02 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG13 | 12 | 0.02 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG11 | 18 | 0.02 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG12 | 18 | 0.02 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG13 | 18 | 0.02 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG11 | 4 | 0.02 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG12 | 4 | 0.02 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG13 | 4 | 0.02 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG11 | 14 | 0.02 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG12 | 14 | 0.02 |
| (1,3789) | 1:A:67:ARG:HA | 1:A:72:VAL:HG13 | 14 | 0.02 |
| (1,3756) | 1:B:69:VAL:H | 1:B:70:GLN:HB2 | 6 | 0.02 |
| (1,3756) | 1:B:69:VAL:H | 1:B:70:GLN:HB3 | 6 | 0.02 |
| (1,3747) | 1:A:69:VAL:HG11 | 1:A:70:GLN:HB2 | 12 | 0.02 |
| (1,3747) | 1:A:69:VAL:HG11 | 1:A:70:GLN:HB3 | 12 | 0.02 |
| (1,3747) | 1:A:69:VAL:HG12 | 1:A:70:GLN:HB2 | 12 | 0.02 |
| (1,3747) | 1:A:69:VAL:HG12 | 1:A:70:GLN:HB3 | 12 | 0.02 |
| (1,3747) | 1:A:69:VAL:HG13 | 1:A:70:GLN:HB2 | 12 | 0.02 |
| (1,3747) | 1:A:69:VAL:HG13 | 1:A:70:GLN:HB3 | 12 | 0.02 |
| (1,3736) | 1:B:66:LEU:HA | 1:B:69:VAL:HB | 12 | 0.02 |
| (1,3735) | 1:A:66:LEU:HA | 1:A:69:VAL:HB | 5 | 0.02 |
| (1,3735) | 1:A:66:LEU:HA | 1:A:69:VAL:HB | 9 | 0.02 |
| (1,3735) | 1:A:66:LEU:HA | 1:A:69:VAL:HB | 13 | 0.02 |
| (1,3735) | 1:A:66:LEU:HA | 1:A:69:VAL:HB | 14 | 0.02 |
| (1,3734) | 1:B:20:ASN:HA | 1:B:22:ILE:HB | 10 | 0.02 |
| (1,3734) | 1:B:20:ASN:HA | 1:B:22:ILE:HB | 11 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|---------|---------|-------|---------------|
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 1 | 0.02 |
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 6 | 0.02 |
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 15 | 0.02 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG11 | 8 | 0.02 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG12 | 8 | 0.02 |
| (1,3712) | 1:B:15:LYS:HD2 | 1:B:69:VAL:HG13 | 8 | 0.02 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG11 | 8 | 0.02 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG12 | 8 | 0.02 |
| (1,3712) | 1:B:15:LYS:HD3 | 1:B:69:VAL:HG13 | 8 | 0.02 |
| (1,3706) | 1:B:68:LYS:HB3 | 1:B:69:VAL:HA | 16 | 0.02 |
| (1,3705) | 1:A:68:LYS:HB3 | 1:A:69:VAL:HA | 2 | 0.02 |
| (1,3702) | 1:B:15:LYS:HE2 | 1:B:18:MET:H | 1 | 0.02 |
| (1,3702) | 1:B:15:LYS:HE3 | 1:B:18:MET:H | 1 | 0.02 |
| (1,3702) | 1:B:15:LYS:HE2 | 1:B:18:MET:H | 10 | 0.02 |
| (1,3702) | 1:B:15:LYS:HE3 | 1:B:18:MET:H | 10 | 0.02 |
| (1,3701) | 1:A:15:LYS:HE2 | 1:A:18:MET:H | 8 | 0.02 |
| (1,3701) | 1:A:15:LYS:HE3 | 1:A:18:MET:H | 8 | 0.02 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE2 | 12 | 0.02 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE3 | 12 | 0.02 |
| (1,3692) | 1:B:68:LYS:HA | 1:B:68:LYS:HE2 | 4 | 0.02 |
| (1,3692) | 1:B:68:LYS:HA | 1:B:68:LYS:HE3 | 4 | 0.02 |
| (1,3690) | 1:A:64:ASP:H | 1:A:65:LYS:HG2 | 5 | 0.02 |
| (1,3653) | 1:B:67:ARG:HD2 | 1:B:75:VAL:HG11 | 6 | 0.02 |
| (1,3653) | 1:B:67:ARG:HD2 | 1:B:75:VAL:HG12 | 6 | 0.02 |
| (1,3653) | 1:B:67:ARG:HD2 | 1:B:75:VAL:HG13 | 6 | 0.02 |
| (1,3653) | 1:B:67:ARG:HD3 | 1:B:75:VAL:HG11 | 6 | 0.02 |
| (1,3653) | 1:B:67:ARG:HD3 | 1:B:75:VAL:HG12 | 6 | 0.02 |
| (1,3653) | 1:B:67:ARG:HD3 | 1:B:75:VAL:HG13 | 6 | 0.02 |
| (1,3652) | 1:A:67:ARG:HD2 | 1:A:75:VAL:HG11 | 13 | 0.02 |
| (1,3652) | 1:A:67:ARG:HD2 | 1:A:75:VAL:HG12 | 13 | 0.02 |
| (1,3652) | 1:A:67:ARG:HD2 | 1:A:75:VAL:HG13 | 13 | 0.02 |
| (1,3652) | 1:A:67:ARG:HD3 | 1:A:75:VAL:HG11 | 13 | 0.02 |
| (1,3652) | 1:A:67:ARG:HD3 | 1:A:75:VAL:HG12 | 13 | 0.02 |
| (1,3652) | 1:A:67:ARG:HD3 | 1:A:75:VAL:HG13 | 13 | 0.02 |
| (1,365) | 1:B:18:MET:HE1 | 1:B:21:GLN:HE22 | 14 | 0.02 |
| (1,365) | 1:B:18:MET:HE2 | 1:B:21:GLN:HE22 | 14 | 0.02 |
| (1,365) | 1:B:18:MET:HE3 | 1:B:21:GLN:HE22 | 14 | 0.02 |
| (1,3648) | 1:A:64:ASP:HA | 1:A:67:ARG:HG3 | 17 | 0.02 |
| (1,364) | 1:A:18:MET:HE1 | 1:A:21:GLN:HE22 | 20 | 0.02 |
| (1,364) | 1:A:18:MET:HE2 | 1:A:21:GLN:HE22 | 20 | 0.02 |
| (1,364) | 1:A:18:MET:HE3 | 1:A:21:GLN:HE22 | 20 | 0.02 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 14 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 14 | 0.02 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 14 | 0.02 |
| (1,3571) | 1:A:62:LEU:HD11 | 1:A:65:LYS:HB3 | 2 | 0.02 |
| (1,3571) | 1:A:62:LEU:HD12 | 1:A:65:LYS:HB3 | 2 | 0.02 |
| (1,3571) | 1:A:62:LEU:HD13 | 1:A:65:LYS:HB3 | 2 | 0.02 |
| (1,3546) | 1:B:61:THR:HA | 1:B:64:ASP:HB3 | 20 | 0.02 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB2 | 1 | 0.02 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB3 | 1 | 0.02 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB2 | 7 | 0.02 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB3 | 7 | 0.02 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB2 | 16 | 0.02 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB3 | 16 | 0.02 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB2 | 15 | 0.02 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB3 | 15 | 0.02 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB2 | 19 | 0.02 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB3 | 19 | 0.02 |
| (1,3537) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HB2 | 8 | 0.02 |
| (1,3537) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HB2 | 13 | 0.02 |
| (1,3537) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HB2 | 17 | 0.02 |
| (1,3537) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HB2 | 18 | 0.02 |
| (1,3536) | 1:A:64:ASP:HB2 | 1:A:65:LYS:HB2 | 11 | 0.02 |
| (1,3536) | 1:A:64:ASP:HB2 | 1:A:65:LYS:HB2 | 20 | 0.02 |
| (1,3530) | 1:B:9:ARG:H | 1:B:63:MET:HE1 | 20 | 0.02 |
| (1,3530) | 1:B:9:ARG:H | 1:B:63:MET:HE2 | 20 | 0.02 |
| (1,3530) | 1:B:9:ARG:H | 1:B:63:MET:HE3 | 20 | 0.02 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE1 | 4 | 0.02 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE2 | 4 | 0.02 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE3 | 4 | 0.02 |
| (1,3528) | 1:B:63:MET:HE1 | 1:B:77:ARG:H | 12 | 0.02 |
| (1,3528) | 1:B:63:MET:HE2 | 1:B:77:ARG:H | 12 | 0.02 |
| (1,3528) | 1:B:63:MET:HE3 | 1:B:77:ARG:H | 12 | 0.02 |
| (1,3528) | 1:B:63:MET:HE1 | 1:B:77:ARG:H | 15 | 0.02 |
| (1,3528) | 1:B:63:MET:HE2 | 1:B:77:ARG:H | 15 | 0.02 |
| (1,3528) | 1:B:63:MET:HE3 | 1:B:77:ARG:H | 15 | 0.02 |
| (1,3528) | 1:B:63:MET:HE1 | 1:B:77:ARG:H | 19 | 0.02 |
| (1,3528) | 1:B:63:MET:HE2 | 1:B:77:ARG:H | 19 | 0.02 |
| (1,3528) | 1:B:63:MET:HE3 | 1:B:77:ARG:H | 19 | 0.02 |
| (1,3527) | 1:A:63:MET:HE1 | 1:A:77:ARG:H | 11 | 0.02 |
| (1,3527) | 1:A:63:MET:HE2 | 1:A:77:ARG:H | 11 | 0.02 |
| (1,3527) | 1:A:63:MET:HE3 | 1:A:77:ARG:H | 11 | 0.02 |
| (1,3527) | 1:A:63:MET:HE1 | 1:A:77:ARG:H | 17 | 0.02 |
| (1,3527) | 1:A:63:MET:HE2 | 1:A:77:ARG:H | 17 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3527) | 1:A:63:MET:HE3 | 1:A:77:ARG:H | 17 | 0.02 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 15 | 0.02 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 15 | 0.02 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 15 | 0.02 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 16 | 0.02 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 16 | 0.02 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 16 | 0.02 |
| (1,3519) | 1:A:63:MET:HE1 | 1:A:76:GLU:HA | 13 | 0.02 |
| (1,3519) | 1:A:63:MET:HE2 | 1:A:76:GLU:HA | 13 | 0.02 |
| (1,3519) | 1:A:63:MET:HE3 | 1:A:76:GLU:HA | 13 | 0.02 |
| (1,3460) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:HD11 | 7 | 0.02 |
| (1,3460) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:HD12 | 7 | 0.02 |
| (1,3460) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:HD13 | 7 | 0.02 |
| (1,3448) | 1:B:62:LEU:HD11 | 1:B:63:MET:HA | 3 | 0.02 |
| (1,3448) | 1:B:62:LEU:HD12 | 1:B:63:MET:HA | 3 | 0.02 |
| (1,3448) | 1:B:62:LEU:HD13 | 1:B:63:MET:HA | 3 | 0.02 |
| (1,3440) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD11 | 3 | 0.02 |
| (1,3440) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD12 | 3 | 0.02 |
| (1,3440) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD13 | 3 | 0.02 |
| (1,3440) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD11 | 18 | 0.02 |
| (1,3440) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD12 | 18 | 0.02 |
| (1,3440) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD13 | 18 | 0.02 |
| (1,3439) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD11 | 12 | 0.02 |
| (1,3439) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD12 | 12 | 0.02 |
| (1,3439) | 1:A:58:LYS:HE2 | 1:A:62:LEU:HD13 | 12 | 0.02 |
| (1,3436) | 1:B:62:LEU:HD11 | 1:B:66:LEU:HG | 11 | 0.02 |
| (1,3436) | 1:B:62:LEU:HD12 | 1:B:66:LEU:HG | 11 | 0.02 |
| (1,3436) | 1:B:62:LEU:HD13 | 1:B:66:LEU:HG | 11 | 0.02 |
| (1,3435) | 1:A:62:LEU:HD11 | 1:A:66:LEU:HG | 4 | 0.02 |
| (1,3435) | 1:A:62:LEU:HD12 | 1:A:66:LEU:HG | 4 | 0.02 |
| (1,3435) | 1:A:62:LEU:HD13 | 1:A:66:LEU:HG | 4 | 0.02 |
| (1,3433) | 1:A:58:LYS:HG3 | 1:A:62:LEU:HD11 | 6 | 0.02 |
| (1,3433) | 1:A:58:LYS:HG3 | 1:A:62:LEU:HD12 | 6 | 0.02 |
| (1,3433) | 1:A:58:LYS:HG3 | 1:A:62:LEU:HD13 | 6 | 0.02 |
| (1,3387) | 1:B:61:THR:HG21 | 1:B:65:LYS:HE2 | 3 | 0.02 |
| (1,3387) | 1:B:61:THR:HG21 | 1:B:65:LYS:HE3 | 3 | 0.02 |
| (1,3387) | 1:B:61:THR:HG22 | 1:B:65:LYS:HE2 | 3 | 0.02 |
| (1,3387) | 1:B:61:THR:HG22 | 1:B:65:LYS:HE3 | 3 | 0.02 |
| (1,3387) | 1:B:61:THR:HG23 | 1:B:65:LYS:HE2 | 3 | 0.02 |
| (1,3387) | 1:B:61:THR:HG23 | 1:B:65:LYS:HE3 | 3 | 0.02 |
| (1,3387) | 1:B:61:THR:HG21 | 1:B:65:LYS:HE2 | 10 | 0.02 |
| (1,3387) | 1:B:61:THR:HG21 | 1:B:65:LYS:HE3 | 10 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3387) | 1:B:61:THR:HG22 | 1:B:65:LYS:HE2 | 10 | 0.02 |
| (1,3387) | 1:B:61:THR:HG22 | 1:B:65:LYS:HE3 | 10 | 0.02 |
| (1,3387) | 1:B:61:THR:HG23 | 1:B:65:LYS:HE2 | 10 | 0.02 |
| (1,3387) | 1:B:61:THR:HG23 | 1:B:65:LYS:HE3 | 10 | 0.02 |
| (1,3364) | 1:A:61:THR:HA | 1:A:64:ASP:HB2 | 18 | 0.02 |
| (1,3354) | 1:A:60:THR:HG21 | 1:A:63:MET:HG3 | 4 | 0.02 |
| (1,3354) | 1:A:60:THR:HG22 | 1:A:63:MET:HG3 | 4 | 0.02 |
| (1,3354) | 1:A:60:THR:HG23 | 1:A:63:MET:HG3 | 4 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD21 | 4 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD22 | 4 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD23 | 4 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD21 | 4 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD22 | 4 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD23 | 4 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD21 | 4 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD22 | 4 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD23 | 4 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD21 | 13 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD22 | 13 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD23 | 13 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD21 | 13 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD22 | 13 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD23 | 13 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD21 | 13 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD22 | 13 | 0.02 |
| (1,3323) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD23 | 13 | 0.02 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD21 | 9 | 0.02 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD22 | 9 | 0.02 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD23 | 9 | 0.02 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD21 | 9 | 0.02 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD22 | 9 | 0.02 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD23 | 9 | 0.02 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD21 | 9 | 0.02 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD22 | 9 | 0.02 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD23 | 9 | 0.02 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD21 | 15 | 0.02 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD22 | 15 | 0.02 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD23 | 15 | 0.02 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD21 | 15 | 0.02 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD22 | 15 | 0.02 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD23 | 15 | 0.02 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD21 | 15 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD22 | 15 | 0.02 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD23 | 15 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD11 | 13 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD12 | 13 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD13 | 13 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD11 | 13 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD12 | 13 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD13 | 13 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD11 | 13 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD12 | 13 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD13 | 13 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD11 | 18 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD12 | 18 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD13 | 18 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD11 | 18 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD12 | 18 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD13 | 18 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD11 | 18 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD12 | 18 | 0.02 |
| (1,3311) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD13 | 18 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD11 | 2 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD12 | 2 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD13 | 2 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD11 | 2 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD12 | 2 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD13 | 2 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD11 | 2 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD12 | 2 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD13 | 2 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD11 | 7 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD12 | 7 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD13 | 7 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD11 | 7 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD12 | 7 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD13 | 7 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD11 | 7 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD12 | 7 | 0.02 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD13 | 7 | 0.02 |
| (1,3284) | 1:A:58:LYS:H | 1:A:58:LYS:HD2 | 6 | 0.02 |
| (1,3284) | 1:A:58:LYS:H | 1:A:58:LYS:HD3 | 6 | 0.02 |
| (1,3275) | 1:B:30:ASP:HB2 | 1:B:58:LYS:HD2 | 9 | 0.02 |
| (1,3275) | 1:B:30:ASP:HB2 | 1:B:58:LYS:HD3 | 9 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3275) | 1:B:30:ASP:HB3 | 1:B:58:LYS:HD2 | 9 | 0.02 |
| (1,3275) | 1:B:30:ASP:HB3 | 1:B:58:LYS:HD3 | 9 | 0.02 |
| (1,3274) | 1:A:30:ASP:HB2 | 1:A:58:LYS:HD2 | 18 | 0.02 |
| (1,3274) | 1:A:30:ASP:HB2 | 1:A:58:LYS:HD3 | 18 | 0.02 |
| (1,3274) | 1:A:30:ASP:HB3 | 1:A:58:LYS:HD2 | 18 | 0.02 |
| (1,3274) | 1:A:30:ASP:HB3 | 1:A:58:LYS:HD3 | 18 | 0.02 |
| (1,3261) | 1:B:58:LYS:HG2 | 1:B:62:LEU:HD11 | 11 | 0.02 |
| (1,3261) | 1:B:58:LYS:HG2 | 1:B:62:LEU:HD12 | 11 | 0.02 |
| (1,3261) | 1:B:58:LYS:HG2 | 1:B:62:LEU:HD13 | 11 | 0.02 |
| (1,3260) | 1:A:58:LYS:HG2 | 1:A:62:LEU:HD11 | 20 | 0.02 |
| (1,3260) | 1:A:58:LYS:HG2 | 1:A:62:LEU:HD12 | 20 | 0.02 |
| (1,3260) | 1:A:58:LYS:HG2 | 1:A:62:LEU:HD13 | 20 | 0.02 |
| (1,3249) | 1:B:31:THR:HG21 | 1:B:58:LYS:HG3 | 2 | 0.02 |
| (1,3249) | 1:B:31:THR:HG22 | 1:B:58:LYS:HG3 | 2 | 0.02 |
| (1,3249) | 1:B:31:THR:HG23 | 1:B:58:LYS:HG3 | 2 | 0.02 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG21 | 11 | 0.02 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG22 | 11 | 0.02 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG23 | 11 | 0.02 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG21 | 11 | 0.02 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG22 | 11 | 0.02 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG23 | 11 | 0.02 |
| (1,3220) | 1:A:4:PHE:HD1 | 1:A:56:THR:HG21 | 10 | 0.02 |
| (1,3220) | 1:A:4:PHE:HD1 | 1:A:56:THR:HG22 | 10 | 0.02 |
| (1,3220) | 1:A:4:PHE:HD1 | 1:A:56:THR:HG23 | 10 | 0.02 |
| (1,3220) | 1:A:4:PHE:HD2 | 1:A:56:THR:HG21 | 10 | 0.02 |
| (1,3220) | 1:A:4:PHE:HD2 | 1:A:56:THR:HG22 | 10 | 0.02 |
| (1,3220) | 1:A:4:PHE:HD2 | 1:A:56:THR:HG23 | 10 | 0.02 |
| (1,3190) | 1:A:54:LYS:H | 1:A:54:LYS:HD2 | 9 | 0.02 |
| (1,3190) | 1:A:54:LYS:H | 1:A:54:LYS:HD3 | 9 | 0.02 |
| (1,3184) | 1:A:15:LYS:HD2 | 1:A:16:ASN:HD22 | 15 | 0.02 |
| (1,3184) | 1:A:15:LYS:HD3 | 1:A:16:ASN:HD22 | 15 | 0.02 |
| (1,3182) | 1:A:54:LYS:HA | 1:A:54:LYS:HD2 | 7 | 0.02 |
| (1,3182) | 1:A:54:LYS:HA | 1:A:54:LYS:HD3 | 7 | 0.02 |
| (1,3182) | 1:A:54:LYS:HA | 1:A:54:LYS:HD2 | 12 | 0.02 |
| (1,3182) | 1:A:54:LYS:HA | 1:A:54:LYS:HD3 | 12 | 0.02 |
| (1,3132) | 1:A:5:LEU:HA | 1:A:53:VAL:HG21 | 9 | 0.02 |
| (1,3132) | 1:A:5:LEU:HA | 1:A:53:VAL:HG22 | 9 | 0.02 |
| (1,3132) | 1:A:5:LEU:HA | 1:A:53:VAL:HG23 | 9 | 0.02 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG11 | 5 | 0.02 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG12 | 5 | 0.02 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG13 | 5 | 0.02 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG11 | 3 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG12 | 3 | 0.02 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG13 | 3 | 0.02 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG11 | 15 | 0.02 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG12 | 15 | 0.02 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG13 | 15 | 0.02 |
| (1,310) | 1:A:33:ILE:HG12 | 1:B:20:ASN:HD22 | 15 | 0.02 |
| (1,3094) | 1:A:53:VAL:HG11 | 1:A:58:LYS:HZ1 | 2 | 0.02 |
| (1,3094) | 1:A:53:VAL:HG12 | 1:A:58:LYS:HZ1 | 2 | 0.02 |
| (1,3094) | 1:A:53:VAL:HG13 | 1:A:58:LYS:HZ1 | 2 | 0.02 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG11 | 6 | 0.02 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG12 | 6 | 0.02 |
| (1,3080) | 1:A:4:PHE:HB2 | 1:A:53:VAL:HG13 | 6 | 0.02 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG11 | 6 | 0.02 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG12 | 6 | 0.02 |
| (1,3080) | 1:A:4:PHE:HB3 | 1:A:53:VAL:HG13 | 6 | 0.02 |
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD11 | 16 | 0.02 |
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD12 | 16 | 0.02 |
| (1,3041) | 1:B:31:THR:H | 1:B:51:ILE:HD13 | 16 | 0.02 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD11 | 3 | 0.02 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD12 | 3 | 0.02 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD13 | 3 | 0.02 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD11 | 11 | 0.02 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD12 | 11 | 0.02 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD13 | 11 | 0.02 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD11 | 13 | 0.02 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD12 | 13 | 0.02 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD13 | 13 | 0.02 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD11 | 16 | 0.02 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD12 | 16 | 0.02 |
| (1,3037) | 1:B:29:PHE:HD1 | 1:B:51:ILE:HD13 | 16 | 0.02 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD11 | 16 | 0.02 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD12 | 16 | 0.02 |
| (1,3037) | 1:B:29:PHE:HD2 | 1:B:51:ILE:HD13 | 16 | 0.02 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD11 | 3 | 0.02 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD12 | 3 | 0.02 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD13 | 3 | 0.02 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD11 | 3 | 0.02 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD12 | 3 | 0.02 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD13 | 3 | 0.02 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD11 | 11 | 0.02 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD12 | 11 | 0.02 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD13 | 11 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD11 | 11 | 0.02 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD12 | 11 | 0.02 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD13 | 11 | 0.02 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD21 | 9 | 0.02 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD22 | 9 | 0.02 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD23 | 9 | 0.02 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD21 | 9 | 0.02 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD22 | 9 | 0.02 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD23 | 9 | 0.02 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD21 | 9 | 0.02 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD22 | 9 | 0.02 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD23 | 9 | 0.02 |
| (1,2991) | 1:A:51:ILE:HG21 | 1:B:20:ASN:HD22 | 18 | 0.02 |
| (1,2991) | 1:A:51:ILE:HG22 | 1:B:20:ASN:HD22 | 18 | 0.02 |
| (1,2991) | 1:A:51:ILE:HG23 | 1:B:20:ASN:HD22 | 18 | 0.02 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG21 | 2 | 0.02 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG22 | 2 | 0.02 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG23 | 2 | 0.02 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG21 | 4 | 0.02 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG22 | 4 | 0.02 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG23 | 4 | 0.02 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG21 | 6 | 0.02 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG22 | 6 | 0.02 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG23 | 6 | 0.02 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG21 | 11 | 0.02 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG22 | 11 | 0.02 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG23 | 11 | 0.02 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG21 | 17 | 0.02 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG22 | 17 | 0.02 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG23 | 17 | 0.02 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG21 | 1 | 0.02 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG22 | 1 | 0.02 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG23 | 1 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG21 | 2 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG22 | 2 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG23 | 2 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG21 | 3 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG22 | 3 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG23 | 3 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG21 | 4 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG22 | 4 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG23 | 4 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG21 | 5 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG22 | 5 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG23 | 5 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG21 | 10 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG22 | 10 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG23 | 10 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG21 | 15 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG22 | 15 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG23 | 15 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG21 | 16 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG22 | 16 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG23 | 16 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG21 | 18 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG22 | 18 | 0.02 |
| (1,2977) | 1:B:33:ILE:HA | 1:B:51:ILE:HG23 | 18 | 0.02 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG21 | 4 | 0.02 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG22 | 4 | 0.02 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG23 | 4 | 0.02 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG21 | 7 | 0.02 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG22 | 7 | 0.02 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG23 | 7 | 0.02 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG21 | 16 | 0.02 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG22 | 16 | 0.02 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG23 | 16 | 0.02 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG21 | 19 | 0.02 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG22 | 19 | 0.02 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG23 | 19 | 0.02 |
| (1,2971) | 1:B:8:ILE:HG21 | 1:B:62:LEU:HD11 | 4 | 0.02 |
| (1,2971) | 1:B:8:ILE:HG21 | 1:B:62:LEU:HD12 | 4 | 0.02 |
| (1,2971) | 1:B:8:ILE:HG21 | 1:B:62:LEU:HD13 | 4 | 0.02 |
| (1,2971) | 1:B:8:ILE:HG22 | 1:B:62:LEU:HD11 | 4 | 0.02 |
| (1,2971) | 1:B:8:ILE:HG22 | 1:B:62:LEU:HD12 | 4 | 0.02 |
| (1,2971) | 1:B:8:ILE:HG22 | 1:B:62:LEU:HD13 | 4 | 0.02 |
| (1,2971) | 1:B:8:ILE:HG23 | 1:B:62:LEU:HD11 | 4 | 0.02 |
| (1,2971) | 1:B:8:ILE:HG23 | 1:B:62:LEU:HD12 | 4 | 0.02 |
| (1,2971) | 1:B:8:ILE:HG23 | 1:B:62:LEU:HD13 | 4 | 0.02 |
| (1,2920) | 1:A:6:ALA:HA | 1:A:50:MET:HE1 | 1 | 0.02 |
| (1,2920) | 1:A:6:ALA:HA | 1:A:50:MET:HE2 | 1 | 0.02 |
| (1,2920) | 1:A:6:ALA:HA | 1:A:50:MET:HE3 | 1 | 0.02 |
| (1,2917) | 1:B:50:MET:HE1 | 1:B:81:LEU:HA | 9 | 0.02 |
| (1,2917) | 1:B:50:MET:HE2 | 1:B:81:LEU:HA | 9 | 0.02 |
| (1,2917) | 1:B:50:MET:HE3 | 1:B:81:LEU:HA | 9 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 9 | 0.02 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 9 | 0.02 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 9 | 0.02 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 20 | 0.02 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 20 | 0.02 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 20 | 0.02 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 2 | 0.02 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 2 | 0.02 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 2 | 0.02 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 6 | 0.02 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 6 | 0.02 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 6 | 0.02 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 7 | 0.02 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 7 | 0.02 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 7 | 0.02 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 16 | 0.02 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 16 | 0.02 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 16 | 0.02 |
| (1,2899) | 1:B:50:MET:HE1 | 1:B:81:LEU:HD21 | 8 | 0.02 |
| (1,2899) | 1:B:50:MET:HE1 | 1:B:81:LEU:HD22 | 8 | 0.02 |
| (1,2899) | 1:B:50:MET:HE1 | 1:B:81:LEU:HD23 | 8 | 0.02 |
| (1,2899) | 1:B:50:MET:HE2 | 1:B:81:LEU:HD21 | 8 | 0.02 |
| (1,2899) | 1:B:50:MET:HE2 | 1:B:81:LEU:HD22 | 8 | 0.02 |
| (1,2899) | 1:B:50:MET:HE2 | 1:B:81:LEU:HD23 | 8 | 0.02 |
| (1,2899) | 1:B:50:MET:HE3 | 1:B:81:LEU:HD21 | 8 | 0.02 |
| (1,2899) | 1:B:50:MET:HE3 | 1:B:81:LEU:HD22 | 8 | 0.02 |
| (1,2899) | 1:B:50:MET:HE3 | 1:B:81:LEU:HD23 | 8 | 0.02 |
| (1,2879) | 1:B:8:ILE:H | 1:B:50:MET:HG3 | 13 | 0.02 |
| (1,2879) | 1:B:8:ILE:H | 1:B:50:MET:HG3 | 19 | 0.02 |
| (1,2878) | 1:A:8:ILE:H | 1:A:50:MET:HG3 | 9 | 0.02 |
| (1,2878) | 1:A:8:ILE:H | 1:A:50:MET:HG3 | 19 | 0.02 |
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 1 | 0.02 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 4 | 0.02 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 11 | 0.02 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 12 | 0.02 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 13 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD11 | 1 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD12 | 1 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD13 | 1 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD11 | 1 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD12 | 1 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD13 | 1 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD11 | 1 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD12 | 1 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD13 | 1 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD11 | 3 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD12 | 3 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD13 | 3 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD11 | 3 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD12 | 3 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD13 | 3 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD11 | 3 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD12 | 3 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD13 | 3 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD11 | 13 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD12 | 13 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD13 | 13 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD11 | 13 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD12 | 13 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD13 | 13 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD11 | 13 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD12 | 13 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD13 | 13 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD11 | 14 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD12 | 14 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD13 | 14 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD11 | 14 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD12 | 14 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD13 | 14 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD11 | 14 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD12 | 14 | 0.02 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD13 | 14 | 0.02 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD11 | 6 | 0.02 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD12 | 6 | 0.02 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD13 | 6 | 0.02 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD11 | 6 | 0.02 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD12 | 6 | 0.02 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD13 | 6 | 0.02 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD11 | 6 | 0.02 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD12 | 6 | 0.02 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD13 | 6 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD21 | 2 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD22 | 2 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD23 | 2 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD21 | 2 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD22 | 2 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD23 | 2 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD21 | 2 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD22 | 2 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD23 | 2 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD21 | 7 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD22 | 7 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD23 | 7 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD21 | 7 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD22 | 7 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD23 | 7 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD21 | 7 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD22 | 7 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD23 | 7 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD21 | 8 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD22 | 8 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD23 | 8 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD21 | 8 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD22 | 8 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD23 | 8 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD21 | 8 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD22 | 8 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD23 | 8 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD21 | 13 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD22 | 13 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD23 | 13 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD21 | 13 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD22 | 13 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD23 | 13 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD21 | 13 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD22 | 13 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD23 | 13 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD21 | 16 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD22 | 16 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD23 | 16 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD21 | 16 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD22 | 16 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD23 | 16 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD21 | 16 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD22 | 16 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD23 | 16 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD21 | 20 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD22 | 20 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD23 | 20 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD21 | 20 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD22 | 20 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD23 | 20 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD21 | 20 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD22 | 20 | 0.02 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD23 | 20 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD21 | 12 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD22 | 12 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD23 | 12 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD21 | 12 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD22 | 12 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD23 | 12 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD21 | 12 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD22 | 12 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD23 | 12 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD21 | 13 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD22 | 13 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD23 | 13 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD21 | 13 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD22 | 13 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD23 | 13 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD21 | 13 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD22 | 13 | 0.02 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD23 | 13 | 0.02 |
| (1,2754) | 1:B:23:THR:HG1 | 1:B:47:CYS:HB3 | 3 | 0.02 |
| (1,2754) | 1:B:23:THR:HG1 | 1:B:47:CYS:HB3 | 9 | 0.02 |
| (1,2753) | 1:A:23:THR:HG1 | 1:A:47:CYS:HB3 | 1 | 0.02 |
| (1,2753) | 1:A:23:THR:HG1 | 1:A:47:CYS:HB3 | 5 | 0.02 |
| (1,2726) | 1:B:46:THR:HG21 | 1:B:47:CYS:H | 5 | 0.02 |
| (1,2726) | 1:B:46:THR:HG22 | 1:B:47:CYS:H | 5 | 0.02 |
| (1,2726) | 1:B:46:THR:HG23 | 1:B:47:CYS:H | 5 | 0.02 |
| (1,2726) | 1:B:46:THR:HG21 | 1:B:47:CYS:H | 8 | 0.02 |
| (1,2726) | 1:B:46:THR:HG22 | 1:B:47:CYS:H | 8 | 0.02 |
| (1,2726) | 1:B:46:THR:HG23 | 1:B:47:CYS:H | 8 | 0.02 |
| (1,2726) | 1:B:46:THR:HG21 | 1:B:47:CYS:H | 17 | 0.02 |
| (1,2726) | 1:B:46:THR:HG22 | 1:B:47:CYS:H | 17 | 0.02 |
| (1,2726) | 1:B:46:THR:HG23 | 1:B:47:CYS:H | 17 | 0.02 |
| (1,2725) | 1:A:46:THR:HG21 | 1:A:47:CYS:H | 4 | 0.02 |
| (1,2725) | 1:A:46:THR:HG22 | 1:A:47:CYS:H | 4 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2725) | 1:A:46:THR:HG23 | 1:A:47:CYS:H | 4 | 0.02 |
| (1,2725) | 1:A:46:THR:HG21 | 1:A:47:CYS:H | 6 | 0.02 |
| (1,2725) | 1:A:46:THR:HG22 | 1:A:47:CYS:H | 6 | 0.02 |
| (1,2725) | 1:A:46:THR:HG23 | 1:A:47:CYS:H | 6 | 0.02 |
| (1,2725) | 1:A:46:THR:HG21 | 1:A:47:CYS:H | 11 | 0.02 |
| (1,2725) | 1:A:46:THR:HG22 | 1:A:47:CYS:H | 11 | 0.02 |
| (1,2725) | 1:A:46:THR:HG23 | 1:A:47:CYS:H | 11 | 0.02 |
| (1,2724) | 1:B:10:ILE:H | 1:B:46:THR:HG21 | 17 | 0.02 |
| (1,2724) | 1:B:10:ILE:H | 1:B:46:THR:HG22 | 17 | 0.02 |
| (1,2724) | 1:B:10:ILE:H | 1:B:46:THR:HG23 | 17 | 0.02 |
| (1,2723) | 1:A:10:ILE:H | 1:A:46:THR:HG21 | 9 | 0.02 |
| (1,2723) | 1:A:10:ILE:H | 1:A:46:THR:HG22 | 9 | 0.02 |
| (1,2723) | 1:A:10:ILE:H | 1:A:46:THR:HG23 | 9 | 0.02 |
| (1,2716) | 1:B:9:ARG:HE | 1:B:46:THR:HG21 | 8 | 0.02 |
| (1,2716) | 1:B:9:ARG:HE | 1:B:46:THR:HG22 | 8 | 0.02 |
| (1,2716) | 1:B:9:ARG:HE | 1:B:46:THR:HG23 | 8 | 0.02 |
| (1,2704) | 1:B:9:ARG:HD2 | 1:B:46:THR:HG21 | 3 | 0.02 |
| (1,2704) | 1:B:9:ARG:HD2 | 1:B:46:THR:HG22 | 3 | 0.02 |
| (1,2704) | 1:B:9:ARG:HD2 | 1:B:46:THR:HG23 | 3 | 0.02 |
| (1,2704) | 1:B:9:ARG:HD3 | 1:B:46:THR:HG21 | 3 | 0.02 |
| (1,2704) | 1:B:9:ARG:HD3 | 1:B:46:THR:HG22 | 3 | 0.02 |
| (1,2704) | 1:B:9:ARG:HD3 | 1:B:46:THR:HG23 | 3 | 0.02 |
| (1,2703) | 1:A:9:ARG:HD2 | 1:A:46:THR:HG21 | 8 | 0.02 |
| (1,2703) | 1:A:9:ARG:HD2 | 1:A:46:THR:HG22 | 8 | 0.02 |
| (1,2703) | 1:A:9:ARG:HD2 | 1:A:46:THR:HG23 | 8 | 0.02 |
| (1,2703) | 1:A:9:ARG:HD3 | 1:A:46:THR:HG21 | 8 | 0.02 |
| (1,2703) | 1:A:9:ARG:HD3 | 1:A:46:THR:HG22 | 8 | 0.02 |
| (1,2703) | 1:A:9:ARG:HD3 | 1:A:46:THR:HG23 | 8 | 0.02 |
| (1,2703) | 1:A:9:ARG:HD2 | 1:A:46:THR:HG21 | 17 | 0.02 |
| (1,2703) | 1:A:9:ARG:HD2 | 1:A:46:THR:HG22 | 17 | 0.02 |
| (1,2703) | 1:A:9:ARG:HD2 | 1:A:46:THR:HG23 | 17 | 0.02 |
| (1,2703) | 1:A:9:ARG:HD3 | 1:A:46:THR:HG21 | 17 | 0.02 |
| (1,2703) | 1:A:9:ARG:HD3 | 1:A:46:THR:HG22 | 17 | 0.02 |
| (1,2703) | 1:A:9:ARG:HD3 | 1:A:46:THR:HG23 | 17 | 0.02 |
| (1,2701) | 1:A:41:LYS:HE2 | 1:A:46:THR:HG21 | 10 | 0.02 |
| (1,2701) | 1:A:41:LYS:HE2 | 1:A:46:THR:HG22 | 10 | 0.02 |
| (1,2701) | 1:A:41:LYS:HE2 | 1:A:46:THR:HG23 | 10 | 0.02 |
| (1,2701) | 1:A:41:LYS:HE3 | 1:A:46:THR:HG21 | 10 | 0.02 |
| (1,2701) | 1:A:41:LYS:HE3 | 1:A:46:THR:HG22 | 10 | 0.02 |
| (1,2701) | 1:A:41:LYS:HE3 | 1:A:46:THR:HG23 | 10 | 0.02 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG21 | 9 | 0.02 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG22 | 9 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG23 | 9 | 0.02 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG21 | 10 | 0.02 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG22 | 10 | 0.02 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG23 | 10 | 0.02 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG21 | 20 | 0.02 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG22 | 20 | 0.02 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG23 | 20 | 0.02 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG21 | 4 | 0.02 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG22 | 4 | 0.02 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG23 | 4 | 0.02 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG21 | 7 | 0.02 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG22 | 7 | 0.02 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG23 | 7 | 0.02 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG21 | 11 | 0.02 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG22 | 11 | 0.02 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG23 | 11 | 0.02 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG21 | 13 | 0.02 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG22 | 13 | 0.02 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG23 | 13 | 0.02 |
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD11 | 6 | 0.02 |
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD12 | 6 | 0.02 |
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD13 | 6 | 0.02 |
| (1,2676) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HD1 | 14 | 0.02 |
| (1,2676) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HD2 | 14 | 0.02 |
| (1,2676) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HD1 | 14 | 0.02 |
| (1,2676) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HD2 | 14 | 0.02 |
| (1,2676) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HD1 | 14 | 0.02 |
| (1,2676) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HD2 | 14 | 0.02 |
| (1,2675) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HD1 | 20 | 0.02 |
| (1,2675) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HD2 | 20 | 0.02 |
| (1,2675) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HD1 | 20 | 0.02 |
| (1,2675) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HD2 | 20 | 0.02 |
| (1,2675) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HD1 | 20 | 0.02 |
| (1,2675) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HD2 | 20 | 0.02 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD11 | 5 | 0.02 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD12 | 5 | 0.02 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD13 | 5 | 0.02 |
| (1,2670) | 1:B:44:ILE:HD11 | 1:B:46:THR:HB | 6 | 0.02 |
| (1,2670) | 1:B:44:ILE:HD12 | 1:B:46:THR:HB | 6 | 0.02 |
| (1,2670) | 1:B:44:ILE:HD13 | 1:B:46:THR:HB | 6 | 0.02 |
| (1,2669) | 1:A:44:ILE:HD11 | 1:A:46:THR:HB | 19 | 0.02 |
| (1,2669) | 1:A:44:ILE:HD12 | 1:A:46:THR:HB | 19 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2669) | 1:A:44:ILE:HD13 | 1:A:46:THR:HB | 19 | 0.02 |
| (1,2662) | 1:B:44:ILE:HG21 | 1:B:45:PHE:H | 14 | 0.02 |
| (1,2662) | 1:B:44:ILE:HG22 | 1:B:45:PHE:H | 14 | 0.02 |
| (1,2662) | 1:B:44:ILE:HG23 | 1:B:45:PHE:H | 14 | 0.02 |
| (1,2658) | 1:B:14:ASP:H | 1:B:44:ILE:HG21 | 17 | 0.02 |
| (1,2658) | 1:B:14:ASP:H | 1:B:44:ILE:HG22 | 17 | 0.02 |
| (1,2658) | 1:B:14:ASP:H | 1:B:44:ILE:HG23 | 17 | 0.02 |
| (1,2638) | 1:B:44:ILE:HG13 | 1:B:45:PHE:H | 13 | 0.02 |
| (1,2612) | 1:B:13:GLU:HA | 1:B:44:ILE:HB | 16 | 0.02 |
| (1,2611) | 1:A:13:GLU:HA | 1:A:44:ILE:HB | 5 | 0.02 |
| (1,2587) | 1:A:15:LYS:H | 1:A:40:ALA:HB1 | 15 | 0.02 |
| (1,2587) | 1:A:15:LYS:H | 1:A:40:ALA:HB2 | 15 | 0.02 |
| (1,2587) | 1:A:15:LYS:H | 1:A:40:ALA:HB3 | 15 | 0.02 |
| (1,2572) | 1:B:40:ALA:HA | 1:B:45:PHE:HA | 8 | 0.02 |
| (1,2572) | 1:B:40:ALA:HA | 1:B:45:PHE:HA | 18 | 0.02 |
| (1,2571) | 1:A:40:ALA:HA | 1:A:45:PHE:HA | 2 | 0.02 |
| (1,2571) | 1:A:40:ALA:HA | 1:A:45:PHE:HA | 4 | 0.02 |
| (1,2571) | 1:A:40:ALA:HA | 1:A:45:PHE:HA | 7 | 0.02 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD21 | 2 | 0.02 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD22 | 2 | 0.02 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD23 | 2 | 0.02 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD21 | 6 | 0.02 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD22 | 6 | 0.02 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD23 | 6 | 0.02 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD21 | 9 | 0.02 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD22 | 9 | 0.02 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD23 | 9 | 0.02 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD21 | 18 | 0.02 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD22 | 18 | 0.02 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD23 | 18 | 0.02 |
| (1,2510) | 1:B:38:LEU:HD11 | 1:B:39:ASN:H | 4 | 0.02 |
| (1,2510) | 1:B:38:LEU:HD12 | 1:B:39:ASN:H | 4 | 0.02 |
| (1,2510) | 1:B:38:LEU:HD13 | 1:B:39:ASN:H | 4 | 0.02 |
| (1,2509) | 1:A:38:LEU:HD11 | 1:A:39:ASN:H | 6 | 0.02 |
| (1,2509) | 1:A:38:LEU:HD12 | 1:A:39:ASN:H | 6 | 0.02 |
| (1,2509) | 1:A:38:LEU:HD13 | 1:A:39:ASN:H | 6 | 0.02 |
| (1,2504) | 1:B:38:LEU:HD11 | 1:B:45:PHE:HZ | 12 | 0.02 |
| (1,2504) | 1:B:38:LEU:HD12 | 1:B:45:PHE:HZ | 12 | 0.02 |
| (1,2504) | 1:B:38:LEU:HD13 | 1:B:45:PHE:HZ | 12 | 0.02 |
| (1,2503) | 1:A:38:LEU:HD11 | 1:A:45:PHE:HZ | 11 | 0.02 |
| (1,2503) | 1:A:38:LEU:HD12 | 1:A:45:PHE:HZ | 11 | 0.02 |
| (1,2503) | 1:A:38:LEU:HD13 | 1:A:45:PHE:HZ | 11 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2474) | 1:B:37:VAL:HG21 | 1:B:38:LEU:H | 1 | 0.02 |
| (1,2474) | 1:B:37:VAL:HG22 | 1:B:38:LEU:H | 1 | 0.02 |
| (1,2474) | 1:B:37:VAL:HG23 | 1:B:38:LEU:H | 1 | 0.02 |
| (1,2474) | 1:B:37:VAL:HG21 | 1:B:38:LEU:H | 20 | 0.02 |
| (1,2474) | 1:B:37:VAL:HG22 | 1:B:38:LEU:H | 20 | 0.02 |
| (1,2474) | 1:B:37:VAL:HG23 | 1:B:38:LEU:H | 20 | 0.02 |
| (1,2473) | 1:A:37:VAL:HG21 | 1:A:38:LEU:H | 4 | 0.02 |
| (1,2473) | 1:A:37:VAL:HG22 | 1:A:38:LEU:H | 4 | 0.02 |
| (1,2473) | 1:A:37:VAL:HG23 | 1:A:38:LEU:H | 4 | 0.02 |
| (1,2473) | 1:A:37:VAL:HG21 | 1:A:38:LEU:H | 5 | 0.02 |
| (1,2473) | 1:A:37:VAL:HG22 | 1:A:38:LEU:H | 5 | 0.02 |
| (1,2473) | 1:A:37:VAL:HG23 | 1:A:38:LEU:H | 5 | 0.02 |
| (1,2473) | 1:A:37:VAL:HG21 | 1:A:38:LEU:H | 15 | 0.02 |
| (1,2473) | 1:A:37:VAL:HG22 | 1:A:38:LEU:H | 15 | 0.02 |
| (1,2473) | 1:A:37:VAL:HG23 | 1:A:38:LEU:H | 15 | 0.02 |
| (1,2473) | 1:A:37:VAL:HG21 | 1:A:38:LEU:H | 17 | 0.02 |
| (1,2473) | 1:A:37:VAL:HG22 | 1:A:38:LEU:H | 17 | 0.02 |
| (1,2473) | 1:A:37:VAL:HG23 | 1:A:38:LEU:H | 17 | 0.02 |
| (1,2471) | 1:A:37:VAL:HG21 | 1:A:48:ASN:H | 15 | 0.02 |
| (1,2471) | 1:A:37:VAL:HG22 | 1:A:48:ASN:H | 15 | 0.02 |
| (1,2471) | 1:A:37:VAL:HG23 | 1:A:48:ASN:H | 15 | 0.02 |
| (1,247) | 1:B:19:THR:H | 1:B:40:ALA:HB1 | 9 | 0.02 |
| (1,247) | 1:B:19:THR:H | 1:B:40:ALA:HB2 | 9 | 0.02 |
| (1,247) | 1:B:19:THR:H | 1:B:40:ALA:HB3 | 9 | 0.02 |
| (1,2466) | 1:B:37:VAL:HG21 | 1:B:48:ASN:HD22 | 7 | 0.02 |
| (1,2466) | 1:B:37:VAL:HG22 | 1:B:48:ASN:HD22 | 7 | 0.02 |
| (1,2466) | 1:B:37:VAL:HG23 | 1:B:48:ASN:HD22 | 7 | 0.02 |
| (1,2465) | 1:A:37:VAL:HG21 | 1:A:48:ASN:HD22 | 4 | 0.02 |
| (1,2465) | 1:A:37:VAL:HG22 | 1:A:48:ASN:HD22 | 4 | 0.02 |
| (1,2465) | 1:A:37:VAL:HG23 | 1:A:48:ASN:HD22 | 4 | 0.02 |
| (1,2465) | 1:A:37:VAL:HG21 | 1:A:48:ASN:HD22 | 5 | 0.02 |
| (1,2465) | 1:A:37:VAL:HG22 | 1:A:48:ASN:HD22 | 5 | 0.02 |
| (1,2465) | 1:A:37:VAL:HG23 | 1:A:48:ASN:HD22 | 5 | 0.02 |
| (1,2465) | 1:A:37:VAL:HG21 | 1:A:48:ASN:HD22 | 7 | 0.02 |
| (1,2465) | 1:A:37:VAL:HG22 | 1:A:48:ASN:HD22 | 7 | 0.02 |
| (1,2465) | 1:A:37:VAL:HG23 | 1:A:48:ASN:HD22 | 7 | 0.02 |
| (1,2465) | 1:A:37:VAL:HG21 | 1:A:48:ASN:HD22 | 12 | 0.02 |
| (1,2465) | 1:A:37:VAL:HG22 | 1:A:48:ASN:HD22 | 12 | 0.02 |
| (1,2465) | 1:A:37:VAL:HG23 | 1:A:48:ASN:HD22 | 12 | 0.02 |
| (1,2415) | 1:A:36:ILE:HD11 | 1:A:38:LEU:H | 12 | 0.02 |
| (1,2415) | 1:A:36:ILE:HD12 | 1:A:38:LEU:H | 12 | 0.02 |
| (1,2415) | 1:A:36:ILE:HD13 | 1:A:38:LEU:H | 12 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 4 | 0.02 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 4 | 0.02 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 4 | 0.02 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 15 | 0.02 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 15 | 0.02 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 15 | 0.02 |
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD11 | 5 | 0.02 |
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD12 | 5 | 0.02 |
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD13 | 5 | 0.02 |
| (1,2390) | 1:B:36:ILE:HG21 | 1:B:48:ASN:H | 6 | 0.02 |
| (1,2390) | 1:B:36:ILE:HG22 | 1:B:48:ASN:H | 6 | 0.02 |
| (1,2390) | 1:B:36:ILE:HG23 | 1:B:48:ASN:H | 6 | 0.02 |
| (1,2390) | 1:B:36:ILE:HG21 | 1:B:48:ASN:H | 10 | 0.02 |
| (1,2390) | 1:B:36:ILE:HG22 | 1:B:48:ASN:H | 10 | 0.02 |
| (1,2390) | 1:B:36:ILE:HG23 | 1:B:48:ASN:H | 10 | 0.02 |
| (1,2389) | 1:A:36:ILE:HG21 | 1:A:48:ASN:H | 15 | 0.02 |
| (1,2389) | 1:A:36:ILE:HG22 | 1:A:48:ASN:H | 15 | 0.02 |
| (1,2389) | 1:A:36:ILE:HG23 | 1:A:48:ASN:H | 15 | 0.02 |
| (1,2374) | 1:B:35:THR:HB | 1:B:36:ILE:HG21 | 12 | 0.02 |
| (1,2374) | 1:B:35:THR:HB | 1:B:36:ILE:HG22 | 12 | 0.02 |
| (1,2374) | 1:B:35:THR:HB | 1:B:36:ILE:HG23 | 12 | 0.02 |
| (1,2368) | 1:B:36:ILE:HG21 | 1:B:37:VAL:HB | 3 | 0.02 |
| (1,2368) | 1:B:36:ILE:HG22 | 1:B:37:VAL:HB | 3 | 0.02 |
| (1,2368) | 1:B:36:ILE:HG23 | 1:B:37:VAL:HB | 3 | 0.02 |
| (1,2368) | 1:B:36:ILE:HG21 | 1:B:37:VAL:HB | 5 | 0.02 |
| (1,2368) | 1:B:36:ILE:HG22 | 1:B:37:VAL:HB | 5 | 0.02 |
| (1,2368) | 1:B:36:ILE:HG23 | 1:B:37:VAL:HB | 5 | 0.02 |
| (1,2367) | 1:A:36:ILE:HG21 | 1:A:37:VAL:HB | 1 | 0.02 |
| (1,2367) | 1:A:36:ILE:HG22 | 1:A:37:VAL:HB | 1 | 0.02 |
| (1,2367) | 1:A:36:ILE:HG23 | 1:A:37:VAL:HB | 1 | 0.02 |
| (1,2344) | 1:B:35:THR:HB | 1:B:50:MET:HB2 | 12 | 0.02 |
| (1,2344) | 1:B:35:THR:HB | 1:B:50:MET:HB2 | 20 | 0.02 |
| (1,2343) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 16 | 0.02 |
| (1,2333) | 1:A:33:ILE:HD11 | 1:A:34:ARG:H | 7 | 0.02 |
| (1,2333) | 1:A:33:ILE:HD12 | 1:A:34:ARG:H | 7 | 0.02 |
| (1,2333) | 1:A:33:ILE:HD13 | 1:A:34:ARG:H | 7 | 0.02 |
| (1,2328) | 1:A:33:ILE:HD11 | 1:B:20:ASN:HD22 | 3 | 0.02 |
| (1,2328) | 1:A:33:ILE:HD12 | 1:B:20:ASN:HD22 | 3 | 0.02 |
| (1,2328) | 1:A:33:ILE:HD13 | 1:B:20:ASN:HD22 | 3 | 0.02 |
| (1,2327) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HD11 | 13 | 0.02 |
| (1,2327) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HD12 | 13 | 0.02 |
| (1,2327) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HD13 | 13 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,227) | 1:B:18:MET:H | 1:B:18:MET:HG3 | 15 | 0.02 |
| (1,227) | 1:B:18:MET:H | 1:B:18:MET:HG3 | 17 | 0.02 |
| (1,2268) | 1:B:29:PHE:HD1 | 1:B:31:THR:HB | 13 | 0.02 |
| (1,2268) | 1:B:29:PHE:HD2 | 1:B:31:THR:HB | 13 | 0.02 |
| (1,2267) | 1:A:29:PHE:HD1 | 1:A:31:THR:HB | 8 | 0.02 |
| (1,2267) | 1:A:29:PHE:HD2 | 1:A:31:THR:HB | 8 | 0.02 |
| (1,2261) | 1:A:25:VAL:HA | 1:A:28:LYS:HE2 | 2 | 0.02 |
| (1,2261) | 1:A:25:VAL:HA | 1:A:28:LYS:HE3 | 2 | 0.02 |
| (1,2229) | 1:A:20:ASN:HD22 | 1:B:27:SER:HA | 12 | 0.02 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 7 | 0.02 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 7 | 0.02 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 7 | 0.02 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 10 | 0.02 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 10 | 0.02 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 10 | 0.02 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 12 | 0.02 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 12 | 0.02 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 12 | 0.02 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 14 | 0.02 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 14 | 0.02 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 14 | 0.02 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 18 | 0.02 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 18 | 0.02 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 18 | 0.02 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 11 | 0.02 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 11 | 0.02 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 11 | 0.02 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 13 | 0.02 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 13 | 0.02 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 13 | 0.02 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 16 | 0.02 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 16 | 0.02 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 16 | 0.02 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 18 | 0.02 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 18 | 0.02 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 18 | 0.02 |
| (1,2186) | 1:B:25:VAL:HG21 | 1:B:29:PHE:HD1 | 2 | 0.02 |
| (1,2186) | 1:B:25:VAL:HG21 | 1:B:29:PHE:HD2 | 2 | 0.02 |
| (1,2186) | 1:B:25:VAL:HG22 | 1:B:29:PHE:HD1 | 2 | 0.02 |
| (1,2186) | 1:B:25:VAL:HG22 | 1:B:29:PHE:HD2 | 2 | 0.02 |
| (1,2186) | 1:B:25:VAL:HG23 | 1:B:29:PHE:HD1 | 2 | 0.02 |
| (1,2186) | 1:B:25:VAL:HG23 | 1:B:29:PHE:HD2 | 2 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2180) | 1:B:22:ILE:HA | 1:B:25:VAL:HG21 | 19 | 0.02 |
| (1,2180) | 1:B:22:ILE:HA | 1:B:25:VAL:HG22 | 19 | 0.02 |
| (1,2180) | 1:B:22:ILE:HA | 1:B:25:VAL:HG23 | 19 | 0.02 |
| (1,2172) | 1:B:25:VAL:HG11 | 1:B:27:SER:H | 4 | 0.02 |
| (1,2172) | 1:B:25:VAL:HG12 | 1:B:27:SER:H | 4 | 0.02 |
| (1,2172) | 1:B:25:VAL:HG13 | 1:B:27:SER:H | 4 | 0.02 |
| (1,2172) | 1:B:25:VAL:HG11 | 1:B:27:SER:H | 12 | 0.02 |
| (1,2172) | 1:B:25:VAL:HG12 | 1:B:27:SER:H | 12 | 0.02 |
| (1,2172) | 1:B:25:VAL:HG13 | 1:B:27:SER:H | 12 | 0.02 |
| (1,2172) | 1:B:25:VAL:HG11 | 1:B:27:SER:H | 16 | 0.02 |
| (1,2172) | 1:B:25:VAL:HG12 | 1:B:27:SER:H | 16 | 0.02 |
| (1,2172) | 1:B:25:VAL:HG13 | 1:B:27:SER:H | 16 | 0.02 |
| (1,2172) | 1:B:25:VAL:HG11 | 1:B:27:SER:H | 20 | 0.02 |
| (1,2172) | 1:B:25:VAL:HG12 | 1:B:27:SER:H | 20 | 0.02 |
| (1,2172) | 1:B:25:VAL:HG13 | 1:B:27:SER:H | 20 | 0.02 |
| (1,2171) | 1:A:25:VAL:HG11 | 1:A:27:SER:H | 8 | 0.02 |
| (1,2171) | 1:A:25:VAL:HG12 | 1:A:27:SER:H | 8 | 0.02 |
| (1,2171) | 1:A:25:VAL:HG13 | 1:A:27:SER:H | 8 | 0.02 |
| (1,2171) | 1:A:25:VAL:HG11 | 1:A:27:SER:H | 11 | 0.02 |
| (1,2171) | 1:A:25:VAL:HG12 | 1:A:27:SER:H | 11 | 0.02 |
| (1,2171) | 1:A:25:VAL:HG13 | 1:A:27:SER:H | 11 | 0.02 |
| (1,2171) | 1:A:25:VAL:HG11 | 1:A:27:SER:H | 12 | 0.02 |
| (1,2171) | 1:A:25:VAL:HG12 | 1:A:27:SER:H | 12 | 0.02 |
| (1,2171) | 1:A:25:VAL:HG13 | 1:A:27:SER:H | 12 | 0.02 |
| (1,2151) | 1:A:25:VAL:HG11 | 1:A:28:LYS:HD3 | 8 | 0.02 |
| (1,2151) | 1:A:25:VAL:HG12 | 1:A:28:LYS:HD3 | 8 | 0.02 |
| (1,2151) | 1:A:25:VAL:HG13 | 1:A:28:LYS:HD3 | 8 | 0.02 |
| (1,2135) | 1:A:67:ARG:HE | 1:A:75:VAL:HG11 | 19 | 0.02 |
| (1,2135) | 1:A:67:ARG:HE | 1:A:75:VAL:HG12 | 19 | 0.02 |
| (1,2135) | 1:A:67:ARG:HE | 1:A:75:VAL:HG13 | 19 | 0.02 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG21 | 4 | 0.02 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG22 | 4 | 0.02 |
| (1,2072) | 1:B:19:THR:HA | 1:B:22:ILE:HG23 | 4 | 0.02 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 4 | 0.02 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 4 | 0.02 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 4 | 0.02 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG21 | 17 | 0.02 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG22 | 17 | 0.02 |
| (1,2071) | 1:A:19:THR:HA | 1:A:22:ILE:HG23 | 17 | 0.02 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 4 | 0.02 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 4 | 0.02 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 4 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 13 | 0.02 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 13 | 0.02 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 13 | 0.02 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 18 | 0.02 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 18 | 0.02 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 18 | 0.02 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 20 | 0.02 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 20 | 0.02 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 20 | 0.02 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG21 | 18 | 0.02 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG22 | 18 | 0.02 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG23 | 18 | 0.02 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG21 | 19 | 0.02 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG22 | 19 | 0.02 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG23 | 19 | 0.02 |
| (1,206) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD22 | 5 | 0.02 |
| (1,206) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD22 | 5 | 0.02 |
| (1,206) | 1:B:15:LYS:HE2 | 1:B:16:ASN:HD22 | 10 | 0.02 |
| (1,206) | 1:B:15:LYS:HE3 | 1:B:16:ASN:HD22 | 10 | 0.02 |
| (1,2025) | 1:B:22:ILE:HB | 1:B:47:CYS:HG | 2 | 0.02 |
| (1,2025) | 1:B:22:ILE:HB | 1:B:47:CYS:HG | 13 | 0.02 |
| (1,2021) | 1:B:19:THR:HG21 | 1:B:22:ILE:HB | 11 | 0.02 |
| (1,2021) | 1:B:19:THR:HG22 | 1:B:22:ILE:HB | 11 | 0.02 |
| (1,2021) | 1:B:19:THR:HG23 | 1:B:22:ILE:HB | 11 | 0.02 |
| (1,2017) | 1:B:21:GLN:HE21 | 1:B:22:ILE:HA | 3 | 0.02 |
| (1,2016) | 1:A:21:GLN:HE21 | 1:A:22:ILE:HA | 2 | 0.02 |
| (1,2016) | 1:A:21:GLN:HE21 | 1:A:22:ILE:HA | 4 | 0.02 |
| (1,2016) | 1:A:21:GLN:HE21 | 1:A:22:ILE:HA | 7 | 0.02 |
| (1,2016) | 1:A:21:GLN:HE21 | 1:A:22:ILE:HA | 14 | 0.02 |
| (1,2009) | 1:B:21:GLN:HG3 | 1:B:25:VAL:H | 18 | 0.02 |
| (1,1926) | 1:A:18:MET:HE1 | 1:A:71:GLY:HA2 | 20 | 0.02 |
| (1,1926) | 1:A:18:MET:HE2 | 1:A:71:GLY:HA2 | 20 | 0.02 |
| (1,1926) | 1:A:18:MET:HE3 | 1:A:71:GLY:HA2 | 20 | 0.02 |
| (1,1910) | 1:B:18:MET:HA | 1:B:21:GLN:HA | 14 | 0.02 |
| (1,1907) | 1:A:18:MET:HA | 1:A:21:GLN:HG2 | 20 | 0.02 |
| (1,1899) | 1:A:16:ASN:HA | 1:A:17:GLY:HA3 | 3 | 0.02 |
| (1,1882) | 1:A:15:LYS:HG2 | 1:A:15:LYS:HE2 | 2 | 0.02 |
| (1,1882) | 1:A:15:LYS:HG2 | 1:A:15:LYS:HE3 | 2 | 0.02 |
| (1,1882) | 1:A:15:LYS:HG3 | 1:A:15:LYS:HE2 | 2 | 0.02 |
| (1,1882) | 1:A:15:LYS:HG3 | 1:A:15:LYS:HE3 | 2 | 0.02 |
| (1,1879) | 1:B:25:VAL:HG21 | 1:B:65:LYS:HE2 | 19 | 0.02 |
| (1,1879) | 1:B:25:VAL:HG21 | 1:B:65:LYS:HE3 | 19 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1879) | 1:B:25:VAL:HG22 | 1:B:65:LYS:HE2 | 19 | 0.02 |
| (1,1879) | 1:B:25:VAL:HG22 | 1:B:65:LYS:HE3 | 19 | 0.02 |
| (1,1879) | 1:B:25:VAL:HG23 | 1:B:65:LYS:HE2 | 19 | 0.02 |
| (1,1879) | 1:B:25:VAL:HG23 | 1:B:65:LYS:HE3 | 19 | 0.02 |
| (1,1878) | 1:A:25:VAL:HG21 | 1:A:65:LYS:HE2 | 3 | 0.02 |
| (1,1878) | 1:A:25:VAL:HG21 | 1:A:65:LYS:HE3 | 3 | 0.02 |
| (1,1878) | 1:A:25:VAL:HG22 | 1:A:65:LYS:HE2 | 3 | 0.02 |
| (1,1878) | 1:A:25:VAL:HG22 | 1:A:65:LYS:HE3 | 3 | 0.02 |
| (1,1878) | 1:A:25:VAL:HG23 | 1:A:65:LYS:HE2 | 3 | 0.02 |
| (1,1878) | 1:A:25:VAL:HG23 | 1:A:65:LYS:HE3 | 3 | 0.02 |
| (1,1875) | 1:B:11:VAL:HG21 | 1:B:41:LYS:HE2 | 14 | 0.02 |
| (1,1875) | 1:B:11:VAL:HG21 | 1:B:41:LYS:HE3 | 14 | 0.02 |
| (1,1875) | 1:B:11:VAL:HG22 | 1:B:41:LYS:HE2 | 14 | 0.02 |
| (1,1875) | 1:B:11:VAL:HG22 | 1:B:41:LYS:HE3 | 14 | 0.02 |
| (1,1875) | 1:B:11:VAL:HG23 | 1:B:41:LYS:HE2 | 14 | 0.02 |
| (1,1875) | 1:B:11:VAL:HG23 | 1:B:41:LYS:HE3 | 14 | 0.02 |
| (1,187) | 1:A:15:LYS:H | 1:A:44:ILE:HA | 4 | 0.02 |
| (1,187) | 1:A:15:LYS:H | 1:A:44:ILE:HA | 6 | 0.02 |
| (1,1856) | 1:B:13:GLU:HG2 | 1:B:15:LYS:HB3 | 5 | 0.02 |
| (1,1856) | 1:B:13:GLU:HG3 | 1:B:15:LYS:HB3 | 5 | 0.02 |
| (1,1856) | 1:B:13:GLU:HG2 | 1:B:15:LYS:HB3 | 16 | 0.02 |
| (1,1856) | 1:B:13:GLU:HG3 | 1:B:15:LYS:HB3 | 16 | 0.02 |
| (1,1855) | 1:A:13:GLU:HG2 | 1:A:15:LYS:HB3 | 11 | 0.02 |
| (1,1855) | 1:A:13:GLU:HG3 | 1:A:15:LYS:HB3 | 11 | 0.02 |
| (1,1855) | 1:A:13:GLU:HG2 | 1:A:15:LYS:HB3 | 12 | 0.02 |
| (1,1855) | 1:A:13:GLU:HG3 | 1:A:15:LYS:HB3 | 12 | 0.02 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG11 | 10 | 0.02 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG12 | 10 | 0.02 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG13 | 10 | 0.02 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG11 | 10 | 0.02 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG12 | 10 | 0.02 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG13 | 10 | 0.02 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG11 | 11 | 0.02 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG12 | 11 | 0.02 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG13 | 11 | 0.02 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG11 | 11 | 0.02 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG12 | 11 | 0.02 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG13 | 11 | 0.02 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG11 | 19 | 0.02 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG12 | 19 | 0.02 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG13 | 19 | 0.02 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG11 | 19 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG12 | 19 | 0.02 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG13 | 19 | 0.02 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG11 | 7 | 0.02 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG12 | 7 | 0.02 |
| (1,1824) | 1:A:13:GLU:HG2 | 1:A:69:VAL:HG13 | 7 | 0.02 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG11 | 7 | 0.02 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG12 | 7 | 0.02 |
| (1,1824) | 1:A:13:GLU:HG3 | 1:A:69:VAL:HG13 | 7 | 0.02 |
| (1,181) | 1:A:15:LYS:H | 1:A:18:MET:HG2 | 17 | 0.02 |
| (1,1806) | 1:A:13:GLU:HB2 | 1:A:15:LYS:HD2 | 3 | 0.02 |
| (1,1806) | 1:A:13:GLU:HB2 | 1:A:15:LYS:HD3 | 3 | 0.02 |
| (1,1798) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HD2 | 7 | 0.02 |
| (1,1798) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HD3 | 7 | 0.02 |
| (1,1796) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HG2 | 3 | 0.02 |
| (1,1796) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HG3 | 3 | 0.02 |
| (1,1796) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HG2 | 10 | 0.02 |
| (1,1796) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HG3 | 10 | 0.02 |
| (1,1796) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HG2 | 17 | 0.02 |
| (1,1796) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HG3 | 17 | 0.02 |
| (1,1762) | 1:A:11:VAL:HG11 | 1:A:73:PHE:HB2 | 4 | 0.02 |
| (1,1762) | 1:A:11:VAL:HG12 | 1:A:73:PHE:HB2 | 4 | 0.02 |
| (1,1762) | 1:A:11:VAL:HG13 | 1:A:73:PHE:HB2 | 4 | 0.02 |
| (1,1762) | 1:A:11:VAL:HG11 | 1:A:73:PHE:HB2 | 16 | 0.02 |
| (1,1762) | 1:A:11:VAL:HG12 | 1:A:73:PHE:HB2 | 16 | 0.02 |
| (1,1762) | 1:A:11:VAL:HG13 | 1:A:73:PHE:HB2 | 16 | 0.02 |
| (1,1761) | 1:B:11:VAL:HG11 | 1:B:41:LYS:HE2 | 1 | 0.02 |
| (1,1761) | 1:B:11:VAL:HG11 | 1:B:41:LYS:HE3 | 1 | 0.02 |
| (1,1761) | 1:B:11:VAL:HG12 | 1:B:41:LYS:HE2 | 1 | 0.02 |
| (1,1761) | 1:B:11:VAL:HG12 | 1:B:41:LYS:HE3 | 1 | 0.02 |
| (1,1761) | 1:B:11:VAL:HG13 | 1:B:41:LYS:HE2 | 1 | 0.02 |
| (1,1761) | 1:B:11:VAL:HG13 | 1:B:41:LYS:HE3 | 1 | 0.02 |
| (1,176) | 1:B:13:GLU:HG2 | 1:B:15:LYS:H | 9 | 0.02 |
| (1,176) | 1:B:13:GLU:HG3 | 1:B:15:LYS:H | 9 | 0.02 |
| (1,175) | 1:A:13:GLU:HG2 | 1:A:15:LYS:H | 12 | 0.02 |
| (1,175) | 1:A:13:GLU:HG3 | 1:A:15:LYS:H | 12 | 0.02 |
| (1,175) | 1:A:13:GLU:HG2 | 1:A:15:LYS:H | 19 | 0.02 |
| (1,175) | 1:A:13:GLU:HG3 | 1:A:15:LYS:H | 19 | 0.02 |
| (1,1749) | 1:B:11:VAL:HG21 | 1:B:40:ALA:HA | 15 | 0.02 |
| (1,1749) | 1:B:11:VAL:HG22 | 1:B:40:ALA:HA | 15 | 0.02 |
| (1,1749) | 1:B:11:VAL:HG23 | 1:B:40:ALA:HA | 15 | 0.02 |
| (1,1744) | 1:A:11:VAL:HG21 | 1:A:46:THR:HB | 1 | 0.02 |
| (1,1744) | 1:A:11:VAL:HG22 | 1:A:46:THR:HB | 1 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1744) | 1:A:11:VAL:HG23 | 1:A:46:THR:HB | 1 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG21 | 6 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG22 | 6 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG23 | 6 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG21 | 6 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG22 | 6 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG23 | 6 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG21 | 6 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG22 | 6 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG23 | 6 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG21 | 9 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG22 | 9 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG23 | 9 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG21 | 9 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG22 | 9 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG23 | 9 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG21 | 9 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG22 | 9 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG23 | 9 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG21 | 18 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG22 | 18 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG23 | 18 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG21 | 18 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG22 | 18 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG23 | 18 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG21 | 18 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG22 | 18 | 0.02 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG23 | 18 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG21 | 8 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG22 | 8 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG23 | 8 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG21 | 8 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG22 | 8 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG23 | 8 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG21 | 8 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG22 | 8 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG23 | 8 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG21 | 10 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG22 | 10 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG23 | 10 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG21 | 10 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG22 | 10 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG23 | 10 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG21 | 10 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG22 | 10 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG23 | 10 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG21 | 15 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG22 | 15 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG23 | 15 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG21 | 15 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG22 | 15 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG23 | 15 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG21 | 15 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG22 | 15 | 0.02 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG23 | 15 | 0.02 |
| (1,171) | 1:A:15:LYS:H | 1:A:18:MET:HE1 | 16 | 0.02 |
| (1,171) | 1:A:15:LYS:H | 1:A:18:MET:HE2 | 16 | 0.02 |
| (1,171) | 1:A:15:LYS:H | 1:A:18:MET:HE3 | 16 | 0.02 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD11 | 3 | 0.02 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD12 | 3 | 0.02 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD13 | 3 | 0.02 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD11 | 18 | 0.02 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD12 | 18 | 0.02 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD13 | 18 | 0.02 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD11 | 5 | 0.02 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD12 | 5 | 0.02 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD13 | 5 | 0.02 |
| (1,1685) | 1:B:9:ARG:HA | 1:B:10:ILE:HG21 | 8 | 0.02 |
| (1,1685) | 1:B:9:ARG:HA | 1:B:10:ILE:HG22 | 8 | 0.02 |
| (1,1685) | 1:B:9:ARG:HA | 1:B:10:ILE:HG23 | 8 | 0.02 |
| (1,1631) | 1:B:9:ARG:HD2 | 1:B:11:VAL:HB | 9 | 0.02 |
| (1,1631) | 1:B:9:ARG:HD3 | 1:B:11:VAL:HB | 9 | 0.02 |
| (1,1631) | 1:B:9:ARG:HD2 | 1:B:11:VAL:HB | 20 | 0.02 |
| (1,1631) | 1:B:9:ARG:HD3 | 1:B:11:VAL:HB | 20 | 0.02 |
| (1,1630) | 1:A:9:ARG:HD2 | 1:A:11:VAL:HB | 11 | 0.02 |
| (1,1630) | 1:A:9:ARG:HD3 | 1:A:11:VAL:HB | 11 | 0.02 |
| (1,1612) | 1:B:24:GLY:H | 1:B:26:ILE:HD11 | 20 | 0.02 |
| (1,1612) | 1:B:24:GLY:H | 1:B:26:ILE:HD12 | 20 | 0.02 |
| (1,1612) | 1:B:24:GLY:H | 1:B:26:ILE:HD13 | 20 | 0.02 |
| (1,1611) | 1:A:24:GLY:H | 1:A:26:ILE:HD11 | 17 | 0.02 |
| (1,1611) | 1:A:24:GLY:H | 1:A:26:ILE:HD12 | 17 | 0.02 |
| (1,1611) | 1:A:24:GLY:H | 1:A:26:ILE:HD13 | 17 | 0.02 |
| (1,1606) | 1:B:8:ILE:HD11 | 1:B:77:ARG:HA | 2 | 0.02 |
| (1,1606) | 1:B:8:ILE:HD12 | 1:B:77:ARG:HA | 2 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1606) | 1:B:8:ILE:HD13 | 1:B:77:ARG:HA | 2 | 0.02 |
| (1,1606) | 1:B:8:ILE:HD11 | 1:B:77:ARG:HA | 6 | 0.02 |
| (1,1606) | 1:B:8:ILE:HD12 | 1:B:77:ARG:HA | 6 | 0.02 |
| (1,1606) | 1:B:8:ILE:HD13 | 1:B:77:ARG:HA | 6 | 0.02 |
| (1,1606) | 1:B:8:ILE:HD11 | 1:B:77:ARG:HA | 15 | 0.02 |
| (1,1606) | 1:B:8:ILE:HD12 | 1:B:77:ARG:HA | 15 | 0.02 |
| (1,1606) | 1:B:8:ILE:HD13 | 1:B:77:ARG:HA | 15 | 0.02 |
| (1,1606) | 1:B:8:ILE:HD11 | 1:B:77:ARG:HA | 20 | 0.02 |
| (1,1606) | 1:B:8:ILE:HD12 | 1:B:77:ARG:HA | 20 | 0.02 |
| (1,1606) | 1:B:8:ILE:HD13 | 1:B:77:ARG:HA | 20 | 0.02 |
| (1,1605) | 1:A:8:ILE:HD11 | 1:A:77:ARG:HA | 13 | 0.02 |
| (1,1605) | 1:A:8:ILE:HD12 | 1:A:77:ARG:HA | 13 | 0.02 |
| (1,1605) | 1:A:8:ILE:HD13 | 1:A:77:ARG:HA | 13 | 0.02 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD21 | 6 | 0.02 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD22 | 6 | 0.02 |
| (1,1590) | 1:B:8:ILE:HD11 | 1:B:62:LEU:HD23 | 6 | 0.02 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD21 | 6 | 0.02 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD22 | 6 | 0.02 |
| (1,1590) | 1:B:8:ILE:HD12 | 1:B:62:LEU:HD23 | 6 | 0.02 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD21 | 6 | 0.02 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD22 | 6 | 0.02 |
| (1,1590) | 1:B:8:ILE:HD13 | 1:B:62:LEU:HD23 | 6 | 0.02 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 14 | 0.02 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 14 | 0.02 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 14 | 0.02 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 14 | 0.02 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 14 | 0.02 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 14 | 0.02 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 14 | 0.02 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 14 | 0.02 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 14 | 0.02 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD2 | 11 | 0.02 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD3 | 11 | 0.02 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD2 | 11 | 0.02 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD3 | 11 | 0.02 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD2 | 11 | 0.02 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD3 | 11 | 0.02 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD2 | 18 | 0.02 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD3 | 18 | 0.02 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD2 | 18 | 0.02 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD3 | 18 | 0.02 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD2 | 18 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD3 | 18 | 0.02 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 8 | 0.02 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 8 | 0.02 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 8 | 0.02 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 8 | 0.02 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 8 | 0.02 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 8 | 0.02 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 10 | 0.02 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 10 | 0.02 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 10 | 0.02 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 10 | 0.02 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 10 | 0.02 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 10 | 0.02 |
| (1,1569) | 1:A:8:ILE:HG21 | 1:A:63:MET:HG3 | 1 | 0.02 |
| (1,1569) | 1:A:8:ILE:HG22 | 1:A:63:MET:HG3 | 1 | 0.02 |
| (1,1569) | 1:A:8:ILE:HG23 | 1:A:63:MET:HG3 | 1 | 0.02 |
| (1,1542) | 1:B:6:ALA:HB1 | 1:B:7:GLY:HA3 | 13 | 0.02 |
| (1,1542) | 1:B:6:ALA:HB2 | 1:B:7:GLY:HA3 | 13 | 0.02 |
| (1,1542) | 1:B:6:ALA:HB3 | 1:B:7:GLY:HA3 | 13 | 0.02 |
| (1,1541) | 1:A:6:ALA:HB1 | 1:A:7:GLY:HA3 | 10 | 0.02 |
| (1,1541) | 1:A:6:ALA:HB2 | 1:A:7:GLY:HA3 | 10 | 0.02 |
| (1,1541) | 1:A:6:ALA:HB3 | 1:A:7:GLY:HA3 | 10 | 0.02 |
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 2 | 0.02 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 2 | 0.02 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 2 | 0.02 |
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 8 | 0.02 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 8 | 0.02 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 8 | 0.02 |
| (1,1527) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HA | 3 | 0.02 |
| (1,1527) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HA | 3 | 0.02 |
| (1,1527) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HA | 3 | 0.02 |
| (1,1527) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HA | 6 | 0.02 |
| (1,1527) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HA | 6 | 0.02 |
| (1,1527) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HA | 6 | 0.02 |
| (1,1527) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HA | 11 | 0.02 |
| (1,1527) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HA | 11 | 0.02 |
| (1,1527) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HA | 11 | 0.02 |
| (1,1527) | 1:A:5:LEU:HD21 | 1:A:52:PHE:HA | 18 | 0.02 |
| (1,1527) | 1:A:5:LEU:HD22 | 1:A:52:PHE:HA | 18 | 0.02 |
| (1,1527) | 1:A:5:LEU:HD23 | 1:A:52:PHE:HA | 18 | 0.02 |
| (1,1456) | 1:B:3:ASP:HB2 | 1:B:53:VAL:H | 8 | 0.02 |
| (1,1381) | 1:A:81:LEU:H | 1:A:81:LEU:HD11 | 2 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1381) | 1:A:81:LEU:H | 1:A:81:LEU:HD12 | 2 | 0.02 |
| (1,1381) | 1:A:81:LEU:H | 1:A:81:LEU:HD13 | 2 | 0.02 |
| (1,1348) | 1:B:77:ARG:H | 1:B:77:ARG:HD2 | 2 | 0.02 |
| (1,1348) | 1:B:77:ARG:H | 1:B:77:ARG:HD3 | 2 | 0.02 |
| (1,1300) | 1:B:74:THR:HG21 | 1:B:75:VAL:H | 6 | 0.02 |
| (1,1300) | 1:B:74:THR:HG22 | 1:B:75:VAL:H | 6 | 0.02 |
| (1,1300) | 1:B:74:THR:HG23 | 1:B:75:VAL:H | 6 | 0.02 |
| (1,1285) | 1:A:12:GLY:HA3 | 1:A:74:THR:H | 11 | 0.02 |
| (1,1257) | 1:A:70:GLN:HA | 1:A:72:VAL:H | 9 | 0.02 |
| (1,1257) | 1:A:70:GLN:HA | 1:A:72:VAL:H | 11 | 0.02 |
| (1,1253) | 1:A:69:VAL:HG21 | 1:A:72:VAL:H | 8 | 0.02 |
| (1,1253) | 1:A:69:VAL:HG22 | 1:A:72:VAL:H | 8 | 0.02 |
| (1,1253) | 1:A:69:VAL:HG23 | 1:A:72:VAL:H | 8 | 0.02 |
| (1,1242) | 1:B:69:VAL:HG11 | 1:B:71:GLY:H | 3 | 0.02 |
| (1,1242) | 1:B:69:VAL:HG12 | 1:B:71:GLY:H | 3 | 0.02 |
| (1,1242) | 1:B:69:VAL:HG13 | 1:B:71:GLY:H | 3 | 0.02 |
| (1,1242) | 1:B:69:VAL:HG11 | 1:B:71:GLY:H | 4 | 0.02 |
| (1,1242) | 1:B:69:VAL:HG12 | 1:B:71:GLY:H | 4 | 0.02 |
| (1,1242) | 1:B:69:VAL:HG13 | 1:B:71:GLY:H | 4 | 0.02 |
| (1,1242) | 1:B:69:VAL:HG11 | 1:B:71:GLY:H | 6 | 0.02 |
| (1,1242) | 1:B:69:VAL:HG12 | 1:B:71:GLY:H | 6 | 0.02 |
| (1,1242) | 1:B:69:VAL:HG13 | 1:B:71:GLY:H | 6 | 0.02 |
| (1,1241) | 1:A:69:VAL:HG11 | 1:A:71:GLY:H | 10 | 0.02 |
| (1,1241) | 1:A:69:VAL:HG12 | 1:A:71:GLY:H | 10 | 0.02 |
| (1,1241) | 1:A:69:VAL:HG13 | 1:A:71:GLY:H | 10 | 0.02 |
| (1,1226) | 1:B:69:VAL:H | 1:B:70:GLN:H | 3 | 0.02 |
| (1,1226) | 1:B:69:VAL:H | 1:B:70:GLN:H | 15 | 0.02 |
| (1,1225) | 1:A:69:VAL:H | 1:A:70:GLN:H | 17 | 0.02 |
| (1,1222) | 1:B:69:VAL:H | 1:B:72:VAL:H | 5 | 0.02 |
| (1,1184) | 1:B:68:LYS:H | 1:B:75:VAL:HG21 | 11 | 0.02 |
| (1,1184) | 1:B:68:LYS:H | 1:B:75:VAL:HG22 | 11 | 0.02 |
| (1,1184) | 1:B:68:LYS:H | 1:B:75:VAL:HG23 | 11 | 0.02 |
| (1,1150) | 1:B:67:ARG:H | 1:B:69:VAL:HG21 | 9 | 0.02 |
| (1,1150) | 1:B:67:ARG:H | 1:B:69:VAL:HG22 | 9 | 0.02 |
| (1,1150) | 1:B:67:ARG:H | 1:B:69:VAL:HG23 | 9 | 0.02 |
| (1,1150) | 1:B:67:ARG:H | 1:B:69:VAL:HG21 | 14 | 0.02 |
| (1,1150) | 1:B:67:ARG:H | 1:B:69:VAL:HG22 | 14 | 0.02 |
| (1,1150) | 1:B:67:ARG:H | 1:B:69:VAL:HG23 | 14 | 0.02 |
| (1,1149) | 1:A:67:ARG:H | 1:A:69:VAL:HG21 | 19 | 0.02 |
| (1,1149) | 1:A:67:ARG:H | 1:A:69:VAL:HG22 | 19 | 0.02 |
| (1,1149) | 1:A:67:ARG:H | 1:A:69:VAL:HG23 | 19 | 0.02 |
| (1,1132) | 1:B:62:LEU:HD11 | 1:B:66:LEU:H | 15 | 0.02 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1132) | 1:B:62:LEU:HD12 | 1:B:66:LEU:H | 15 | 0.02 |
| (1,1132) | 1:B:62:LEU:HD13 | 1:B:66:LEU:H | 15 | 0.02 |
| (1,1132) | 1:B:62:LEU:HD11 | 1:B:66:LEU:H | 18 | 0.02 |
| (1,1132) | 1:B:62:LEU:HD12 | 1:B:66:LEU:H | 18 | 0.02 |
| (1,1132) | 1:B:62:LEU:HD13 | 1:B:66:LEU:H | 18 | 0.02 |
| (1,1131) | 1:A:62:LEU:HD11 | 1:A:66:LEU:H | 1 | 0.02 |
| (1,1131) | 1:A:62:LEU:HD12 | 1:A:66:LEU:H | 1 | 0.02 |
| (1,1131) | 1:A:62:LEU:HD13 | 1:A:66:LEU:H | 1 | 0.02 |
| (1,1131) | 1:A:62:LEU:HD11 | 1:A:66:LEU:H | 8 | 0.02 |
| (1,1131) | 1:A:62:LEU:HD12 | 1:A:66:LEU:H | 8 | 0.02 |
| (1,1131) | 1:A:62:LEU:HD13 | 1:A:66:LEU:H | 8 | 0.02 |
| (1,1131) | 1:A:62:LEU:HD11 | 1:A:66:LEU:H | 17 | 0.02 |
| (1,1131) | 1:A:62:LEU:HD12 | 1:A:66:LEU:H | 17 | 0.02 |
| (1,1131) | 1:A:62:LEU:HD13 | 1:A:66:LEU:H | 17 | 0.02 |
| (1,1130) | 1:B:62:LEU:HD11 | 1:B:65:LYS:H | 13 | 0.02 |
| (1,1130) | 1:B:62:LEU:HD12 | 1:B:65:LYS:H | 13 | 0.02 |
| (1,1130) | 1:B:62:LEU:HD13 | 1:B:65:LYS:H | 13 | 0.02 |
| (1,1130) | 1:B:62:LEU:HD11 | 1:B:65:LYS:H | 19 | 0.02 |
| (1,1130) | 1:B:62:LEU:HD12 | 1:B:65:LYS:H | 19 | 0.02 |
| (1,1130) | 1:B:62:LEU:HD13 | 1:B:65:LYS:H | 19 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD11 | 1:A:65:LYS:H | 5 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD12 | 1:A:65:LYS:H | 5 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD13 | 1:A:65:LYS:H | 5 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD11 | 1:A:65:LYS:H | 8 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD12 | 1:A:65:LYS:H | 8 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD13 | 1:A:65:LYS:H | 8 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD11 | 1:A:65:LYS:H | 10 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD12 | 1:A:65:LYS:H | 10 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD13 | 1:A:65:LYS:H | 10 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD11 | 1:A:65:LYS:H | 12 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD12 | 1:A:65:LYS:H | 12 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD13 | 1:A:65:LYS:H | 12 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD11 | 1:A:65:LYS:H | 14 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD12 | 1:A:65:LYS:H | 14 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD13 | 1:A:65:LYS:H | 14 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD11 | 1:A:65:LYS:H | 17 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD12 | 1:A:65:LYS:H | 17 | 0.02 |
| (1,1129) | 1:A:62:LEU:HD13 | 1:A:65:LYS:H | 17 | 0.02 |
| (1,1091) | 1:B:64:ASP:H | 1:B:75:VAL:HG11 | 9 | 0.02 |
| (1,1091) | 1:B:64:ASP:H | 1:B:75:VAL:HG12 | 9 | 0.02 |
| (1,1091) | 1:B:64:ASP:H | 1:B:75:VAL:HG13 | 9 | 0.02 |
| (1,979) | 1:B:58:LYS:H | 1:B:58:LYS:HG3 | 5 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,979) | 1:B:58:LYS:H | 1:B:58:LYS:HG3 | 8 | 0.01 |
| (1,979) | 1:B:58:LYS:H | 1:B:58:LYS:HG3 | 9 | 0.01 |
| (1,979) | 1:B:58:LYS:H | 1:B:58:LYS:HG3 | 15 | 0.01 |
| (1,979) | 1:B:58:LYS:H | 1:B:58:LYS:HG3 | 17 | 0.01 |
| (1,978) | 1:A:58:LYS:H | 1:A:58:LYS:HG3 | 4 | 0.01 |
| (1,978) | 1:A:58:LYS:H | 1:A:58:LYS:HG3 | 8 | 0.01 |
| (1,978) | 1:A:58:LYS:H | 1:A:58:LYS:HG3 | 13 | 0.01 |
| (1,915) | 1:B:51:ILE:HG12 | 1:B:52:PHE:H | 2 | 0.01 |
| (1,914) | 1:A:51:ILE:HG12 | 1:A:52:PHE:H | 7 | 0.01 |
| (1,914) | 1:A:51:ILE:HG12 | 1:A:52:PHE:H | 10 | 0.01 |
| (1,914) | 1:A:51:ILE:HG12 | 1:A:52:PHE:H | 14 | 0.01 |
| (1,85) | 1:B:9:ARG:HE | 1:B:11:VAL:HG21 | 8 | 0.01 |
| (1,85) | 1:B:9:ARG:HE | 1:B:11:VAL:HG22 | 8 | 0.01 |
| (1,85) | 1:B:9:ARG:HE | 1:B:11:VAL:HG23 | 8 | 0.01 |
| (1,849) | 1:B:47:CYS:HG | 1:B:48:ASN:H | 14 | 0.01 |
| (1,849) | 1:B:47:CYS:HG | 1:B:48:ASN:H | 17 | 0.01 |
| (1,848) | 1:A:47:CYS:HG | 1:A:48:ASN:H | 5 | 0.01 |
| (1,845) | 1:B:36:ILE:HD11 | 1:B:48:ASN:H | 8 | 0.01 |
| (1,845) | 1:B:36:ILE:HD12 | 1:B:48:ASN:H | 8 | 0.01 |
| (1,845) | 1:B:36:ILE:HD13 | 1:B:48:ASN:H | 8 | 0.01 |
| (1,845) | 1:B:36:ILE:HD11 | 1:B:48:ASN:H | 20 | 0.01 |
| (1,845) | 1:B:36:ILE:HD12 | 1:B:48:ASN:H | 20 | 0.01 |
| (1,845) | 1:B:36:ILE:HD13 | 1:B:48:ASN:H | 20 | 0.01 |
| (1,839) | 1:B:45:PHE:HZ | 1:B:47:CYS:H | 6 | 0.01 |
| (1,777) | 1:B:43:GLY:H | 1:B:44:ILE:H | 1 | 0.01 |
| (1,761) | 1:B:44:ILE:H | 1:B:44:ILE:HG21 | 15 | 0.01 |
| (1,761) | 1:B:44:ILE:H | 1:B:44:ILE:HG22 | 15 | 0.01 |
| (1,761) | 1:B:44:ILE:H | 1:B:44:ILE:HG23 | 15 | 0.01 |
| (1,760) | 1:A:44:ILE:H | 1:A:44:ILE:HG21 | 10 | 0.01 |
| (1,760) | 1:A:44:ILE:H | 1:A:44:ILE:HG22 | 10 | 0.01 |
| (1,760) | 1:A:44:ILE:H | 1:A:44:ILE:HG23 | 10 | 0.01 |
| (1,739) | 1:B:41:LYS:H | 1:B:43:GLY:H | 14 | 0.01 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD1 | 15 | 0.01 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD2 | 15 | 0.01 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD1 | 20 | 0.01 |
| (1,733) | 1:B:41:LYS:H | 1:B:45:PHE:HD2 | 20 | 0.01 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD1 | 6 | 0.01 |
| (1,732) | 1:A:41:LYS:H | 1:A:45:PHE:HD2 | 6 | 0.01 |
| (1,711) | 1:B:41:LYS:H | 1:B:44:ILE:HG21 | 1 | 0.01 |
| (1,711) | 1:B:41:LYS:H | 1:B:44:ILE:HG22 | 1 | 0.01 |
| (1,711) | 1:B:41:LYS:H | 1:B:44:ILE:HG23 | 1 | 0.01 |
| (1,631) | 1:B:35:THR:H | 1:B:83:HIS:HE1 | 20 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|------------------|------------------|-------|---------------|
| (1,593) | 1:A:32:ASN:HD22 | 1:B:17:GLY:H | 3 | 0.01 |
| (1,581) | 1:B:32:ASN:HA | 1:B:32:ASN:HD21 | 4 | 0.01 |
| (1,581) | 1:B:32:ASN:HA | 1:B:32:ASN:HD21 | 6 | 0.01 |
| (1,579) | 1:A:32:ASN:HD21 | 1:A:33:ILE:HB | 6 | 0.01 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD11 | 1 | 0.01 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD12 | 1 | 0.01 |
| (1,568) | 1:B:32:ASN:H | 1:B:51:ILE:HD13 | 1 | 0.01 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD11 | 6 | 0.01 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD12 | 6 | 0.01 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD13 | 6 | 0.01 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD11 | 16 | 0.01 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD12 | 16 | 0.01 |
| (1,567) | 1:A:32:ASN:H | 1:A:51:ILE:HD13 | 16 | 0.01 |
| (1,562) | 1:B:29:PHE:HD1 | 1:B:31:THR:H | 2 | 0.01 |
| (1,562) | 1:B:29:PHE:HD2 | 1:B:31:THR:H | 2 | 0.01 |
| (1,562) | 1:B:29:PHE:HD1 | 1:B:31:THR:H | 7 | 0.01 |
| (1,562) | 1:B:29:PHE:HD2 | 1:B:31:THR:H | 7 | 0.01 |
| (1,562) | 1:B:29:PHE:HD1 | 1:B:31:THR:H | 13 | 0.01 |
| (1,562) | 1:B:29:PHE:HD2 | 1:B:31:THR:H | 13 | 0.01 |
| (1,562) | 1:B:29:PHE:HD1 | 1:B:31:THR:H | 14 | 0.01 |
| (1,562) | 1:B:29:PHE:HD2 | 1:B:31:THR:H | 14 | 0.01 |
| (1,562) | 1:B:29:PHE:HD1 | 1:B:31:THR:H | 17 | 0.01 |
| (1,562) | 1:B:29:PHE:HD2 | 1:B:31:THR:H | 17 | 0.01 |
| (1,561) | 1:A:29:PHE:HD1 | 1:A:31:THR:H | 5 | 0.01 |
| (1,561) | 1:A:29:PHE:HD2 | 1:A:31:THR:H | 5 | 0.01 |
| (1,561) | 1:A:29:PHE:HD1 | 1:A:31:THR:H | 7 | 0.01 |
| (1,561) | 1:A:29:PHE:HD2 | 1:A:31:THR:H | 7 | 0.01 |
| (1,561) | 1:A:29:PHE:HD1 | 1:A:31:THR:H | 11 | 0.01 |
| (1,561) | 1:A:29:PHE:HD2 | 1:A:31:THR:H | 11 | 0.01 |
| (1,558) | 1:B:30:ASP:HA | 1:B:31:THR:H | 3 | 0.01 |
| (1,557) | 1:A:30:ASP:HA | 1:A:31:THR:H | 9 | 0.01 |
| (1,557) | 1:A:30:ASP:HA | 1:A:31:THR:H | 18 | 0.01 |
| (1,5242) | 1:B:68:LYS:HA | 1:B:68:LYS:HG2 | 8 | 0.01 |
| (1,5242) | 1:B:68:LYS:HA | 1:B:68:LYS:HG2 | 11 | 0.01 |
| (1,5242) | 1:B:68:LYS:HA | 1:B:68:LYS:HG2 | 12 | 0.01 |
| (1,5242) | 1:B:68:LYS:HA | 1:B:68:LYS:HG2 | 19 | 0.01 |
| (1,5231) | 1:B:66:LEU:HB2 | 1:B:75:VAL:HG11 | 20 | 0.01 |
| (1,5231) | 1:B:66:LEU:HB2 | 1:B:75:VAL:HG12 | 20 | 0.01 |
| (1,5231) | 1:B:66:LEU:HB2 | 1:B:75:VAL:HG13 | 20 | 0.01 |
| (1,5223) | 1:B:65:LYS:H | 1:B:65:LYS:HD2 | 1 | 0.01 |
| (1,5223) | 1:B:65:LYS:H | 1:B:65:LYS:HD2 | 3 | 0.01 |
| (1,5223) | 1:B:65:LYS:H | 1:B:65:LYS:HD2 | 17 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5216) | 1:B:63:MET:HE1 | 1:B:77:ARG:HB2 | 6 | 0.01 |
| (1,5216) | 1:B:63:MET:HE2 | 1:B:77:ARG:HB2 | 6 | 0.01 |
| (1,5216) | 1:B:63:MET:HE3 | 1:B:77:ARG:HB2 | 6 | 0.01 |
| (1,5205) | 1:B:62:LEU:H | 1:B:65:LYS:HD2 | 8 | 0.01 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD21 | 7 | 0.01 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD22 | 7 | 0.01 |
| (1,5195) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD23 | 7 | 0.01 |
| (1,5192) | 1:B:58:LYS:HE2 | 1:B:59:LEU:HA | 3 | 0.01 |
| (1,5182) | 1:B:55:ASN:HD21 | 1:B:58:LYS:HG3 | 5 | 0.01 |
| (1,5170) | 1:B:54:LYS:HB2 | 1:B:55:ASN:HB2 | 9 | 0.01 |
| (1,5167) | 1:B:53:VAL:HG21 | 1:B:58:LYS:HB2 | 14 | 0.01 |
| (1,5167) | 1:B:53:VAL:HG22 | 1:B:58:LYS:HB2 | 14 | 0.01 |
| (1,5167) | 1:B:53:VAL:HG23 | 1:B:58:LYS:HB2 | 14 | 0.01 |
| (1,5165) | 1:B:53:VAL:HG21 | 1:B:54:LYS:HB2 | 12 | 0.01 |
| (1,5165) | 1:B:53:VAL:HG22 | 1:B:54:LYS:HB2 | 12 | 0.01 |
| (1,5165) | 1:B:53:VAL:HG23 | 1:B:54:LYS:HB2 | 12 | 0.01 |
| (1,5164) | 1:B:53:VAL:HG11 | 1:B:58:LYS:HE2 | 6 | 0.01 |
| (1,5164) | 1:B:53:VAL:HG12 | 1:B:58:LYS:HE2 | 6 | 0.01 |
| (1,5164) | 1:B:53:VAL:HG13 | 1:B:58:LYS:HE2 | 6 | 0.01 |
| (1,5122) | 1:B:37:VAL:HB | 1:B:48:ASN:HB2 | 10 | 0.01 |
| (1,5122) | 1:B:37:VAL:HB | 1:B:48:ASN:HB2 | 19 | 0.01 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG21 | 1 | 0.01 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG22 | 1 | 0.01 |
| (1,5119) | 1:B:36:ILE:HG12 | 1:B:37:VAL:HG23 | 1 | 0.01 |
| (1,5114) | 1:B:35:THR:HB | 1:B:50:MET:HB2 | 18 | 0.01 |
| (1,5108) | 1:B:34:ARG:HB2 | 1:B:51:ILE:H | 2 | 0.01 |
| (1,5092) | 1:B:32:ASN:HA | 1:B:32:ASN:HD21 | 4 | 0.01 |
| (1,5092) | 1:B:32:ASN:HA | 1:B:32:ASN:HD21 | 6 | 0.01 |
| (1,5067) | 1:B:28:LYS:H | 1:B:28:LYS:HG2 | 10 | 0.01 |
| (1,5067) | 1:B:28:LYS:H | 1:B:28:LYS:HG2 | 12 | 0.01 |
| (1,5067) | 1:B:28:LYS:H | 1:B:28:LYS:HG2 | 15 | 0.01 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD11 | 20 | 0.01 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD12 | 20 | 0.01 |
| (1,5064) | 1:B:27:SER:HB2 | 1:B:33:ILE:HD13 | 20 | 0.01 |
| (1,5063) | 1:B:27:SER:HB2 | 1:B:28:LYS:H | 19 | 0.01 |
| (1,5063) | 1:B:27:SER:HB2 | 1:B:28:LYS:H | 20 | 0.01 |
| (1,5056) | 1:B:26:ILE:HG12 | 1:B:27:SER:H | 12 | 0.01 |
| (1,5052) | 1:B:25:VAL:HG21 | 1:B:28:LYS:HG2 | 4 | 0.01 |
| (1,5052) | 1:B:25:VAL:HG22 | 1:B:28:LYS:HG2 | 4 | 0.01 |
| (1,5052) | 1:B:25:VAL:HG23 | 1:B:28:LYS:HG2 | 4 | 0.01 |
| (1,5051) | 1:B:25:VAL:HG11 | 1:B:28:LYS:HD2 | 10 | 0.01 |
| (1,5051) | 1:B:25:VAL:HG12 | 1:B:28:LYS:HD2 | 10 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,5051) | 1:B:25:VAL:HG13 | 1:B:28:LYS:HD2 | 10 | 0.01 |
| (1,5041) | 1:B:24:GLY:HA2 | 1:B:28:LYS:HG2 | 14 | 0.01 |
| (1,5029) | 1:B:20:ASN:HB2 | 1:B:21:GLN:HE21 | 1 | 0.01 |
| (1,5029) | 1:B:20:ASN:HB2 | 1:B:21:GLN:HE21 | 20 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 1 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 1 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 1 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 2 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 2 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 2 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 4 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 4 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 4 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 11 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 11 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 11 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 15 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 15 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 15 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 18 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 18 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 18 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE1 | 20 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE2 | 20 | 0.01 |
| (1,5020) | 1:B:18:MET:HG2 | 1:B:18:MET:HE3 | 20 | 0.01 |
| (1,5019) | 1:B:17:GLY:HA2 | 1:B:21:GLN:HE22 | 1 | 0.01 |
| (1,5007) | 1:B:15:LYS:HD2 | 1:B:16:ASN:HB2 | 8 | 0.01 |
| (1,5007) | 1:B:15:LYS:HD3 | 1:B:16:ASN:HB2 | 8 | 0.01 |
| (1,5006) | 1:B:15:LYS:HG2 | 1:B:18:MET:HG2 | 18 | 0.01 |
| (1,5006) | 1:B:15:LYS:HG3 | 1:B:18:MET:HG2 | 18 | 0.01 |
| (1,5002) | 1:B:15:LYS:HB2 | 1:B:18:MET:HG2 | 15 | 0.01 |
| (1,4977) | 1:B:8:ILE:HG12 | 1:B:77:ARG:HB2 | 7 | 0.01 |
| (1,4972) | 1:B:8:ILE:HG12 | 1:B:49:LEU:HB3 | 18 | 0.01 |
| (1,4930) | 1:A:68:LYS:HA | 1:A:68:LYS:HG2 | 13 | 0.01 |
| (1,4930) | 1:A:68:LYS:HA | 1:A:68:LYS:HG2 | 17 | 0.01 |
| (1,4929) | 1:A:68:LYS:H | 1:A:68:LYS:HD2 | 12 | 0.01 |
| (1,4923) | 1:A:67:ARG:HG2 | 1:A:68:LYS:H | 12 | 0.01 |
| (1,4923) | 1:A:67:ARG:HG2 | 1:A:68:LYS:H | 15 | 0.01 |
| (1,4919) | 1:A:66:LEU:HB2 | 1:A:75:VAL:HG11 | 2 | 0.01 |
| (1,4919) | 1:A:66:LEU:HB2 | 1:A:75:VAL:HG12 | 2 | 0.01 |
| (1,4919) | 1:A:66:LEU:HB2 | 1:A:75:VAL:HG13 | 2 | 0.01 |
| (1,4912) | 1:A:65:LYS:H | 1:A:65:LYS:HD2 | 19 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,4909) | 1:A:63:MET:HE1 | 1:A:77:ARG:HB2 | 9 | 0.01 |
| (1,4909) | 1:A:63:MET:HE2 | 1:A:77:ARG:HB2 | 9 | 0.01 |
| (1,4909) | 1:A:63:MET:HE3 | 1:A:77:ARG:HB2 | 9 | 0.01 |
| (1,4902) | 1:A:62:LEU:H | 1:A:65:LYS:HD2 | 10 | 0.01 |
| (1,4882) | 1:A:56:THR:HG21 | 1:A:59:LEU:HB2 | 9 | 0.01 |
| (1,4882) | 1:A:56:THR:HG22 | 1:A:59:LEU:HB2 | 9 | 0.01 |
| (1,4882) | 1:A:56:THR:HG23 | 1:A:59:LEU:HB2 | 9 | 0.01 |
| (1,4869) | 1:A:54:LYS:HG2 | 1:A:55:ASN:H | 1 | 0.01 |
| (1,4867) | 1:A:54:LYS:HB2 | 1:A:55:ASN:HB2 | 15 | 0.01 |
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 1 | 0.01 |
| (1,4859) | 1:A:53:VAL:HA | 1:A:54:LYS:HB2 | 6 | 0.01 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG21 | 3 | 0.01 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG22 | 3 | 0.01 |
| (1,4815) | 1:A:36:ILE:HG12 | 1:A:37:VAL:HG23 | 3 | 0.01 |
| (1,4813) | 1:A:36:ILE:HG12 | 1:A:37:VAL:H | 19 | 0.01 |
| (1,4809) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 4 | 0.01 |
| (1,4809) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 8 | 0.01 |
| (1,4809) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 13 | 0.01 |
| (1,4809) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 15 | 0.01 |
| (1,4809) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 19 | 0.01 |
| (1,4809) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 20 | 0.01 |
| (1,4787) | 1:A:29:PHE:HE1 | 1:A:65:LYS:HD2 | 14 | 0.01 |
| (1,4786) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 4 | 0.01 |
| (1,4786) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 4 | 0.01 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD11 | 15 | 0.01 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD12 | 15 | 0.01 |
| (1,4784) | 1:A:29:PHE:HB2 | 1:A:62:LEU:HD13 | 15 | 0.01 |
| (1,478) | 1:B:25:VAL:HB | 1:B:27:SER:H | 9 | 0.01 |
| (1,478) | 1:B:25:VAL:HB | 1:B:27:SER:H | 20 | 0.01 |
| (1,4774) | 1:A:28:LYS:HB2 | 1:A:28:LYS:HD2 | 2 | 0.01 |
| (1,477) | 1:A:25:VAL:HB | 1:A:27:SER:H | 4 | 0.01 |
| (1,4769) | 1:A:28:LYS:H | 1:A:28:LYS:HG2 | 19 | 0.01 |
| (1,4762) | 1:A:27:SER:HB2 | 1:A:28:LYS:H | 1 | 0.01 |
| (1,4762) | 1:A:27:SER:HB2 | 1:A:28:LYS:H | 13 | 0.01 |
| (1,4724) | 1:A:20:ASN:HB2 | 1:A:21:GLN:HE21 | 10 | 0.01 |
| (1,4723) | 1:A:20:ASN:HB2 | 1:A:21:GLN:H | 14 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE1 | 5 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE2 | 5 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE3 | 5 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE1 | 7 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE2 | 7 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE3 | 7 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE1 | 8 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE2 | 8 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE3 | 8 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE1 | 10 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE2 | 10 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE3 | 10 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE1 | 13 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE2 | 13 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE3 | 13 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE1 | 14 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE2 | 14 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE3 | 14 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE1 | 16 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE2 | 16 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE3 | 16 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE1 | 18 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE2 | 18 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE3 | 18 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE1 | 19 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE2 | 19 | 0.01 |
| (1,4712) | 1:A:18:MET:HG2 | 1:A:18:MET:HE3 | 19 | 0.01 |
| (1,4710) | 1:A:18:MET:HB2 | 1:A:22:ILE:HG12 | 7 | 0.01 |
| (1,4672) | 1:A:14:ASP:HB2 | 1:A:43:GLY:HA2 | 18 | 0.01 |
| (1,4671) | 1:A:14:ASP:HB2 | 1:A:43:GLY:H | 14 | 0.01 |
| (1,4627) | 1:A:3:ASP:HA | 1:A:54:LYS:HB2 | 5 | 0.01 |
| (1,4624) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HE1 | 19 | 0.01 |
| (1,4624) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HE1 | 19 | 0.01 |
| (1,4624) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HE1 | 19 | 0.01 |
| (1,4610) | 1:B:81:LEU:HB3 | 1:B:83:HIS:HD2 | 10 | 0.01 |
| (1,4610) | 1:B:81:LEU:HB3 | 1:B:83:HIS:HD2 | 19 | 0.01 |
| (1,4609) | 1:A:81:LEU:HB3 | 1:A:83:HIS:HD2 | 6 | 0.01 |
| (1,4609) | 1:A:81:LEU:HB3 | 1:A:83:HIS:HD2 | 8 | 0.01 |
| (1,4609) | 1:A:81:LEU:HB3 | 1:A:83:HIS:HD2 | 11 | 0.01 |
| (1,4609) | 1:A:81:LEU:HB3 | 1:A:83:HIS:HD2 | 16 | 0.01 |
| (1,4608) | 1:B:5:LEU:HG | 1:B:83:HIS:HD2 | 6 | 0.01 |
| (1,4607) | 1:A:5:LEU:HG | 1:A:83:HIS:HD2 | 14 | 0.01 |
| (1,4607) | 1:A:5:LEU:HG | 1:A:83:HIS:HD2 | 18 | 0.01 |
| (1,4607) | 1:A:5:LEU:HG | 1:A:83:HIS:HD2 | 20 | 0.01 |
| (1,4606) | 1:B:81:LEU:HD11 | 1:B:83:HIS:HD2 | 5 | 0.01 |
| (1,4606) | 1:B:81:LEU:HD12 | 1:B:83:HIS:HD2 | 5 | 0.01 |
| (1,4606) | 1:B:81:LEU:HD13 | 1:B:83:HIS:HD2 | 5 | 0.01 |
| (1,4601) | 1:A:5:LEU:HD21 | 1:A:83:HIS:HD2 | 2 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,4601) | 1:A:5:LEU:HD22 | 1:A:83:HIS:HD2 | 2 | 0.01 |
| (1,4601) | 1:A:5:LEU:HD23 | 1:A:83:HIS:HD2 | 2 | 0.01 |
| (1,4601) | 1:A:5:LEU:HD21 | 1:A:83:HIS:HD2 | 5 | 0.01 |
| (1,4601) | 1:A:5:LEU:HD22 | 1:A:83:HIS:HD2 | 5 | 0.01 |
| (1,4601) | 1:A:5:LEU:HD23 | 1:A:83:HIS:HD2 | 5 | 0.01 |
| (1,4588) | 1:B:13:GLU:HB3 | 1:B:73:PHE:HZ | 17 | 0.01 |
| (1,4587) | 1:A:13:GLU:HB3 | 1:A:73:PHE:HZ | 20 | 0.01 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG21 | 11 | 0.01 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG22 | 11 | 0.01 |
| (1,4586) | 1:B:73:PHE:HZ | 1:B:74:THR:HG23 | 11 | 0.01 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG21 | 5 | 0.01 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG22 | 5 | 0.01 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG23 | 5 | 0.01 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG21 | 18 | 0.01 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG22 | 18 | 0.01 |
| (1,4585) | 1:A:73:PHE:HZ | 1:A:74:THR:HG23 | 18 | 0.01 |
| (1,4567) | 1:A:44:ILE:HG21 | 1:A:73:PHE:HE1 | 13 | 0.01 |
| (1,4567) | 1:A:44:ILE:HG22 | 1:A:73:PHE:HE1 | 13 | 0.01 |
| (1,4567) | 1:A:44:ILE:HG23 | 1:A:73:PHE:HE1 | 13 | 0.01 |
| (1,4544) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HE1 | 11 | 0.01 |
| (1,4544) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HE1 | 11 | 0.01 |
| (1,4544) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HE1 | 11 | 0.01 |
| (1,4540) | 1:B:6:ALA:H | 1:B:52:PHE:HD1 | 2 | 0.01 |
| (1,4540) | 1:B:6:ALA:H | 1:B:52:PHE:HD2 | 2 | 0.01 |
| (1,4539) | 1:A:6:ALA:H | 1:A:52:PHE:HD1 | 7 | 0.01 |
| (1,4539) | 1:A:6:ALA:H | 1:A:52:PHE:HD2 | 7 | 0.01 |
| (1,4538) | 1:B:52:PHE:HD1 | 1:B:53:VAL:H | 17 | 0.01 |
| (1,4538) | 1:B:52:PHE:HD2 | 1:B:53:VAL:H | 17 | 0.01 |
| (1,4537) | 1:A:52:PHE:HD1 | 1:A:53:VAL:H | 3 | 0.01 |
| (1,4537) | 1:A:52:PHE:HD2 | 1:A:53:VAL:H | 3 | 0.01 |
| (1,4537) | 1:A:52:PHE:HD1 | 1:A:53:VAL:H | 14 | 0.01 |
| (1,4537) | 1:A:52:PHE:HD2 | 1:A:53:VAL:H | 14 | 0.01 |
| (1,4526) | 1:B:5:LEU:HA | 1:B:52:PHE:HD1 | 11 | 0.01 |
| (1,4526) | 1:B:5:LEU:HA | 1:B:52:PHE:HD2 | 11 | 0.01 |
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD1 | 8 | 0.01 |
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD2 | 8 | 0.01 |
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD1 | 19 | 0.01 |
| (1,4525) | 1:A:5:LEU:HA | 1:A:52:PHE:HD2 | 19 | 0.01 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 3 | 0.01 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 5 | 0.01 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 6 | 0.01 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 11 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 15 | 0.01 |
| (1,4508) | 1:B:22:ILE:HG13 | 1:B:45:PHE:HZ | 18 | 0.01 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 16 | 0.01 |
| (1,4507) | 1:A:22:ILE:HG13 | 1:A:45:PHE:HZ | 19 | 0.01 |
| (1,4496) | 1:B:12:GLY:H | 1:B:45:PHE:HE1 | 3 | 0.01 |
| (1,4496) | 1:B:12:GLY:H | 1:B:45:PHE:HE1 | 17 | 0.01 |
| (1,4496) | 1:B:12:GLY:H | 1:B:45:PHE:HE1 | 20 | 0.01 |
| (1,4477) | 1:A:19:THR:HG21 | 1:A:45:PHE:HE1 | 8 | 0.01 |
| (1,4477) | 1:A:19:THR:HG22 | 1:A:45:PHE:HE1 | 8 | 0.01 |
| (1,4477) | 1:A:19:THR:HG23 | 1:A:45:PHE:HE1 | 8 | 0.01 |
| (1,4476) | 1:B:22:ILE:HD11 | 1:B:45:PHE:HE1 | 10 | 0.01 |
| (1,4476) | 1:B:22:ILE:HD12 | 1:B:45:PHE:HE1 | 10 | 0.01 |
| (1,4476) | 1:B:22:ILE:HD13 | 1:B:45:PHE:HE1 | 10 | 0.01 |
| (1,4473) | 1:A:38:LEU:HD11 | 1:A:45:PHE:HE1 | 11 | 0.01 |
| (1,4473) | 1:A:38:LEU:HD12 | 1:A:45:PHE:HE1 | 11 | 0.01 |
| (1,4473) | 1:A:38:LEU:HD13 | 1:A:45:PHE:HE1 | 11 | 0.01 |
| (1,4447) | 1:B:40:ALA:HB1 | 1:B:45:PHE:HD1 | 13 | 0.01 |
| (1,4447) | 1:B:40:ALA:HB1 | 1:B:45:PHE:HD2 | 13 | 0.01 |
| (1,4447) | 1:B:40:ALA:HB2 | 1:B:45:PHE:HD1 | 13 | 0.01 |
| (1,4447) | 1:B:40:ALA:HB2 | 1:B:45:PHE:HD2 | 13 | 0.01 |
| (1,4447) | 1:B:40:ALA:HB3 | 1:B:45:PHE:HD1 | 13 | 0.01 |
| (1,4447) | 1:B:40:ALA:HB3 | 1:B:45:PHE:HD2 | 13 | 0.01 |
| (1,4419) | 1:B:29:PHE:H | 1:B:29:PHE:HD1 | 12 | 0.01 |
| (1,4419) | 1:B:29:PHE:H | 1:B:29:PHE:HD2 | 12 | 0.01 |
| (1,4418) | 1:A:29:PHE:H | 1:A:29:PHE:HD1 | 20 | 0.01 |
| (1,4418) | 1:A:29:PHE:H | 1:A:29:PHE:HD2 | 20 | 0.01 |
| (1,4416) | 1:A:29:PHE:HA | 1:A:29:PHE:HD1 | 12 | 0.01 |
| (1,4416) | 1:A:29:PHE:HA | 1:A:29:PHE:HD2 | 12 | 0.01 |
| (1,4413) | 1:B:29:PHE:HD1 | 1:B:65:LYS:HD2 | 17 | 0.01 |
| (1,4413) | 1:B:29:PHE:HD2 | 1:B:65:LYS:HD2 | 17 | 0.01 |
| (1,4412) | 1:A:29:PHE:HD1 | 1:A:65:LYS:HD2 | 20 | 0.01 |
| (1,4412) | 1:A:29:PHE:HD2 | 1:A:65:LYS:HD2 | 20 | 0.01 |
| (1,4393) | 1:B:4:PHE:HZ | 1:B:6:ALA:HA | 6 | 0.01 |
| (1,4393) | 1:B:4:PHE:HZ | 1:B:6:ALA:HA | 17 | 0.01 |
| (1,4393) | 1:B:4:PHE:HZ | 1:B:6:ALA:HA | 18 | 0.01 |
| (1,4392) | 1:A:4:PHE:HZ | 1:A:6:ALA:HA | 1 | 0.01 |
| (1,4392) | 1:A:4:PHE:HZ | 1:A:6:ALA:HA | 8 | 0.01 |
| (1,4392) | 1:A:4:PHE:HZ | 1:A:6:ALA:HA | 9 | 0.01 |
| (1,4392) | 1:A:4:PHE:HZ | 1:A:6:ALA:HA | 17 | 0.01 |
| (1,4388) | 1:A:4:PHE:HZ | 1:A:56:THR:HA | 15 | 0.01 |
| (1,4385) | 1:B:4:PHE:HZ | 1:B:59:LEU:HD21 | 4 | 0.01 |
| (1,4385) | 1:B:4:PHE:HZ | 1:B:59:LEU:HD22 | 4 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4385) | 1:B:4:PHE:HZ | 1:B:59:LEU:HD23 | 4 | 0.01 |
| (1,4363) | 1:B:29:PHE:HE1 | 1:B:66:LEU:HG | 12 | 0.01 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD21 | 10 | 0.01 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD22 | 10 | 0.01 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD23 | 10 | 0.01 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD21 | 15 | 0.01 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD22 | 15 | 0.01 |
| (1,4357) | 1:B:4:PHE:HE1 | 1:B:59:LEU:HD23 | 15 | 0.01 |
| (1,4351) | 1:B:4:PHE:HD1 | 1:B:5:LEU:H | 3 | 0.01 |
| (1,4351) | 1:B:4:PHE:HD2 | 1:B:5:LEU:H | 3 | 0.01 |
| (1,4351) | 1:B:4:PHE:HD1 | 1:B:5:LEU:H | 4 | 0.01 |
| (1,4351) | 1:B:4:PHE:HD2 | 1:B:5:LEU:H | 4 | 0.01 |
| (1,4351) | 1:B:4:PHE:HD1 | 1:B:5:LEU:H | 5 | 0.01 |
| (1,4351) | 1:B:4:PHE:HD2 | 1:B:5:LEU:H | 5 | 0.01 |
| (1,4351) | 1:B:4:PHE:HD1 | 1:B:5:LEU:H | 8 | 0.01 |
| (1,4351) | 1:B:4:PHE:HD2 | 1:B:5:LEU:H | 8 | 0.01 |
| (1,4351) | 1:B:4:PHE:HD1 | 1:B:5:LEU:H | 10 | 0.01 |
| (1,4351) | 1:B:4:PHE:HD2 | 1:B:5:LEU:H | 10 | 0.01 |
| (1,4351) | 1:B:4:PHE:HD1 | 1:B:5:LEU:H | 17 | 0.01 |
| (1,4351) | 1:B:4:PHE:HD2 | 1:B:5:LEU:H | 17 | 0.01 |
| (1,4351) | 1:B:4:PHE:HD1 | 1:B:5:LEU:H | 20 | 0.01 |
| (1,4351) | 1:B:4:PHE:HD2 | 1:B:5:LEU:H | 20 | 0.01 |
| (1,4350) | 1:A:4:PHE:HD1 | 1:A:5:LEU:H | 2 | 0.01 |
| (1,4350) | 1:A:4:PHE:HD2 | 1:A:5:LEU:H | 2 | 0.01 |
| (1,4350) | 1:A:4:PHE:HD1 | 1:A:5:LEU:H | 5 | 0.01 |
| (1,4350) | 1:A:4:PHE:HD2 | 1:A:5:LEU:H | 5 | 0.01 |
| (1,4350) | 1:A:4:PHE:HD1 | 1:A:5:LEU:H | 8 | 0.01 |
| (1,4350) | 1:A:4:PHE:HD2 | 1:A:5:LEU:H | 8 | 0.01 |
| (1,4350) | 1:A:4:PHE:HD1 | 1:A:5:LEU:H | 18 | 0.01 |
| (1,4350) | 1:A:4:PHE:HD2 | 1:A:5:LEU:H | 18 | 0.01 |
| (1,4345) | 1:B:4:PHE:HD1 | 1:B:54:LYS:HA | 9 | 0.01 |
| (1,4345) | 1:B:4:PHE:HD2 | 1:B:54:LYS:HA | 9 | 0.01 |
| (1,4344) | 1:A:4:PHE:HD1 | 1:A:54:LYS:HA | 2 | 0.01 |
| (1,4344) | 1:A:4:PHE:HD2 | 1:A:54:LYS:HA | 2 | 0.01 |
| (1,4344) | 1:A:4:PHE:HD1 | 1:A:54:LYS:HA | 7 | 0.01 |
| (1,4344) | 1:A:4:PHE:HD2 | 1:A:54:LYS:HA | 7 | 0.01 |
| (1,4344) | 1:A:4:PHE:HD1 | 1:A:54:LYS:HA | 16 | 0.01 |
| (1,4344) | 1:A:4:PHE:HD2 | 1:A:54:LYS:HA | 16 | 0.01 |
| (1,4344) | 1:A:4:PHE:HD1 | 1:A:54:LYS:HA | 19 | 0.01 |
| (1,4344) | 1:A:4:PHE:HD2 | 1:A:54:LYS:HA | 19 | 0.01 |
| (1,4342) | 1:A:4:PHE:HD1 | 1:A:5:LEU:HB3 | 12 | 0.01 |
| (1,4342) | 1:A:4:PHE:HD2 | 1:A:5:LEU:HB3 | 12 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4335) | 1:B:83:HIS:HA | 1:B:83:HIS:HD2 | 7 | 0.01 |
| (1,4335) | 1:B:83:HIS:HA | 1:B:83:HIS:HD2 | 20 | 0.01 |
| (1,4334) | 1:A:83:HIS:HA | 1:A:83:HIS:HD2 | 3 | 0.01 |
| (1,4334) | 1:A:83:HIS:HA | 1:A:83:HIS:HD2 | 14 | 0.01 |
| (1,4325) | 1:B:80:ASN:HA | 1:B:81:LEU:HG | 14 | 0.01 |
| (1,4324) | 1:A:80:ASN:HA | 1:A:81:LEU:HG | 2 | 0.01 |
| (1,432) | 1:A:24:GLY:H | 1:A:27:SER:HG | 4 | 0.01 |
| (1,432) | 1:A:24:GLY:H | 1:A:27:SER:HG | 12 | 0.01 |
| (1,432) | 1:A:24:GLY:H | 1:A:27:SER:HG | 15 | 0.01 |
| (1,4319) | 1:B:77:ARG:HG3 | 1:B:79:SER:HA | 5 | 0.01 |
| (1,4319) | 1:B:77:ARG:HG3 | 1:B:79:SER:HA | 11 | 0.01 |
| (1,4318) | 1:A:77:ARG:HG3 | 1:A:79:SER:HA | 8 | 0.01 |
| (1,4318) | 1:A:77:ARG:HG3 | 1:A:79:SER:HA | 17 | 0.01 |
| (1,4314) | 1:A:79:SER:HA | 1:A:81:LEU:HD21 | 2 | 0.01 |
| (1,4314) | 1:A:79:SER:HA | 1:A:81:LEU:HD22 | 2 | 0.01 |
| (1,4314) | 1:A:79:SER:HA | 1:A:81:LEU:HD23 | 2 | 0.01 |
| (1,4299) | 1:B:74:THR:HA | 1:B:75:VAL:HG21 | 4 | 0.01 |
| (1,4299) | 1:B:74:THR:HA | 1:B:75:VAL:HG22 | 4 | 0.01 |
| (1,4299) | 1:B:74:THR:HA | 1:B:75:VAL:HG23 | 4 | 0.01 |
| (1,4297) | 1:B:73:PHE:HA | 1:B:73:PHE:HD1 | 5 | 0.01 |
| (1,4297) | 1:B:73:PHE:HA | 1:B:73:PHE:HD2 | 5 | 0.01 |
| (1,4296) | 1:A:73:PHE:HA | 1:A:73:PHE:HD1 | 18 | 0.01 |
| (1,4296) | 1:A:73:PHE:HA | 1:A:73:PHE:HD2 | 18 | 0.01 |
| (1,4292) | 1:A:73:PHE:HA | 1:A:75:VAL:HG21 | 2 | 0.01 |
| (1,4292) | 1:A:73:PHE:HA | 1:A:75:VAL:HG22 | 2 | 0.01 |
| (1,4292) | 1:A:73:PHE:HA | 1:A:75:VAL:HG23 | 2 | 0.01 |
| (1,4258) | 1:A:41:LYS:HG2 | 1:A:42:ASP:HA | 2 | 0.01 |
| (1,4258) | 1:A:41:LYS:HG3 | 1:A:42:ASP:HA | 2 | 0.01 |
| (1,4255) | 1:B:41:LYS:HA | 1:B:41:LYS:HD2 | 1 | 0.01 |
| (1,4255) | 1:B:41:LYS:HA | 1:B:41:LYS:HD3 | 1 | 0.01 |
| (1,4255) | 1:B:41:LYS:HA | 1:B:41:LYS:HD2 | 10 | 0.01 |
| (1,4255) | 1:B:41:LYS:HA | 1:B:41:LYS:HD3 | 10 | 0.01 |
| (1,4254) | 1:A:41:LYS:HA | 1:A:41:LYS:HD2 | 20 | 0.01 |
| (1,4254) | 1:A:41:LYS:HA | 1:A:41:LYS:HD3 | 20 | 0.01 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG2 | 8 | 0.01 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG3 | 8 | 0.01 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG2 | 11 | 0.01 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG3 | 11 | 0.01 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG2 | 14 | 0.01 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG3 | 14 | 0.01 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG2 | 20 | 0.01 |
| (1,4253) | 1:B:41:LYS:HA | 1:B:41:LYS:HG3 | 20 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG2 | 4 | 0.01 |
| (1,4252) | 1:A:41:LYS:HA | 1:A:41:LYS:HG3 | 4 | 0.01 |
| (1,4243) | 1:B:15:LYS:HA | 1:B:17:GLY:H | 5 | 0.01 |
| (1,4242) | 1:A:15:LYS:HA | 1:A:17:GLY:H | 14 | 0.01 |
| (1,4216) | 1:A:8:ILE:HA | 1:A:78:LEU:HB2 | 8 | 0.01 |
| (1,4199) | 1:B:82:GLU:H | 1:B:83:HIS:HB3 | 7 | 0.01 |
| (1,4199) | 1:B:82:GLU:H | 1:B:83:HIS:HB3 | 9 | 0.01 |
| (1,4199) | 1:B:82:GLU:H | 1:B:83:HIS:HB3 | 17 | 0.01 |
| (1,4199) | 1:B:82:GLU:H | 1:B:83:HIS:HB3 | 19 | 0.01 |
| (1,4193) | 1:B:5:LEU:HB2 | 1:B:83:HIS:HB3 | 9 | 0.01 |
| (1,4192) | 1:A:5:LEU:HB2 | 1:A:83:HIS:HB3 | 4 | 0.01 |
| (1,4192) | 1:A:5:LEU:HB2 | 1:A:83:HIS:HB3 | 7 | 0.01 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD11 | 1 | 0.01 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD12 | 1 | 0.01 |
| (1,4189) | 1:B:5:LEU:HD11 | 1:B:81:LEU:HD13 | 1 | 0.01 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD11 | 1 | 0.01 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD12 | 1 | 0.01 |
| (1,4189) | 1:B:5:LEU:HD12 | 1:B:81:LEU:HD13 | 1 | 0.01 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD11 | 1 | 0.01 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD12 | 1 | 0.01 |
| (1,4189) | 1:B:5:LEU:HD13 | 1:B:81:LEU:HD13 | 1 | 0.01 |
| (1,4171) | 1:B:72:VAL:HG21 | 1:B:73:PHE:HB3 | 6 | 0.01 |
| (1,4171) | 1:B:72:VAL:HG22 | 1:B:73:PHE:HB3 | 6 | 0.01 |
| (1,4171) | 1:B:72:VAL:HG23 | 1:B:73:PHE:HB3 | 6 | 0.01 |
| (1,4170) | 1:A:72:VAL:HG21 | 1:A:73:PHE:HB3 | 5 | 0.01 |
| (1,4170) | 1:A:72:VAL:HG22 | 1:A:73:PHE:HB3 | 5 | 0.01 |
| (1,4170) | 1:A:72:VAL:HG23 | 1:A:73:PHE:HB3 | 5 | 0.01 |
| (1,4170) | 1:A:72:VAL:HG21 | 1:A:73:PHE:HB3 | 10 | 0.01 |
| (1,4170) | 1:A:72:VAL:HG22 | 1:A:73:PHE:HB3 | 10 | 0.01 |
| (1,4170) | 1:A:72:VAL:HG23 | 1:A:73:PHE:HB3 | 10 | 0.01 |
| (1,4170) | 1:A:72:VAL:HG21 | 1:A:73:PHE:HB3 | 11 | 0.01 |
| (1,4170) | 1:A:72:VAL:HG22 | 1:A:73:PHE:HB3 | 11 | 0.01 |
| (1,4170) | 1:A:72:VAL:HG23 | 1:A:73:PHE:HB3 | 11 | 0.01 |
| (1,4170) | 1:A:72:VAL:HG21 | 1:A:73:PHE:HB3 | 14 | 0.01 |
| (1,4170) | 1:A:72:VAL:HG22 | 1:A:73:PHE:HB3 | 14 | 0.01 |
| (1,4170) | 1:A:72:VAL:HG23 | 1:A:73:PHE:HB3 | 14 | 0.01 |
| (1,4147) | 1:B:61:THR:HG21 | 1:B:65:LYS:HB3 | 19 | 0.01 |
| (1,4147) | 1:B:61:THR:HG22 | 1:B:65:LYS:HB3 | 19 | 0.01 |
| (1,4147) | 1:B:61:THR:HG23 | 1:B:65:LYS:HB3 | 19 | 0.01 |
| (1,4146) | 1:A:61:THR:HG21 | 1:A:65:LYS:HB3 | 14 | 0.01 |
| (1,4146) | 1:A:61:THR:HG22 | 1:A:65:LYS:HB3 | 14 | 0.01 |
| (1,4146) | 1:A:61:THR:HG23 | 1:A:65:LYS:HB3 | 14 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD11 | 7 | 0.01 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD12 | 7 | 0.01 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD13 | 7 | 0.01 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD11 | 20 | 0.01 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD12 | 20 | 0.01 |
| (1,4135) | 1:B:11:VAL:HA | 1:B:44:ILE:HD13 | 20 | 0.01 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD11 | 2 | 0.01 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD12 | 2 | 0.01 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD13 | 2 | 0.01 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD11 | 5 | 0.01 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD12 | 5 | 0.01 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD13 | 5 | 0.01 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD11 | 11 | 0.01 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD12 | 11 | 0.01 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD13 | 11 | 0.01 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD11 | 17 | 0.01 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD12 | 17 | 0.01 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD13 | 17 | 0.01 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD11 | 19 | 0.01 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD12 | 19 | 0.01 |
| (1,4134) | 1:A:11:VAL:HA | 1:A:44:ILE:HD13 | 19 | 0.01 |
| (1,4124) | 1:A:23:THR:H | 1:B:33:ILE:HD11 | 18 | 0.01 |
| (1,4124) | 1:A:23:THR:H | 1:B:33:ILE:HD12 | 18 | 0.01 |
| (1,4124) | 1:A:23:THR:H | 1:B:33:ILE:HD13 | 18 | 0.01 |
| (1,4116) | 1:B:18:MET:HA | 1:B:21:GLN:HB2 | 7 | 0.01 |
| (1,4111) | 1:A:18:MET:HE1 | 1:A:21:GLN:HE21 | 10 | 0.01 |
| (1,4111) | 1:A:18:MET:HE2 | 1:A:21:GLN:HE21 | 10 | 0.01 |
| (1,4111) | 1:A:18:MET:HE3 | 1:A:21:GLN:HE21 | 10 | 0.01 |
| (1,4110) | 1:B:18:MET:HE1 | 1:B:72:VAL:HG21 | 4 | 0.01 |
| (1,4110) | 1:B:18:MET:HE1 | 1:B:72:VAL:HG22 | 4 | 0.01 |
| (1,4110) | 1:B:18:MET:HE1 | 1:B:72:VAL:HG23 | 4 | 0.01 |
| (1,4110) | 1:B:18:MET:HE2 | 1:B:72:VAL:HG21 | 4 | 0.01 |
| (1,4110) | 1:B:18:MET:HE2 | 1:B:72:VAL:HG22 | 4 | 0.01 |
| (1,4110) | 1:B:18:MET:HE2 | 1:B:72:VAL:HG23 | 4 | 0.01 |
| (1,4110) | 1:B:18:MET:HE3 | 1:B:72:VAL:HG21 | 4 | 0.01 |
| (1,4110) | 1:B:18:MET:HE3 | 1:B:72:VAL:HG22 | 4 | 0.01 |
| (1,4110) | 1:B:18:MET:HE3 | 1:B:72:VAL:HG23 | 4 | 0.01 |
| (1,4107) | 1:A:18:MET:HE1 | 1:A:69:VAL:HG11 | 10 | 0.01 |
| (1,4107) | 1:A:18:MET:HE1 | 1:A:69:VAL:HG12 | 10 | 0.01 |
| (1,4107) | 1:A:18:MET:HE1 | 1:A:69:VAL:HG13 | 10 | 0.01 |
| (1,4107) | 1:A:18:MET:HE2 | 1:A:69:VAL:HG11 | 10 | 0.01 |
| (1,4107) | 1:A:18:MET:HE2 | 1:A:69:VAL:HG12 | 10 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4107) | 1:A:18:MET:HE2 | 1:A:69:VAL:HG13 | 10 | 0.01 |
| (1,4107) | 1:A:18:MET:HE3 | 1:A:69:VAL:HG11 | 10 | 0.01 |
| (1,4107) | 1:A:18:MET:HE3 | 1:A:69:VAL:HG12 | 10 | 0.01 |
| (1,4107) | 1:A:18:MET:HE3 | 1:A:69:VAL:HG13 | 10 | 0.01 |
| (1,4107) | 1:A:18:MET:HE1 | 1:A:69:VAL:HG11 | 17 | 0.01 |
| (1,4107) | 1:A:18:MET:HE1 | 1:A:69:VAL:HG12 | 17 | 0.01 |
| (1,4107) | 1:A:18:MET:HE1 | 1:A:69:VAL:HG13 | 17 | 0.01 |
| (1,4107) | 1:A:18:MET:HE2 | 1:A:69:VAL:HG11 | 17 | 0.01 |
| (1,4107) | 1:A:18:MET:HE2 | 1:A:69:VAL:HG12 | 17 | 0.01 |
| (1,4107) | 1:A:18:MET:HE2 | 1:A:69:VAL:HG13 | 17 | 0.01 |
| (1,4107) | 1:A:18:MET:HE3 | 1:A:69:VAL:HG11 | 17 | 0.01 |
| (1,4107) | 1:A:18:MET:HE3 | 1:A:69:VAL:HG12 | 17 | 0.01 |
| (1,4107) | 1:A:18:MET:HE3 | 1:A:69:VAL:HG13 | 17 | 0.01 |
| (1,4106) | 1:B:15:LYS:HB3 | 1:B:18:MET:HB3 | 9 | 0.01 |
| (1,4087) | 1:B:82:GLU:H | 1:B:82:GLU:HG3 | 1 | 0.01 |
| (1,4087) | 1:B:82:GLU:H | 1:B:82:GLU:HG3 | 5 | 0.01 |
| (1,4075) | 1:B:82:GLU:HA | 1:B:83:HIS:HB2 | 1 | 0.01 |
| (1,4075) | 1:B:82:GLU:HA | 1:B:83:HIS:HB2 | 17 | 0.01 |
| (1,4074) | 1:A:82:GLU:HA | 1:A:83:HIS:HB2 | 2 | 0.01 |
| (1,4074) | 1:A:82:GLU:HA | 1:A:83:HIS:HB2 | 10 | 0.01 |
| (1,4074) | 1:A:82:GLU:HA | 1:A:83:HIS:HB2 | 15 | 0.01 |
| (1,4073) | 1:B:8:ILE:H | 1:B:81:LEU:HD21 | 9 | 0.01 |
| (1,4073) | 1:B:8:ILE:H | 1:B:81:LEU:HD22 | 9 | 0.01 |
| (1,4073) | 1:B:8:ILE:H | 1:B:81:LEU:HD23 | 9 | 0.01 |
| (1,4073) | 1:B:8:ILE:H | 1:B:81:LEU:HD21 | 10 | 0.01 |
| (1,4073) | 1:B:8:ILE:H | 1:B:81:LEU:HD22 | 10 | 0.01 |
| (1,4073) | 1:B:8:ILE:H | 1:B:81:LEU:HD23 | 10 | 0.01 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD21 | 12 | 0.01 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD22 | 12 | 0.01 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD23 | 12 | 0.01 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD21 | 17 | 0.01 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD22 | 17 | 0.01 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD23 | 17 | 0.01 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD21 | 19 | 0.01 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD22 | 19 | 0.01 |
| (1,4072) | 1:A:8:ILE:H | 1:A:81:LEU:HD23 | 19 | 0.01 |
| (1,4071) | 1:B:79:SER:H | 1:B:81:LEU:HD21 | 6 | 0.01 |
| (1,4071) | 1:B:79:SER:H | 1:B:81:LEU:HD22 | 6 | 0.01 |
| (1,4071) | 1:B:79:SER:H | 1:B:81:LEU:HD23 | 6 | 0.01 |
| (1,4059) | 1:B:50:MET:HG3 | 1:B:81:LEU:HD21 | 18 | 0.01 |
| (1,4059) | 1:B:50:MET:HG3 | 1:B:81:LEU:HD22 | 18 | 0.01 |
| (1,4059) | 1:B:50:MET:HG3 | 1:B:81:LEU:HD23 | 18 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,4036) | 1:A:50:MET:HG2 | 1:A:81:LEU:HD11 | 10 | 0.01 |
| (1,4036) | 1:A:50:MET:HG2 | 1:A:81:LEU:HD12 | 10 | 0.01 |
| (1,4036) | 1:A:50:MET:HG2 | 1:A:81:LEU:HD13 | 10 | 0.01 |
| (1,4023) | 1:B:80:ASN:HB3 | 1:B:81:LEU:HD21 | 1 | 0.01 |
| (1,4023) | 1:B:80:ASN:HB3 | 1:B:81:LEU:HD22 | 1 | 0.01 |
| (1,4023) | 1:B:80:ASN:HB3 | 1:B:81:LEU:HD23 | 1 | 0.01 |
| (1,4019) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 9 | 0.01 |
| (1,4019) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 9 | 0.01 |
| (1,4019) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 9 | 0.01 |
| (1,4019) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD21 | 16 | 0.01 |
| (1,4019) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD22 | 16 | 0.01 |
| (1,4019) | 1:B:80:ASN:HB2 | 1:B:81:LEU:HD23 | 16 | 0.01 |
| (1,4014) | 1:A:78:LEU:HB3 | 1:A:79:SER:HB2 | 10 | 0.01 |
| (1,4014) | 1:A:78:LEU:HB3 | 1:A:79:SER:HB3 | 10 | 0.01 |
| (1,4013) | 1:B:9:ARG:H | 1:B:78:LEU:HD21 | 6 | 0.01 |
| (1,4013) | 1:B:9:ARG:H | 1:B:78:LEU:HD22 | 6 | 0.01 |
| (1,4013) | 1:B:9:ARG:H | 1:B:78:LEU:HD23 | 6 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD21 | 8 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD22 | 8 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD23 | 8 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD21 | 8 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD22 | 8 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD23 | 8 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD21 | 12 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD22 | 12 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD23 | 12 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD21 | 12 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD22 | 12 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD23 | 12 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD21 | 18 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD22 | 18 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB2 | 1:B:78:LEU:HD23 | 18 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD21 | 18 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD22 | 18 | 0.01 |
| (1,3999) | 1:B:9:ARG:HB3 | 1:B:78:LEU:HD23 | 18 | 0.01 |
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD21 | 6 | 0.01 |
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD22 | 6 | 0.01 |
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD23 | 6 | 0.01 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD21 | 6 | 0.01 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD22 | 6 | 0.01 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD23 | 6 | 0.01 |
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD21 | 16 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD22 | 16 | 0.01 |
| (1,3998) | 1:A:9:ARG:HB2 | 1:A:78:LEU:HD23 | 16 | 0.01 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD21 | 16 | 0.01 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD22 | 16 | 0.01 |
| (1,3998) | 1:A:9:ARG:HB3 | 1:A:78:LEU:HD23 | 16 | 0.01 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD11 | 1 | 0.01 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD12 | 1 | 0.01 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD13 | 1 | 0.01 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD11 | 5 | 0.01 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD12 | 5 | 0.01 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD13 | 5 | 0.01 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD11 | 11 | 0.01 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD12 | 11 | 0.01 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD13 | 11 | 0.01 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD11 | 17 | 0.01 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD12 | 17 | 0.01 |
| (1,3995) | 1:B:76:GLU:H | 1:B:78:LEU:HD13 | 17 | 0.01 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD11 | 3 | 0.01 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD12 | 3 | 0.01 |
| (1,3994) | 1:A:76:GLU:H | 1:A:78:LEU:HD13 | 3 | 0.01 |
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD11 | 12 | 0.01 |
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD12 | 12 | 0.01 |
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD13 | 12 | 0.01 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD11 | 12 | 0.01 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD12 | 12 | 0.01 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD13 | 12 | 0.01 |
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD11 | 18 | 0.01 |
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD12 | 18 | 0.01 |
| (1,3973) | 1:B:9:ARG:HD2 | 1:B:78:LEU:HD13 | 18 | 0.01 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD11 | 18 | 0.01 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD12 | 18 | 0.01 |
| (1,3973) | 1:B:9:ARG:HD3 | 1:B:78:LEU:HD13 | 18 | 0.01 |
| (1,3972) | 1:A:9:ARG:HD2 | 1:A:78:LEU:HD11 | 2 | 0.01 |
| (1,3972) | 1:A:9:ARG:HD2 | 1:A:78:LEU:HD12 | 2 | 0.01 |
| (1,3972) | 1:A:9:ARG:HD2 | 1:A:78:LEU:HD13 | 2 | 0.01 |
| (1,3972) | 1:A:9:ARG:HD3 | 1:A:78:LEU:HD11 | 2 | 0.01 |
| (1,3972) | 1:A:9:ARG:HD3 | 1:A:78:LEU:HD12 | 2 | 0.01 |
| (1,3972) | 1:A:9:ARG:HD3 | 1:A:78:LEU:HD13 | 2 | 0.01 |
| (1,397) | 1:B:22:ILE:H | 1:B:23:THR:HG1 | 9 | 0.01 |
| (1,397) | 1:B:22:ILE:H | 1:B:23:THR:HG1 | 10 | 0.01 |
| (1,397) | 1:B:22:ILE:H | 1:B:23:THR:HG1 | 15 | 0.01 |
| (1,396) | 1:A:22:ILE:H | 1:A:23:THR:HG1 | 1 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,396) | 1:A:22:ILE:H | 1:A:23:THR:HG1 | 7 | 0.01 |
| (1,396) | 1:A:22:ILE:H | 1:A:23:THR:HG1 | 9 | 0.01 |
| (1,396) | 1:A:22:ILE:H | 1:A:23:THR:HG1 | 17 | 0.01 |
| (1,3952) | 1:A:78:LEU:HB2 | 1:A:80:ASN:H | 20 | 0.01 |
| (1,3945) | 1:B:9:ARG:H | 1:B:78:LEU:HB3 | 2 | 0.01 |
| (1,3937) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HB3 | 15 | 0.01 |
| (1,3937) | 1:B:7:GLY:HA2 | 1:B:78:LEU:HB3 | 16 | 0.01 |
| (1,3936) | 1:A:7:GLY:HA2 | 1:A:78:LEU:HB3 | 17 | 0.01 |
| (1,3931) | 1:B:77:ARG:HD2 | 1:B:78:LEU:H | 17 | 0.01 |
| (1,3931) | 1:B:77:ARG:HD3 | 1:B:78:LEU:H | 17 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB1 | 1:A:77:ARG:HD2 | 11 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB1 | 1:A:77:ARG:HD3 | 11 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB2 | 1:A:77:ARG:HD2 | 11 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB2 | 1:A:77:ARG:HD3 | 11 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB3 | 1:A:77:ARG:HD2 | 11 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB3 | 1:A:77:ARG:HD3 | 11 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB1 | 1:A:77:ARG:HD2 | 12 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB1 | 1:A:77:ARG:HD3 | 12 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB2 | 1:A:77:ARG:HD2 | 12 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB2 | 1:A:77:ARG:HD3 | 12 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB3 | 1:A:77:ARG:HD2 | 12 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB3 | 1:A:77:ARG:HD3 | 12 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB1 | 1:A:77:ARG:HD2 | 13 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB1 | 1:A:77:ARG:HD3 | 13 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB2 | 1:A:77:ARG:HD2 | 13 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB2 | 1:A:77:ARG:HD3 | 13 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB3 | 1:A:77:ARG:HD2 | 13 | 0.01 |
| (1,3920) | 1:A:6:ALA:HB3 | 1:A:77:ARG:HD3 | 13 | 0.01 |
| (1,3916) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HD2 | 15 | 0.01 |
| (1,3916) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HD3 | 15 | 0.01 |
| (1,3916) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HD2 | 15 | 0.01 |
| (1,3916) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HD3 | 15 | 0.01 |
| (1,3916) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HD2 | 15 | 0.01 |
| (1,3916) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HD3 | 15 | 0.01 |
| (1,3901) | 1:B:59:LEU:HD11 | 1:B:77:ARG:HG2 | 16 | 0.01 |
| (1,3901) | 1:B:59:LEU:HD12 | 1:B:77:ARG:HG2 | 16 | 0.01 |
| (1,3901) | 1:B:59:LEU:HD13 | 1:B:77:ARG:HG2 | 16 | 0.01 |
| (1,3900) | 1:A:59:LEU:HD11 | 1:A:77:ARG:HG2 | 1 | 0.01 |
| (1,3900) | 1:A:59:LEU:HD12 | 1:A:77:ARG:HG2 | 1 | 0.01 |
| (1,3900) | 1:A:59:LEU:HD13 | 1:A:77:ARG:HG2 | 1 | 0.01 |
| (1,3897) | 1:B:74:THR:HA | 1:B:76:GLU:HG2 | 1 | 0.01 |
| (1,3897) | 1:B:74:THR:HA | 1:B:76:GLU:HG3 | 1 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3897) | 1:B:74:THR:HA | 1:B:76:GLU:HG2 | 3 | 0.01 |
| (1,3897) | 1:B:74:THR:HA | 1:B:76:GLU:HG3 | 3 | 0.01 |
| (1,3894) | 1:A:9:ARG:HB2 | 1:A:76:GLU:HG2 | 17 | 0.01 |
| (1,3894) | 1:A:9:ARG:HB2 | 1:A:76:GLU:HG3 | 17 | 0.01 |
| (1,3894) | 1:A:9:ARG:HB3 | 1:A:76:GLU:HG2 | 17 | 0.01 |
| (1,3894) | 1:A:9:ARG:HB3 | 1:A:76:GLU:HG3 | 17 | 0.01 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG21 | 19 | 0.01 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG22 | 19 | 0.01 |
| (1,3860) | 1:B:73:PHE:HD1 | 1:B:74:THR:HG23 | 19 | 0.01 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG21 | 19 | 0.01 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG22 | 19 | 0.01 |
| (1,3860) | 1:B:73:PHE:HD2 | 1:B:74:THR:HG23 | 19 | 0.01 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG21 | 6 | 0.01 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG22 | 6 | 0.01 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG23 | 6 | 0.01 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG21 | 6 | 0.01 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG22 | 6 | 0.01 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG23 | 6 | 0.01 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG21 | 14 | 0.01 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG22 | 14 | 0.01 |
| (1,3859) | 1:A:73:PHE:HD1 | 1:A:74:THR:HG23 | 14 | 0.01 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG21 | 14 | 0.01 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG22 | 14 | 0.01 |
| (1,3859) | 1:A:73:PHE:HD2 | 1:A:74:THR:HG23 | 14 | 0.01 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG21 | 7 | 0.01 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG22 | 7 | 0.01 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG23 | 7 | 0.01 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG21 | 9 | 0.01 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG22 | 9 | 0.01 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG23 | 9 | 0.01 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG21 | 18 | 0.01 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG22 | 18 | 0.01 |
| (1,3858) | 1:B:73:PHE:HA | 1:B:74:THR:HG23 | 18 | 0.01 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG21 | 5 | 0.01 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG22 | 5 | 0.01 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG23 | 5 | 0.01 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG21 | 7 | 0.01 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG22 | 7 | 0.01 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG23 | 7 | 0.01 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG21 | 8 | 0.01 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG22 | 8 | 0.01 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG23 | 8 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG21 | 13 | 0.01 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG22 | 13 | 0.01 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG23 | 13 | 0.01 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG21 | 17 | 0.01 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG22 | 17 | 0.01 |
| (1,3852) | 1:B:73:PHE:HB3 | 1:B:74:THR:HG23 | 17 | 0.01 |
| (1,3848) | 1:B:74:THR:HB | 1:B:75:VAL:H | 17 | 0.01 |
| (1,3846) | 1:B:10:ILE:HA | 1:B:74:THR:HB | 9 | 0.01 |
| (1,3845) | 1:A:10:ILE:HA | 1:A:74:THR:HB | 12 | 0.01 |
| (1,3814) | 1:B:66:LEU:HA | 1:B:72:VAL:HG21 | 13 | 0.01 |
| (1,3814) | 1:B:66:LEU:HA | 1:B:72:VAL:HG22 | 13 | 0.01 |
| (1,3814) | 1:B:66:LEU:HA | 1:B:72:VAL:HG23 | 13 | 0.01 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG11 | 11 | 0.01 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG12 | 11 | 0.01 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG13 | 11 | 0.01 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG11 | 13 | 0.01 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG12 | 13 | 0.01 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG13 | 13 | 0.01 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG11 | 14 | 0.01 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG12 | 14 | 0.01 |
| (1,3790) | 1:B:67:ARG:HA | 1:B:72:VAL:HG13 | 14 | 0.01 |
| (1,3756) | 1:B:69:VAL:H | 1:B:70:GLN:HB2 | 3 | 0.01 |
| (1,3756) | 1:B:69:VAL:H | 1:B:70:GLN:HB3 | 3 | 0.01 |
| (1,3756) | 1:B:69:VAL:H | 1:B:70:GLN:HB2 | 18 | 0.01 |
| (1,3756) | 1:B:69:VAL:H | 1:B:70:GLN:HB3 | 18 | 0.01 |
| (1,3756) | 1:B:69:VAL:H | 1:B:70:GLN:HB2 | 19 | 0.01 |
| (1,3756) | 1:B:69:VAL:H | 1:B:70:GLN:HB3 | 19 | 0.01 |
| (1,3755) | 1:A:69:VAL:H | 1:A:70:GLN:HB2 | 6 | 0.01 |
| (1,3755) | 1:A:69:VAL:H | 1:A:70:GLN:HB3 | 6 | 0.01 |
| (1,3748) | 1:B:69:VAL:HG11 | 1:B:70:GLN:HB2 | 1 | 0.01 |
| (1,3748) | 1:B:69:VAL:HG11 | 1:B:70:GLN:HB3 | 1 | 0.01 |
| (1,3748) | 1:B:69:VAL:HG12 | 1:B:70:GLN:HB2 | 1 | 0.01 |
| (1,3748) | 1:B:69:VAL:HG12 | 1:B:70:GLN:HB3 | 1 | 0.01 |
| (1,3748) | 1:B:69:VAL:HG13 | 1:B:70:GLN:HB2 | 1 | 0.01 |
| (1,3748) | 1:B:69:VAL:HG13 | 1:B:70:GLN:HB3 | 1 | 0.01 |
| (1,3736) | 1:B:66:LEU:HA | 1:B:69:VAL:HB | 3 | 0.01 |
| (1,3735) | 1:A:66:LEU:HA | 1:A:69:VAL:HB | 20 | 0.01 |
| (1,3734) | 1:B:20:ASN:HA | 1:B:22:ILE:HB | 7 | 0.01 |
| (1,3734) | 1:B:20:ASN:HA | 1:B:22:ILE:HB | 16 | 0.01 |
| (1,3734) | 1:B:20:ASN:HA | 1:B:22:ILE:HB | 19 | 0.01 |
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 7 | 0.01 |
| (1,3733) | 1:A:20:ASN:HA | 1:A:22:ILE:HB | 18 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3724) | 1:B:66:LEU:HA | 1:B:69:VAL:HG21 | 14 | 0.01 |
| (1,3724) | 1:B:66:LEU:HA | 1:B:69:VAL:HG22 | 14 | 0.01 |
| (1,3724) | 1:B:66:LEU:HA | 1:B:69:VAL:HG23 | 14 | 0.01 |
| (1,3723) | 1:A:66:LEU:HA | 1:A:69:VAL:HG21 | 18 | 0.01 |
| (1,3723) | 1:A:66:LEU:HA | 1:A:69:VAL:HG22 | 18 | 0.01 |
| (1,3723) | 1:A:66:LEU:HA | 1:A:69:VAL:HG23 | 18 | 0.01 |
| (1,3705) | 1:A:68:LYS:HB3 | 1:A:69:VAL:HA | 7 | 0.01 |
| (1,3702) | 1:B:15:LYS:HE2 | 1:B:18:MET:H | 16 | 0.01 |
| (1,3702) | 1:B:15:LYS:HE3 | 1:B:18:MET:H | 16 | 0.01 |
| (1,3702) | 1:B:15:LYS:HE2 | 1:B:18:MET:H | 17 | 0.01 |
| (1,3702) | 1:B:15:LYS:HE3 | 1:B:18:MET:H | 17 | 0.01 |
| (1,3701) | 1:A:15:LYS:HE2 | 1:A:18:MET:H | 7 | 0.01 |
| (1,3701) | 1:A:15:LYS:HE3 | 1:A:18:MET:H | 7 | 0.01 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE2 | 17 | 0.01 |
| (1,3698) | 1:B:15:LYS:H | 1:B:15:LYS:HE3 | 17 | 0.01 |
| (1,3668) | 1:A:68:LYS:HA | 1:A:68:LYS:HD3 | 2 | 0.01 |
| (1,3667) | 1:B:68:LYS:HA | 1:B:68:LYS:HG3 | 14 | 0.01 |
| (1,3667) | 1:B:68:LYS:HA | 1:B:68:LYS:HG3 | 16 | 0.01 |
| (1,365) | 1:B:18:MET:HE1 | 1:B:21:GLN:HE22 | 4 | 0.01 |
| (1,365) | 1:B:18:MET:HE2 | 1:B:21:GLN:HE22 | 4 | 0.01 |
| (1,365) | 1:B:18:MET:HE3 | 1:B:21:GLN:HE22 | 4 | 0.01 |
| (1,3621) | 1:B:41:LYS:HE2 | 1:B:44:ILE:H | 4 | 0.01 |
| (1,3621) | 1:B:41:LYS:HE3 | 1:B:44:ILE:H | 4 | 0.01 |
| (1,3620) | 1:A:41:LYS:HE2 | 1:A:44:ILE:H | 12 | 0.01 |
| (1,3620) | 1:A:41:LYS:HE3 | 1:A:44:ILE:H | 12 | 0.01 |
| (1,3602) | 1:A:29:PHE:HZ | 1:A:65:LYS:HG2 | 17 | 0.01 |
| (1,3572) | 1:B:62:LEU:HD11 | 1:B:65:LYS:HB3 | 1 | 0.01 |
| (1,3572) | 1:B:62:LEU:HD12 | 1:B:65:LYS:HB3 | 1 | 0.01 |
| (1,3572) | 1:B:62:LEU:HD13 | 1:B:65:LYS:HB3 | 1 | 0.01 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB2 | 10 | 0.01 |
| (1,3542) | 1:B:64:ASP:HB3 | 1:B:67:ARG:HB3 | 10 | 0.01 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB2 | 11 | 0.01 |
| (1,3541) | 1:A:64:ASP:HB3 | 1:A:67:ARG:HB3 | 11 | 0.01 |
| (1,3537) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HB2 | 4 | 0.01 |
| (1,3537) | 1:B:64:ASP:HB2 | 1:B:65:LYS:HB2 | 5 | 0.01 |
| (1,3536) | 1:A:64:ASP:HB2 | 1:A:65:LYS:HB2 | 4 | 0.01 |
| (1,3536) | 1:A:64:ASP:HB2 | 1:A:65:LYS:HB2 | 8 | 0.01 |
| (1,3532) | 1:B:61:THR:HG21 | 1:B:64:ASP:HB2 | 4 | 0.01 |
| (1,3532) | 1:B:61:THR:HG22 | 1:B:64:ASP:HB2 | 4 | 0.01 |
| (1,3532) | 1:B:61:THR:HG23 | 1:B:64:ASP:HB2 | 4 | 0.01 |
| (1,3532) | 1:B:61:THR:HG21 | 1:B:64:ASP:HB2 | 6 | 0.01 |
| (1,3532) | 1:B:61:THR:HG22 | 1:B:64:ASP:HB2 | 6 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3532) | 1:B:61:THR:HG23 | 1:B:64:ASP:HB2 | 6 | 0.01 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE1 | 2 | 0.01 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE2 | 2 | 0.01 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE3 | 2 | 0.01 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE1 | 11 | 0.01 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE2 | 11 | 0.01 |
| (1,3529) | 1:A:9:ARG:H | 1:A:63:MET:HE3 | 11 | 0.01 |
| (1,3528) | 1:B:63:MET:HE1 | 1:B:77:ARG:H | 1 | 0.01 |
| (1,3528) | 1:B:63:MET:HE2 | 1:B:77:ARG:H | 1 | 0.01 |
| (1,3528) | 1:B:63:MET:HE3 | 1:B:77:ARG:H | 1 | 0.01 |
| (1,3528) | 1:B:63:MET:HE1 | 1:B:77:ARG:H | 11 | 0.01 |
| (1,3528) | 1:B:63:MET:HE2 | 1:B:77:ARG:H | 11 | 0.01 |
| (1,3528) | 1:B:63:MET:HE3 | 1:B:77:ARG:H | 11 | 0.01 |
| (1,3527) | 1:A:63:MET:HE1 | 1:A:77:ARG:H | 3 | 0.01 |
| (1,3527) | 1:A:63:MET:HE2 | 1:A:77:ARG:H | 3 | 0.01 |
| (1,3527) | 1:A:63:MET:HE3 | 1:A:77:ARG:H | 3 | 0.01 |
| (1,3527) | 1:A:63:MET:HE1 | 1:A:77:ARG:H | 20 | 0.01 |
| (1,3527) | 1:A:63:MET:HE2 | 1:A:77:ARG:H | 20 | 0.01 |
| (1,3527) | 1:A:63:MET:HE3 | 1:A:77:ARG:H | 20 | 0.01 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 7 | 0.01 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 7 | 0.01 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 7 | 0.01 |
| (1,3520) | 1:B:63:MET:HE1 | 1:B:76:GLU:HA | 17 | 0.01 |
| (1,3520) | 1:B:63:MET:HE2 | 1:B:76:GLU:HA | 17 | 0.01 |
| (1,3520) | 1:B:63:MET:HE3 | 1:B:76:GLU:HA | 17 | 0.01 |
| (1,3519) | 1:A:63:MET:HE1 | 1:A:76:GLU:HA | 11 | 0.01 |
| (1,3519) | 1:A:63:MET:HE2 | 1:A:76:GLU:HA | 11 | 0.01 |
| (1,3519) | 1:A:63:MET:HE3 | 1:A:76:GLU:HA | 11 | 0.01 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE1 | 15 | 0.01 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE2 | 15 | 0.01 |
| (1,3501) | 1:A:8:ILE:HD11 | 1:A:63:MET:HE3 | 15 | 0.01 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE1 | 15 | 0.01 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE2 | 15 | 0.01 |
| (1,3501) | 1:A:8:ILE:HD12 | 1:A:63:MET:HE3 | 15 | 0.01 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE1 | 15 | 0.01 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE2 | 15 | 0.01 |
| (1,3501) | 1:A:8:ILE:HD13 | 1:A:63:MET:HE3 | 15 | 0.01 |
| (1,3440) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD11 | 14 | 0.01 |
| (1,3440) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD12 | 14 | 0.01 |
| (1,3440) | 1:B:58:LYS:HE2 | 1:B:62:LEU:HD13 | 14 | 0.01 |
| (1,3436) | 1:B:62:LEU:HD11 | 1:B:66:LEU:HG | 6 | 0.01 |
| (1,3436) | 1:B:62:LEU:HD12 | 1:B:66:LEU:HG | 6 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,3436) | 1:B:62:LEU:HD13 | 1:B:66:LEU:HG | 6 | 0.01 |
| (1,3436) | 1:B:62:LEU:HD11 | 1:B:66:LEU:HG | 7 | 0.01 |
| (1,3436) | 1:B:62:LEU:HD12 | 1:B:66:LEU:HG | 7 | 0.01 |
| (1,3436) | 1:B:62:LEU:HD13 | 1:B:66:LEU:HG | 7 | 0.01 |
| (1,3436) | 1:B:62:LEU:HD11 | 1:B:66:LEU:HG | 12 | 0.01 |
| (1,3436) | 1:B:62:LEU:HD12 | 1:B:66:LEU:HG | 12 | 0.01 |
| (1,3436) | 1:B:62:LEU:HD13 | 1:B:66:LEU:HG | 12 | 0.01 |
| (1,3435) | 1:A:62:LEU:HD11 | 1:A:66:LEU:HG | 15 | 0.01 |
| (1,3435) | 1:A:62:LEU:HD12 | 1:A:66:LEU:HG | 15 | 0.01 |
| (1,3435) | 1:A:62:LEU:HD13 | 1:A:66:LEU:HG | 15 | 0.01 |
| (1,3435) | 1:A:62:LEU:HD11 | 1:A:66:LEU:HG | 16 | 0.01 |
| (1,3435) | 1:A:62:LEU:HD12 | 1:A:66:LEU:HG | 16 | 0.01 |
| (1,3435) | 1:A:62:LEU:HD13 | 1:A:66:LEU:HG | 16 | 0.01 |
| (1,3387) | 1:B:61:THR:HG21 | 1:B:65:LYS:HE2 | 9 | 0.01 |
| (1,3387) | 1:B:61:THR:HG21 | 1:B:65:LYS:HE3 | 9 | 0.01 |
| (1,3387) | 1:B:61:THR:HG22 | 1:B:65:LYS:HE2 | 9 | 0.01 |
| (1,3387) | 1:B:61:THR:HG22 | 1:B:65:LYS:HE3 | 9 | 0.01 |
| (1,3387) | 1:B:61:THR:HG23 | 1:B:65:LYS:HE2 | 9 | 0.01 |
| (1,3387) | 1:B:61:THR:HG23 | 1:B:65:LYS:HE3 | 9 | 0.01 |
| (1,3386) | 1:A:61:THR:HG21 | 1:A:65:LYS:HE2 | 2 | 0.01 |
| (1,3386) | 1:A:61:THR:HG21 | 1:A:65:LYS:HE3 | 2 | 0.01 |
| (1,3386) | 1:A:61:THR:HG22 | 1:A:65:LYS:HE2 | 2 | 0.01 |
| (1,3386) | 1:A:61:THR:HG22 | 1:A:65:LYS:HE3 | 2 | 0.01 |
| (1,3386) | 1:A:61:THR:HG23 | 1:A:65:LYS:HE2 | 2 | 0.01 |
| (1,3386) | 1:A:61:THR:HG23 | 1:A:65:LYS:HE3 | 2 | 0.01 |
| (1,3386) | 1:A:61:THR:HG21 | 1:A:65:LYS:HE2 | 14 | 0.01 |
| (1,3386) | 1:A:61:THR:HG21 | 1:A:65:LYS:HE3 | 14 | 0.01 |
| (1,3386) | 1:A:61:THR:HG22 | 1:A:65:LYS:HE2 | 14 | 0.01 |
| (1,3386) | 1:A:61:THR:HG22 | 1:A:65:LYS:HE3 | 14 | 0.01 |
| (1,3386) | 1:A:61:THR:HG23 | 1:A:65:LYS:HE2 | 14 | 0.01 |
| (1,3386) | 1:A:61:THR:HG23 | 1:A:65:LYS:HE3 | 14 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD21 | 8 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD22 | 8 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD23 | 8 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD21 | 8 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD22 | 8 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD23 | 8 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD21 | 8 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD22 | 8 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD23 | 8 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD21 | 16 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD22 | 16 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD23 | 16 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD21 | 16 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD22 | 16 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD23 | 16 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD21 | 16 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD22 | 16 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD23 | 16 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD21 | 17 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD22 | 17 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD23 | 17 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD21 | 17 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD22 | 17 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD23 | 17 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD21 | 17 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD22 | 17 | 0.01 |
| (1,3322) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD23 | 17 | 0.01 |
| (1,3311) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD11 | 8 | 0.01 |
| (1,3311) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD12 | 8 | 0.01 |
| (1,3311) | 1:B:6:ALA:HB1 | 1:B:59:LEU:HD13 | 8 | 0.01 |
| (1,3311) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD11 | 8 | 0.01 |
| (1,3311) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD12 | 8 | 0.01 |
| (1,3311) | 1:B:6:ALA:HB2 | 1:B:59:LEU:HD13 | 8 | 0.01 |
| (1,3311) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD11 | 8 | 0.01 |
| (1,3311) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD12 | 8 | 0.01 |
| (1,3311) | 1:B:6:ALA:HB3 | 1:B:59:LEU:HD13 | 8 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD11 | 1 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD12 | 1 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD13 | 1 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD11 | 1 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD12 | 1 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD13 | 1 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD11 | 1 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD12 | 1 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD13 | 1 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD11 | 10 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD12 | 10 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD13 | 10 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD11 | 10 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD12 | 10 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD13 | 10 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD11 | 10 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD12 | 10 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD13 | 10 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD11 | 13 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD12 | 13 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD13 | 13 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD11 | 13 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD12 | 13 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD13 | 13 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD11 | 13 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD12 | 13 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD13 | 13 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD11 | 17 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD12 | 17 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB1 | 1:A:59:LEU:HD13 | 17 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD11 | 17 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD12 | 17 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB2 | 1:A:59:LEU:HD13 | 17 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD11 | 17 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD12 | 17 | 0.01 |
| (1,3310) | 1:A:6:ALA:HB3 | 1:A:59:LEU:HD13 | 17 | 0.01 |
| (1,3261) | 1:B:58:LYS:HG2 | 1:B:62:LEU:HD11 | 4 | 0.01 |
| (1,3261) | 1:B:58:LYS:HG2 | 1:B:62:LEU:HD12 | 4 | 0.01 |
| (1,3261) | 1:B:58:LYS:HG2 | 1:B:62:LEU:HD13 | 4 | 0.01 |
| (1,3260) | 1:A:58:LYS:HG2 | 1:A:62:LEU:HD11 | 3 | 0.01 |
| (1,3260) | 1:A:58:LYS:HG2 | 1:A:62:LEU:HD12 | 3 | 0.01 |
| (1,3260) | 1:A:58:LYS:HG2 | 1:A:62:LEU:HD13 | 3 | 0.01 |
| (1,3260) | 1:A:58:LYS:HG2 | 1:A:62:LEU:HD11 | 15 | 0.01 |
| (1,3260) | 1:A:58:LYS:HG2 | 1:A:62:LEU:HD12 | 15 | 0.01 |
| (1,3260) | 1:A:58:LYS:HG2 | 1:A:62:LEU:HD13 | 15 | 0.01 |
| (1,3231) | 1:B:57:ASP:HB2 | 1:B:58:LYS:HG3 | 7 | 0.01 |
| (1,3231) | 1:B:57:ASP:HB3 | 1:B:58:LYS:HG3 | 7 | 0.01 |
| (1,3231) | 1:B:57:ASP:HB2 | 1:B:58:LYS:HG3 | 9 | 0.01 |
| (1,3231) | 1:B:57:ASP:HB3 | 1:B:58:LYS:HG3 | 9 | 0.01 |
| (1,3231) | 1:B:57:ASP:HB2 | 1:B:58:LYS:HG3 | 19 | 0.01 |
| (1,3231) | 1:B:57:ASP:HB3 | 1:B:58:LYS:HG3 | 19 | 0.01 |
| (1,3230) | 1:A:57:ASP:HB2 | 1:A:58:LYS:HG3 | 8 | 0.01 |
| (1,3230) | 1:A:57:ASP:HB3 | 1:A:58:LYS:HG3 | 8 | 0.01 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG21 | 1 | 0.01 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG22 | 1 | 0.01 |
| (1,3221) | 1:B:4:PHE:HD1 | 1:B:56:THR:HG23 | 1 | 0.01 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG21 | 1 | 0.01 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG22 | 1 | 0.01 |
| (1,3221) | 1:B:4:PHE:HD2 | 1:B:56:THR:HG23 | 1 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,3220) | 1:A:4:PHE:HD1 | 1:A:56:THR:HG21 | 5 | 0.01 |
| (1,3220) | 1:A:4:PHE:HD1 | 1:A:56:THR:HG22 | 5 | 0.01 |
| (1,3220) | 1:A:4:PHE:HD1 | 1:A:56:THR:HG23 | 5 | 0.01 |
| (1,3220) | 1:A:4:PHE:HD2 | 1:A:56:THR:HG21 | 5 | 0.01 |
| (1,3220) | 1:A:4:PHE:HD2 | 1:A:56:THR:HG22 | 5 | 0.01 |
| (1,3220) | 1:A:4:PHE:HD2 | 1:A:56:THR:HG23 | 5 | 0.01 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD2 | 7 | 0.01 |
| (1,3183) | 1:B:54:LYS:HA | 1:B:54:LYS:HD3 | 7 | 0.01 |
| (1,3125) | 1:B:53:VAL:HG21 | 1:B:59:LEU:HA | 14 | 0.01 |
| (1,3125) | 1:B:53:VAL:HG22 | 1:B:59:LEU:HA | 14 | 0.01 |
| (1,3125) | 1:B:53:VAL:HG23 | 1:B:59:LEU:HA | 14 | 0.01 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG11 | 4 | 0.01 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG12 | 4 | 0.01 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG13 | 4 | 0.01 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG11 | 7 | 0.01 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG12 | 7 | 0.01 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG13 | 7 | 0.01 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG11 | 9 | 0.01 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG12 | 9 | 0.01 |
| (1,3105) | 1:B:4:PHE:H | 1:B:53:VAL:HG13 | 9 | 0.01 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG11 | 12 | 0.01 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG12 | 12 | 0.01 |
| (1,3104) | 1:A:4:PHE:H | 1:A:53:VAL:HG13 | 12 | 0.01 |
| (1,3099) | 1:B:52:PHE:H | 1:B:53:VAL:HG11 | 9 | 0.01 |
| (1,3099) | 1:B:52:PHE:H | 1:B:53:VAL:HG12 | 9 | 0.01 |
| (1,3099) | 1:B:52:PHE:H | 1:B:53:VAL:HG13 | 9 | 0.01 |
| (1,3098) | 1:A:52:PHE:H | 1:A:53:VAL:HG11 | 7 | 0.01 |
| (1,3098) | 1:A:52:PHE:H | 1:A:53:VAL:HG12 | 7 | 0.01 |
| (1,3098) | 1:A:52:PHE:H | 1:A:53:VAL:HG13 | 7 | 0.01 |
| (1,3096) | 1:A:53:VAL:HG11 | 1:A:55:ASN:H | 1 | 0.01 |
| (1,3096) | 1:A:53:VAL:HG12 | 1:A:55:ASN:H | 1 | 0.01 |
| (1,3096) | 1:A:53:VAL:HG13 | 1:A:55:ASN:H | 1 | 0.01 |
| (1,3094) | 1:A:53:VAL:HG11 | 1:A:58:LYS:HZ1 | 4 | 0.01 |
| (1,3094) | 1:A:53:VAL:HG12 | 1:A:58:LYS:HZ1 | 4 | 0.01 |
| (1,3094) | 1:A:53:VAL:HG13 | 1:A:58:LYS:HZ1 | 4 | 0.01 |
| (1,3094) | 1:A:53:VAL:HG11 | 1:A:58:LYS:HZ1 | 20 | 0.01 |
| (1,3094) | 1:A:53:VAL:HG12 | 1:A:58:LYS:HZ1 | 20 | 0.01 |
| (1,3094) | 1:A:53:VAL:HG13 | 1:A:58:LYS:HZ1 | 20 | 0.01 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD11 | 18 | 0.01 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD12 | 18 | 0.01 |
| (1,3040) | 1:A:31:THR:H | 1:A:51:ILE:HD13 | 18 | 0.01 |
| (1,3038) | 1:A:51:ILE:HD11 | 1:A:58:LYS:HZ1 | 18 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3038) | 1:A:51:ILE:HD12 | 1:A:58:LYS:HZ1 | 18 | 0.01 |
| (1,3038) | 1:A:51:ILE:HD13 | 1:A:58:LYS:HZ1 | 18 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD11 | 14 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD12 | 14 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD13 | 14 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD11 | 14 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD12 | 14 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD13 | 14 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD11 | 15 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD12 | 15 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD13 | 15 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD11 | 15 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD12 | 15 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD13 | 15 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD11 | 20 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD12 | 20 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD1 | 1:A:51:ILE:HD13 | 20 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD11 | 20 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD12 | 20 | 0.01 |
| (1,3036) | 1:A:29:PHE:HD2 | 1:A:51:ILE:HD13 | 20 | 0.01 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD11 | 9 | 0.01 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD12 | 9 | 0.01 |
| (1,3032) | 1:A:7:GLY:HA3 | 1:A:51:ILE:HD13 | 9 | 0.01 |
| (1,3013) | 1:B:51:ILE:HD11 | 1:B:62:LEU:HD21 | 15 | 0.01 |
| (1,3013) | 1:B:51:ILE:HD11 | 1:B:62:LEU:HD22 | 15 | 0.01 |
| (1,3013) | 1:B:51:ILE:HD11 | 1:B:62:LEU:HD23 | 15 | 0.01 |
| (1,3013) | 1:B:51:ILE:HD12 | 1:B:62:LEU:HD21 | 15 | 0.01 |
| (1,3013) | 1:B:51:ILE:HD12 | 1:B:62:LEU:HD22 | 15 | 0.01 |
| (1,3013) | 1:B:51:ILE:HD12 | 1:B:62:LEU:HD23 | 15 | 0.01 |
| (1,3013) | 1:B:51:ILE:HD13 | 1:B:62:LEU:HD21 | 15 | 0.01 |
| (1,3013) | 1:B:51:ILE:HD13 | 1:B:62:LEU:HD22 | 15 | 0.01 |
| (1,3013) | 1:B:51:ILE:HD13 | 1:B:62:LEU:HD23 | 15 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD21 | 8 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD22 | 8 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD23 | 8 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD21 | 8 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD22 | 8 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD23 | 8 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD21 | 8 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD22 | 8 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD23 | 8 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD21 | 14 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD22 | 14 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD23 | 14 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD21 | 14 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD22 | 14 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD23 | 14 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD21 | 14 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD22 | 14 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD23 | 14 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD21 | 15 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD22 | 15 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD23 | 15 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD21 | 15 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD22 | 15 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD23 | 15 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD21 | 15 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD22 | 15 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD23 | 15 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD21 | 16 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD22 | 16 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD23 | 16 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD21 | 16 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD22 | 16 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD23 | 16 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD21 | 16 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD22 | 16 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD23 | 16 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD21 | 17 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD22 | 17 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD11 | 1:A:62:LEU:HD23 | 17 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD21 | 17 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD22 | 17 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD12 | 1:A:62:LEU:HD23 | 17 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD21 | 17 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD22 | 17 | 0.01 |
| (1,3012) | 1:A:51:ILE:HD13 | 1:A:62:LEU:HD23 | 17 | 0.01 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG21 | 7 | 0.01 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG22 | 7 | 0.01 |
| (1,2979) | 1:B:31:THR:HB | 1:B:51:ILE:HG23 | 7 | 0.01 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG21 | 10 | 0.01 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG22 | 10 | 0.01 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG23 | 10 | 0.01 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG21 | 12 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG22 | 12 | 0.01 |
| (1,2978) | 1:A:31:THR:HB | 1:A:51:ILE:HG23 | 12 | 0.01 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG21 | 6 | 0.01 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG22 | 6 | 0.01 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG23 | 6 | 0.01 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG21 | 9 | 0.01 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG22 | 9 | 0.01 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG23 | 9 | 0.01 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG21 | 17 | 0.01 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG22 | 17 | 0.01 |
| (1,2976) | 1:A:33:ILE:HA | 1:A:51:ILE:HG23 | 17 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD11 | 2 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD12 | 2 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD13 | 2 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD11 | 2 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD12 | 2 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD13 | 2 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD11 | 2 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD12 | 2 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD13 | 2 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD11 | 9 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD12 | 9 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD13 | 9 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD11 | 9 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD12 | 9 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD13 | 9 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD11 | 9 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD12 | 9 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD13 | 9 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD11 | 15 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD12 | 15 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG21 | 1:A:62:LEU:HD13 | 15 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD11 | 15 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD12 | 15 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG22 | 1:A:62:LEU:HD13 | 15 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD11 | 15 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD12 | 15 | 0.01 |
| (1,2970) | 1:A:8:ILE:HG23 | 1:A:62:LEU:HD13 | 15 | 0.01 |
| (1,2916) | 1:A:50:MET:HE1 | 1:A:81:LEU:HA | 12 | 0.01 |
| (1,2916) | 1:A:50:MET:HE2 | 1:A:81:LEU:HA | 12 | 0.01 |
| (1,2916) | 1:A:50:MET:HE3 | 1:A:81:LEU:HA | 12 | 0.01 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 13 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 13 | 0.01 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 13 | 0.01 |
| (1,2903) | 1:B:50:MET:HE1 | 1:B:51:ILE:HG13 | 16 | 0.01 |
| (1,2903) | 1:B:50:MET:HE2 | 1:B:51:ILE:HG13 | 16 | 0.01 |
| (1,2903) | 1:B:50:MET:HE3 | 1:B:51:ILE:HG13 | 16 | 0.01 |
| (1,2902) | 1:A:50:MET:HE1 | 1:A:51:ILE:HG13 | 13 | 0.01 |
| (1,2902) | 1:A:50:MET:HE2 | 1:A:51:ILE:HG13 | 13 | 0.01 |
| (1,2902) | 1:A:50:MET:HE3 | 1:A:51:ILE:HG13 | 13 | 0.01 |
| (1,2877) | 1:B:50:MET:HG3 | 1:B:51:ILE:H | 6 | 0.01 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 3 | 0.01 |
| (1,2876) | 1:A:50:MET:HG3 | 1:A:51:ILE:H | 18 | 0.01 |
| (1,2859) | 1:B:50:MET:HG3 | 1:B:78:LEU:HD11 | 15 | 0.01 |
| (1,2859) | 1:B:50:MET:HG3 | 1:B:78:LEU:HD12 | 15 | 0.01 |
| (1,2859) | 1:B:50:MET:HG3 | 1:B:78:LEU:HD13 | 15 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD11 | 12 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD12 | 12 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD13 | 12 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD11 | 12 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD12 | 12 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD13 | 12 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD11 | 12 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD12 | 12 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD13 | 12 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD11 | 18 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD12 | 18 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG21 | 1:B:49:LEU:HD13 | 18 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD11 | 18 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD12 | 18 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG22 | 1:B:49:LEU:HD13 | 18 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD11 | 18 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD12 | 18 | 0.01 |
| (1,2800) | 1:B:26:ILE:HG23 | 1:B:49:LEU:HD13 | 18 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD11 | 1 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD12 | 1 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD13 | 1 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD11 | 1 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD12 | 1 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD13 | 1 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD11 | 1 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD12 | 1 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD13 | 1 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD11 | 2 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD12 | 2 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD13 | 2 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD11 | 2 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD12 | 2 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD13 | 2 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD11 | 2 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD12 | 2 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD13 | 2 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD11 | 9 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD12 | 9 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD13 | 9 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD11 | 9 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD12 | 9 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD13 | 9 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD11 | 9 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD12 | 9 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD13 | 9 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD11 | 12 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD12 | 12 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD13 | 12 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD11 | 12 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD12 | 12 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD13 | 12 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD11 | 12 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD12 | 12 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD13 | 12 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD11 | 14 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD12 | 14 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD13 | 14 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD11 | 14 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD12 | 14 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD13 | 14 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD11 | 14 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD12 | 14 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD13 | 14 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD11 | 16 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD12 | 16 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD13 | 16 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD11 | 16 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD12 | 16 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD13 | 16 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD11 | 16 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD12 | 16 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD13 | 16 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD11 | 20 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD12 | 20 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG21 | 1:A:49:LEU:HD13 | 20 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD11 | 20 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD12 | 20 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG22 | 1:A:49:LEU:HD13 | 20 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD11 | 20 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD12 | 20 | 0.01 |
| (1,2799) | 1:A:26:ILE:HG23 | 1:A:49:LEU:HD13 | 20 | 0.01 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD21 | 9 | 0.01 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD22 | 9 | 0.01 |
| (1,2798) | 1:B:49:LEU:HD11 | 1:B:62:LEU:HD23 | 9 | 0.01 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD21 | 9 | 0.01 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD22 | 9 | 0.01 |
| (1,2798) | 1:B:49:LEU:HD12 | 1:B:62:LEU:HD23 | 9 | 0.01 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD21 | 9 | 0.01 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD22 | 9 | 0.01 |
| (1,2798) | 1:B:49:LEU:HD13 | 1:B:62:LEU:HD23 | 9 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD21 | 8 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD22 | 8 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD23 | 8 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD21 | 8 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD22 | 8 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD23 | 8 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD21 | 8 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD22 | 8 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD23 | 8 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD21 | 15 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD22 | 15 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD23 | 15 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD21 | 15 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD22 | 15 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD23 | 15 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD21 | 15 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD22 | 15 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD23 | 15 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD21 | 17 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD22 | 17 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD11 | 1:A:62:LEU:HD23 | 17 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD21 | 17 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD22 | 17 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD12 | 1:A:62:LEU:HD23 | 17 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD21 | 17 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD22 | 17 | 0.01 |
| (1,2797) | 1:A:49:LEU:HD13 | 1:A:62:LEU:HD23 | 17 | 0.01 |
| (1,2760) | 1:B:10:ILE:HD11 | 1:B:48:ASN:HA | 2 | 0.01 |
| (1,2760) | 1:B:10:ILE:HD12 | 1:B:48:ASN:HA | 2 | 0.01 |
| (1,2760) | 1:B:10:ILE:HD13 | 1:B:48:ASN:HA | 2 | 0.01 |
| (1,2753) | 1:A:23:THR:HG1 | 1:A:47:CYS:HB3 | 10 | 0.01 |
| (1,2726) | 1:B:46:THR:HG21 | 1:B:47:CYS:H | 10 | 0.01 |
| (1,2726) | 1:B:46:THR:HG22 | 1:B:47:CYS:H | 10 | 0.01 |
| (1,2726) | 1:B:46:THR:HG23 | 1:B:47:CYS:H | 10 | 0.01 |
| (1,2726) | 1:B:46:THR:HG21 | 1:B:47:CYS:H | 13 | 0.01 |
| (1,2726) | 1:B:46:THR:HG22 | 1:B:47:CYS:H | 13 | 0.01 |
| (1,2726) | 1:B:46:THR:HG23 | 1:B:47:CYS:H | 13 | 0.01 |
| (1,2725) | 1:A:46:THR:HG21 | 1:A:47:CYS:H | 3 | 0.01 |
| (1,2725) | 1:A:46:THR:HG22 | 1:A:47:CYS:H | 3 | 0.01 |
| (1,2725) | 1:A:46:THR:HG23 | 1:A:47:CYS:H | 3 | 0.01 |
| (1,2725) | 1:A:46:THR:HG21 | 1:A:47:CYS:H | 8 | 0.01 |
| (1,2725) | 1:A:46:THR:HG22 | 1:A:47:CYS:H | 8 | 0.01 |
| (1,2725) | 1:A:46:THR:HG23 | 1:A:47:CYS:H | 8 | 0.01 |
| (1,2725) | 1:A:46:THR:HG21 | 1:A:47:CYS:H | 17 | 0.01 |
| (1,2725) | 1:A:46:THR:HG22 | 1:A:47:CYS:H | 17 | 0.01 |
| (1,2725) | 1:A:46:THR:HG23 | 1:A:47:CYS:H | 17 | 0.01 |
| (1,2725) | 1:A:46:THR:HG21 | 1:A:47:CYS:H | 18 | 0.01 |
| (1,2725) | 1:A:46:THR:HG22 | 1:A:47:CYS:H | 18 | 0.01 |
| (1,2725) | 1:A:46:THR:HG23 | 1:A:47:CYS:H | 18 | 0.01 |
| (1,2704) | 1:B:9:ARG:HD2 | 1:B:46:THR:HG21 | 13 | 0.01 |
| (1,2704) | 1:B:9:ARG:HD2 | 1:B:46:THR:HG22 | 13 | 0.01 |
| (1,2704) | 1:B:9:ARG:HD2 | 1:B:46:THR:HG23 | 13 | 0.01 |
| (1,2704) | 1:B:9:ARG:HD3 | 1:B:46:THR:HG21 | 13 | 0.01 |
| (1,2704) | 1:B:9:ARG:HD3 | 1:B:46:THR:HG22 | 13 | 0.01 |
| (1,2704) | 1:B:9:ARG:HD3 | 1:B:46:THR:HG23 | 13 | 0.01 |
| (1,2703) | 1:A:9:ARG:HD2 | 1:A:46:THR:HG21 | 19 | 0.01 |
| (1,2703) | 1:A:9:ARG:HD2 | 1:A:46:THR:HG22 | 19 | 0.01 |
| (1,2703) | 1:A:9:ARG:HD2 | 1:A:46:THR:HG23 | 19 | 0.01 |
| (1,2703) | 1:A:9:ARG:HD3 | 1:A:46:THR:HG21 | 19 | 0.01 |
| (1,2703) | 1:A:9:ARG:HD3 | 1:A:46:THR:HG22 | 19 | 0.01 |
| (1,2703) | 1:A:9:ARG:HD3 | 1:A:46:THR:HG23 | 19 | 0.01 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG21 | 4 | 0.01 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG22 | 4 | 0.01 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG23 | 4 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG21 | 18 | 0.01 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG22 | 18 | 0.01 |
| (1,2698) | 1:B:44:ILE:HB | 1:B:46:THR:HG23 | 18 | 0.01 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG21 | 2 | 0.01 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG22 | 2 | 0.01 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG23 | 2 | 0.01 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG21 | 17 | 0.01 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG22 | 17 | 0.01 |
| (1,2697) | 1:A:44:ILE:HB | 1:A:46:THR:HG23 | 17 | 0.01 |
| (1,2684) | 1:B:44:ILE:HD11 | 1:B:45:PHE:H | 7 | 0.01 |
| (1,2684) | 1:B:44:ILE:HD12 | 1:B:45:PHE:H | 7 | 0.01 |
| (1,2684) | 1:B:44:ILE:HD13 | 1:B:45:PHE:H | 7 | 0.01 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 2 | 0.01 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 2 | 0.01 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 2 | 0.01 |
| (1,2683) | 1:A:44:ILE:HD11 | 1:A:45:PHE:H | 16 | 0.01 |
| (1,2683) | 1:A:44:ILE:HD12 | 1:A:45:PHE:H | 16 | 0.01 |
| (1,2683) | 1:A:44:ILE:HD13 | 1:A:45:PHE:H | 16 | 0.01 |
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD11 | 3 | 0.01 |
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD12 | 3 | 0.01 |
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD13 | 3 | 0.01 |
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD11 | 17 | 0.01 |
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD12 | 17 | 0.01 |
| (1,2682) | 1:B:44:ILE:H | 1:B:44:ILE:HD13 | 17 | 0.01 |
| (1,2681) | 1:A:44:ILE:H | 1:A:44:ILE:HD11 | 10 | 0.01 |
| (1,2681) | 1:A:44:ILE:H | 1:A:44:ILE:HD12 | 10 | 0.01 |
| (1,2681) | 1:A:44:ILE:H | 1:A:44:ILE:HD13 | 10 | 0.01 |
| (1,2681) | 1:A:44:ILE:H | 1:A:44:ILE:HD11 | 18 | 0.01 |
| (1,2681) | 1:A:44:ILE:H | 1:A:44:ILE:HD12 | 18 | 0.01 |
| (1,2681) | 1:A:44:ILE:H | 1:A:44:ILE:HD13 | 18 | 0.01 |
| (1,2676) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HD1 | 12 | 0.01 |
| (1,2676) | 1:B:44:ILE:HD11 | 1:B:73:PHE:HD2 | 12 | 0.01 |
| (1,2676) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HD1 | 12 | 0.01 |
| (1,2676) | 1:B:44:ILE:HD12 | 1:B:73:PHE:HD2 | 12 | 0.01 |
| (1,2676) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HD1 | 12 | 0.01 |
| (1,2676) | 1:B:44:ILE:HD13 | 1:B:73:PHE:HD2 | 12 | 0.01 |
| (1,2675) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HD1 | 2 | 0.01 |
| (1,2675) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HD2 | 2 | 0.01 |
| (1,2675) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HD1 | 2 | 0.01 |
| (1,2675) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HD2 | 2 | 0.01 |
| (1,2675) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HD1 | 2 | 0.01 |
| (1,2675) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HD2 | 2 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2675) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HD1 | 14 | 0.01 |
| (1,2675) | 1:A:44:ILE:HD11 | 1:A:73:PHE:HD2 | 14 | 0.01 |
| (1,2675) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HD1 | 14 | 0.01 |
| (1,2675) | 1:A:44:ILE:HD12 | 1:A:73:PHE:HD2 | 14 | 0.01 |
| (1,2675) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HD1 | 14 | 0.01 |
| (1,2675) | 1:A:44:ILE:HD13 | 1:A:73:PHE:HD2 | 14 | 0.01 |
| (1,2673) | 1:A:44:ILE:HA | 1:A:44:ILE:HD11 | 15 | 0.01 |
| (1,2673) | 1:A:44:ILE:HA | 1:A:44:ILE:HD12 | 15 | 0.01 |
| (1,2673) | 1:A:44:ILE:HA | 1:A:44:ILE:HD13 | 15 | 0.01 |
| (1,2672) | 1:B:13:GLU:HA | 1:B:44:ILE:HD11 | 14 | 0.01 |
| (1,2672) | 1:B:13:GLU:HA | 1:B:44:ILE:HD12 | 14 | 0.01 |
| (1,2672) | 1:B:13:GLU:HA | 1:B:44:ILE:HD13 | 14 | 0.01 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD11 | 2 | 0.01 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD12 | 2 | 0.01 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD13 | 2 | 0.01 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD11 | 20 | 0.01 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD12 | 20 | 0.01 |
| (1,2671) | 1:A:13:GLU:HA | 1:A:44:ILE:HD13 | 20 | 0.01 |
| (1,2670) | 1:B:44:ILE:HD11 | 1:B:46:THR:HB | 18 | 0.01 |
| (1,2670) | 1:B:44:ILE:HD12 | 1:B:46:THR:HB | 18 | 0.01 |
| (1,2670) | 1:B:44:ILE:HD13 | 1:B:46:THR:HB | 18 | 0.01 |
| (1,2669) | 1:A:44:ILE:HD11 | 1:A:46:THR:HB | 4 | 0.01 |
| (1,2669) | 1:A:44:ILE:HD12 | 1:A:46:THR:HB | 4 | 0.01 |
| (1,2669) | 1:A:44:ILE:HD13 | 1:A:46:THR:HB | 4 | 0.01 |
| (1,2669) | 1:A:44:ILE:HD11 | 1:A:46:THR:HB | 12 | 0.01 |
| (1,2669) | 1:A:44:ILE:HD12 | 1:A:46:THR:HB | 12 | 0.01 |
| (1,2669) | 1:A:44:ILE:HD13 | 1:A:46:THR:HB | 12 | 0.01 |
| (1,2669) | 1:A:44:ILE:HD11 | 1:A:46:THR:HB | 13 | 0.01 |
| (1,2669) | 1:A:44:ILE:HD12 | 1:A:46:THR:HB | 13 | 0.01 |
| (1,2669) | 1:A:44:ILE:HD13 | 1:A:46:THR:HB | 13 | 0.01 |
| (1,2669) | 1:A:44:ILE:HD11 | 1:A:46:THR:HB | 17 | 0.01 |
| (1,2669) | 1:A:44:ILE:HD12 | 1:A:46:THR:HB | 17 | 0.01 |
| (1,2669) | 1:A:44:ILE:HD13 | 1:A:46:THR:HB | 17 | 0.01 |
| (1,2666) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HD11 | 14 | 0.01 |
| (1,2666) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HD12 | 14 | 0.01 |
| (1,2666) | 1:B:42:ASP:HB2 | 1:B:44:ILE:HD13 | 14 | 0.01 |
| (1,2638) | 1:B:44:ILE:HG13 | 1:B:45:PHE:H | 9 | 0.01 |
| (1,2638) | 1:B:44:ILE:HG13 | 1:B:45:PHE:H | 10 | 0.01 |
| (1,2637) | 1:A:44:ILE:HG13 | 1:A:45:PHE:H | 3 | 0.01 |
| (1,2637) | 1:A:44:ILE:HG13 | 1:A:45:PHE:H | 8 | 0.01 |
| (1,2637) | 1:A:44:ILE:HG13 | 1:A:45:PHE:H | 18 | 0.01 |
| (1,2613) | 1:A:12:GLY:H | 1:A:44:ILE:HB | 13 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|------|--------|--------|-------|---------------|
| (1,2612) | 1:B:13:GLU:HA | 1:B:44:ILE:HB | 9 | 0.01 |
| (1,2612) | 1:B:13:GLU:HA | 1:B:44:ILE:HB | 11 | 0.01 |
| (1,2611) | 1:A:13:GLU:HA | 1:A:44:ILE:HB | 3 | 0.01 |
| (1,2605) | 1:A:14:ASP:HB2 | 1:A:43:GLY:HA3 | 4 | 0.01 |
| (1,2572) | 1:B:40:ALA:HA | 1:B:45:PHE:HA | 9 | 0.01 |
| (1,2572) | 1:B:40:ALA:HA | 1:B:45:PHE:HA | 16 | 0.01 |
| (1,2571) | 1:A:40:ALA:HA | 1:A:45:PHE:HA | 6 | 0.01 |
| (1,2571) | 1:A:40:ALA:HA | 1:A:45:PHE:HA | 8 | 0.01 |
| (1,2571) | 1:A:40:ALA:HA | 1:A:45:PHE:HA | 11 | 0.01 |
| (1,2571) | 1:A:40:ALA:HA | 1:A:45:PHE:HA | 18 | 0.01 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD21 | 12 | 0.01 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD22 | 12 | 0.01 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD23 | 12 | 0.01 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD21 | 20 | 0.01 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD22 | 20 | 0.01 |
| (1,2536) | 1:B:37:VAL:HA | 1:B:38:LEU:HD23 | 20 | 0.01 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD21 | 6 | 0.01 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD22 | 6 | 0.01 |
| (1,2535) | 1:A:37:VAL:HA | 1:A:38:LEU:HD23 | 6 | 0.01 |
| (1,2534) | 1:B:23:THR:HG1 | 1:B:38:LEU:HD21 | 10 | 0.01 |
| (1,2534) | 1:B:23:THR:HG1 | 1:B:38:LEU:HD22 | 10 | 0.01 |
| (1,2534) | 1:B:23:THR:HG1 | 1:B:38:LEU:HD23 | 10 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD21 | 1:B:35:THR:HG21 | 2 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD21 | 1:B:35:THR:HG22 | 2 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD21 | 1:B:35:THR:HG23 | 2 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD22 | 1:B:35:THR:HG21 | 2 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD22 | 1:B:35:THR:HG22 | 2 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD22 | 1:B:35:THR:HG23 | 2 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD23 | 1:B:35:THR:HG21 | 2 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD23 | 1:B:35:THR:HG22 | 2 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD23 | 1:B:35:THR:HG23 | 2 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD21 | 1:B:35:THR:HG21 | 16 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD21 | 1:B:35:THR:HG22 | 16 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD21 | 1:B:35:THR:HG23 | 16 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD22 | 1:B:35:THR:HG21 | 16 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD22 | 1:B:35:THR:HG22 | 16 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD22 | 1:B:35:THR:HG23 | 16 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD23 | 1:B:35:THR:HG21 | 16 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD23 | 1:B:35:THR:HG22 | 16 | 0.01 |
| (1,2518) | 1:A:38:LEU:HD23 | 1:B:35:THR:HG23 | 16 | 0.01 |
| (1,2510) | 1:B:38:LEU:HD11 | 1:B:39:ASN:H | 15 | 0.01 |
| (1,2510) | 1:B:38:LEU:HD12 | 1:B:39:ASN:H | 15 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2510) | 1:B:38:LEU:HD13 | 1:B:39:ASN:H | 15 | 0.01 |
| (1,2510) | 1:B:38:LEU:HD11 | 1:B:39:ASN:H | 17 | 0.01 |
| (1,2510) | 1:B:38:LEU:HD12 | 1:B:39:ASN:H | 17 | 0.01 |
| (1,2510) | 1:B:38:LEU:HD13 | 1:B:39:ASN:H | 17 | 0.01 |
| (1,2510) | 1:B:38:LEU:HD11 | 1:B:39:ASN:H | 18 | 0.01 |
| (1,2510) | 1:B:38:LEU:HD12 | 1:B:39:ASN:H | 18 | 0.01 |
| (1,2510) | 1:B:38:LEU:HD13 | 1:B:39:ASN:H | 18 | 0.01 |
| (1,2503) | 1:A:38:LEU:HD11 | 1:A:45:PHE:HZ | 13 | 0.01 |
| (1,2503) | 1:A:38:LEU:HD12 | 1:A:45:PHE:HZ | 13 | 0.01 |
| (1,2503) | 1:A:38:LEU:HD13 | 1:A:45:PHE:HZ | 13 | 0.01 |
| (1,2503) | 1:A:38:LEU:HD11 | 1:A:45:PHE:HZ | 18 | 0.01 |
| (1,2503) | 1:A:38:LEU:HD12 | 1:A:45:PHE:HZ | 18 | 0.01 |
| (1,2503) | 1:A:38:LEU:HD13 | 1:A:45:PHE:HZ | 18 | 0.01 |
| (1,2485) | 1:A:38:LEU:HD11 | 1:A:47:CYS:HG | 2 | 0.01 |
| (1,2485) | 1:A:38:LEU:HD12 | 1:A:47:CYS:HG | 2 | 0.01 |
| (1,2485) | 1:A:38:LEU:HD13 | 1:A:47:CYS:HG | 2 | 0.01 |
| (1,2474) | 1:B:37:VAL:HG21 | 1:B:38:LEU:H | 3 | 0.01 |
| (1,2474) | 1:B:37:VAL:HG22 | 1:B:38:LEU:H | 3 | 0.01 |
| (1,2474) | 1:B:37:VAL:HG23 | 1:B:38:LEU:H | 3 | 0.01 |
| (1,2474) | 1:B:37:VAL:HG21 | 1:B:38:LEU:H | 6 | 0.01 |
| (1,2474) | 1:B:37:VAL:HG22 | 1:B:38:LEU:H | 6 | 0.01 |
| (1,2474) | 1:B:37:VAL:HG23 | 1:B:38:LEU:H | 6 | 0.01 |
| (1,2474) | 1:B:37:VAL:HG21 | 1:B:38:LEU:H | 8 | 0.01 |
| (1,2474) | 1:B:37:VAL:HG22 | 1:B:38:LEU:H | 8 | 0.01 |
| (1,2474) | 1:B:37:VAL:HG23 | 1:B:38:LEU:H | 8 | 0.01 |
| (1,2473) | 1:A:37:VAL:HG21 | 1:A:38:LEU:H | 1 | 0.01 |
| (1,2473) | 1:A:37:VAL:HG22 | 1:A:38:LEU:H | 1 | 0.01 |
| (1,2473) | 1:A:37:VAL:HG23 | 1:A:38:LEU:H | 1 | 0.01 |
| (1,2473) | 1:A:37:VAL:HG21 | 1:A:38:LEU:H | 2 | 0.01 |
| (1,2473) | 1:A:37:VAL:HG22 | 1:A:38:LEU:H | 2 | 0.01 |
| (1,2473) | 1:A:37:VAL:HG23 | 1:A:38:LEU:H | 2 | 0.01 |
| (1,2473) | 1:A:37:VAL:HG21 | 1:A:38:LEU:H | 16 | 0.01 |
| (1,2473) | 1:A:37:VAL:HG22 | 1:A:38:LEU:H | 16 | 0.01 |
| (1,2473) | 1:A:37:VAL:HG23 | 1:A:38:LEU:H | 16 | 0.01 |
| (1,2473) | 1:A:37:VAL:HG21 | 1:A:38:LEU:H | 19 | 0.01 |
| (1,2473) | 1:A:37:VAL:HG22 | 1:A:38:LEU:H | 19 | 0.01 |
| (1,2473) | 1:A:37:VAL:HG23 | 1:A:38:LEU:H | 19 | 0.01 |
| (1,2473) | 1:A:37:VAL:HG21 | 1:A:38:LEU:H | 20 | 0.01 |
| (1,2473) | 1:A:37:VAL:HG22 | 1:A:38:LEU:H | 20 | 0.01 |
| (1,2473) | 1:A:37:VAL:HG23 | 1:A:38:LEU:H | 20 | 0.01 |
| (1,2466) | 1:B:37:VAL:HG21 | 1:B:48:ASN:HD22 | 1 | 0.01 |
| (1,2466) | 1:B:37:VAL:HG22 | 1:B:48:ASN:HD22 | 1 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2466) | 1:B:37:VAL:HG23 | 1:B:48:ASN:HD22 | 1 | 0.01 |
| (1,2466) | 1:B:37:VAL:HG21 | 1:B:48:ASN:HD22 | 10 | 0.01 |
| (1,2466) | 1:B:37:VAL:HG22 | 1:B:48:ASN:HD22 | 10 | 0.01 |
| (1,2466) | 1:B:37:VAL:HG23 | 1:B:48:ASN:HD22 | 10 | 0.01 |
| (1,2465) | 1:A:37:VAL:HG21 | 1:A:48:ASN:HD22 | 2 | 0.01 |
| (1,2465) | 1:A:37:VAL:HG22 | 1:A:48:ASN:HD22 | 2 | 0.01 |
| (1,2465) | 1:A:37:VAL:HG23 | 1:A:48:ASN:HD22 | 2 | 0.01 |
| (1,2465) | 1:A:37:VAL:HG21 | 1:A:48:ASN:HD22 | 16 | 0.01 |
| (1,2465) | 1:A:37:VAL:HG22 | 1:A:48:ASN:HD22 | 16 | 0.01 |
| (1,2465) | 1:A:37:VAL:HG23 | 1:A:48:ASN:HD22 | 16 | 0.01 |
| (1,2465) | 1:A:37:VAL:HG21 | 1:A:48:ASN:HD22 | 17 | 0.01 |
| (1,2465) | 1:A:37:VAL:HG22 | 1:A:48:ASN:HD22 | 17 | 0.01 |
| (1,2465) | 1:A:37:VAL:HG23 | 1:A:48:ASN:HD22 | 17 | 0.01 |
| (1,2465) | 1:A:37:VAL:HG21 | 1:A:48:ASN:HD22 | 20 | 0.01 |
| (1,2465) | 1:A:37:VAL:HG22 | 1:A:48:ASN:HD22 | 20 | 0.01 |
| (1,2465) | 1:A:37:VAL:HG23 | 1:A:48:ASN:HD22 | 20 | 0.01 |
| (1,2451) | 1:A:37:VAL:HG21 | 1:A:48:ASN:HB3 | 14 | 0.01 |
| (1,2451) | 1:A:37:VAL:HG22 | 1:A:48:ASN:HB3 | 14 | 0.01 |
| (1,2451) | 1:A:37:VAL:HG23 | 1:A:48:ASN:HB3 | 14 | 0.01 |
| (1,245) | 1:B:15:LYS:HG2 | 1:B:19:THR:H | 1 | 0.01 |
| (1,245) | 1:B:15:LYS:HG3 | 1:B:19:THR:H | 1 | 0.01 |
| (1,245) | 1:B:15:LYS:HG2 | 1:B:19:THR:H | 12 | 0.01 |
| (1,245) | 1:B:15:LYS:HG3 | 1:B:19:THR:H | 12 | 0.01 |
| (1,244) | 1:A:15:LYS:HG2 | 1:A:19:THR:H | 11 | 0.01 |
| (1,244) | 1:A:15:LYS:HG3 | 1:A:19:THR:H | 11 | 0.01 |
| (1,2420) | 1:B:37:VAL:HB | 1:B:48:ASN:HB2 | 10 | 0.01 |
| (1,2420) | 1:B:37:VAL:HB | 1:B:48:ASN:HB2 | 19 | 0.01 |
| (1,2412) | 1:B:23:THR:H | 1:B:36:ILE:HD11 | 4 | 0.01 |
| (1,2412) | 1:B:23:THR:H | 1:B:36:ILE:HD12 | 4 | 0.01 |
| (1,2412) | 1:B:23:THR:H | 1:B:36:ILE:HD13 | 4 | 0.01 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 16 | 0.01 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 16 | 0.01 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 16 | 0.01 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD11 | 17 | 0.01 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD12 | 17 | 0.01 |
| (1,241) | 1:B:19:THR:H | 1:B:38:LEU:HD13 | 17 | 0.01 |
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD11 | 6 | 0.01 |
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD12 | 6 | 0.01 |
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD13 | 6 | 0.01 |
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD11 | 8 | 0.01 |
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD12 | 8 | 0.01 |
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD13 | 8 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD11 | 13 | 0.01 |
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD12 | 13 | 0.01 |
| (1,2401) | 1:A:23:THR:HG1 | 1:A:36:ILE:HD13 | 13 | 0.01 |
| (1,2390) | 1:B:36:ILE:HG21 | 1:B:48:ASN:H | 14 | 0.01 |
| (1,2390) | 1:B:36:ILE:HG22 | 1:B:48:ASN:H | 14 | 0.01 |
| (1,2390) | 1:B:36:ILE:HG23 | 1:B:48:ASN:H | 14 | 0.01 |
| (1,2389) | 1:A:36:ILE:HG21 | 1:A:48:ASN:H | 2 | 0.01 |
| (1,2389) | 1:A:36:ILE:HG22 | 1:A:48:ASN:H | 2 | 0.01 |
| (1,2389) | 1:A:36:ILE:HG23 | 1:A:48:ASN:H | 2 | 0.01 |
| (1,2373) | 1:A:35:THR:HB | 1:A:36:ILE:HG21 | 13 | 0.01 |
| (1,2373) | 1:A:35:THR:HB | 1:A:36:ILE:HG22 | 13 | 0.01 |
| (1,2373) | 1:A:35:THR:HB | 1:A:36:ILE:HG23 | 13 | 0.01 |
| (1,2368) | 1:B:36:ILE:HG21 | 1:B:37:VAL:HB | 1 | 0.01 |
| (1,2368) | 1:B:36:ILE:HG22 | 1:B:37:VAL:HB | 1 | 0.01 |
| (1,2368) | 1:B:36:ILE:HG23 | 1:B:37:VAL:HB | 1 | 0.01 |
| (1,2368) | 1:B:36:ILE:HG21 | 1:B:37:VAL:HB | 4 | 0.01 |
| (1,2368) | 1:B:36:ILE:HG22 | 1:B:37:VAL:HB | 4 | 0.01 |
| (1,2368) | 1:B:36:ILE:HG23 | 1:B:37:VAL:HB | 4 | 0.01 |
| (1,2367) | 1:A:36:ILE:HG21 | 1:A:37:VAL:HB | 8 | 0.01 |
| (1,2367) | 1:A:36:ILE:HG22 | 1:A:37:VAL:HB | 8 | 0.01 |
| (1,2367) | 1:A:36:ILE:HG23 | 1:A:37:VAL:HB | 8 | 0.01 |
| (1,2344) | 1:B:35:THR:HB | 1:B:50:MET:HB2 | 18 | 0.01 |
| (1,2343) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 4 | 0.01 |
| (1,2343) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 8 | 0.01 |
| (1,2343) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 13 | 0.01 |
| (1,2343) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 15 | 0.01 |
| (1,2343) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 19 | 0.01 |
| (1,2343) | 1:A:35:THR:HB | 1:A:50:MET:HB2 | 20 | 0.01 |
| (1,2334) | 1:B:33:ILE:HD11 | 1:B:34:ARG:H | 7 | 0.01 |
| (1,2334) | 1:B:33:ILE:HD12 | 1:B:34:ARG:H | 7 | 0.01 |
| (1,2334) | 1:B:33:ILE:HD13 | 1:B:34:ARG:H | 7 | 0.01 |
| (1,2331) | 1:A:33:ILE:H | 1:A:33:ILE:HD11 | 6 | 0.01 |
| (1,2331) | 1:A:33:ILE:H | 1:A:33:ILE:HD12 | 6 | 0.01 |
| (1,2331) | 1:A:33:ILE:H | 1:A:33:ILE:HD13 | 6 | 0.01 |
| (1,2331) | 1:A:33:ILE:H | 1:A:33:ILE:HD11 | 15 | 0.01 |
| (1,2331) | 1:A:33:ILE:H | 1:A:33:ILE:HD12 | 15 | 0.01 |
| (1,2331) | 1:A:33:ILE:H | 1:A:33:ILE:HD13 | 15 | 0.01 |
| (1,2328) | 1:A:33:ILE:HD11 | 1:B:20:ASN:HD22 | 14 | 0.01 |
| (1,2328) | 1:A:33:ILE:HD12 | 1:B:20:ASN:HD22 | 14 | 0.01 |
| (1,2328) | 1:A:33:ILE:HD13 | 1:B:20:ASN:HD22 | 14 | 0.01 |
| (1,2327) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HD11 | 2 | 0.01 |
| (1,2327) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HD12 | 2 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,2327) | 1:A:20:ASN:HD22 | 1:B:33:ILE:HD13 | 2 | 0.01 |
| (1,2323) | 1:A:20:ASN:HA | 1:B:33:ILE:HD11 | 16 | 0.01 |
| (1,2323) | 1:A:20:ASN:HA | 1:B:33:ILE:HD12 | 16 | 0.01 |
| (1,2323) | 1:A:20:ASN:HA | 1:B:33:ILE:HD13 | 16 | 0.01 |
| (1,2323) | 1:A:20:ASN:HA | 1:B:33:ILE:HD11 | 20 | 0.01 |
| (1,2323) | 1:A:20:ASN:HA | 1:B:33:ILE:HD12 | 20 | 0.01 |
| (1,2323) | 1:A:20:ASN:HA | 1:B:33:ILE:HD13 | 20 | 0.01 |
| (1,2287) | 1:A:31:THR:HG21 | 1:A:52:PHE:H | 15 | 0.01 |
| (1,2287) | 1:A:31:THR:HG22 | 1:A:52:PHE:H | 15 | 0.01 |
| (1,2287) | 1:A:31:THR:HG23 | 1:A:52:PHE:H | 15 | 0.01 |
| (1,227) | 1:B:18:MET:H | 1:B:18:MET:HG3 | 4 | 0.01 |
| (1,227) | 1:B:18:MET:H | 1:B:18:MET:HG3 | 5 | 0.01 |
| (1,227) | 1:B:18:MET:H | 1:B:18:MET:HG3 | 20 | 0.01 |
| (1,2268) | 1:B:29:PHE:HD1 | 1:B:31:THR:HB | 9 | 0.01 |
| (1,2268) | 1:B:29:PHE:HD2 | 1:B:31:THR:HB | 9 | 0.01 |
| (1,2268) | 1:B:29:PHE:HD1 | 1:B:31:THR:HB | 10 | 0.01 |
| (1,2268) | 1:B:29:PHE:HD2 | 1:B:31:THR:HB | 10 | 0.01 |
| (1,2267) | 1:A:29:PHE:HD1 | 1:A:31:THR:HB | 5 | 0.01 |
| (1,2267) | 1:A:29:PHE:HD2 | 1:A:31:THR:HB | 5 | 0.01 |
| (1,2263) | 1:A:28:LYS:HA | 1:A:28:LYS:HE2 | 13 | 0.01 |
| (1,2263) | 1:A:28:LYS:HA | 1:A:28:LYS:HE3 | 13 | 0.01 |
| (1,2261) | 1:A:25:VAL:HA | 1:A:28:LYS:HE2 | 17 | 0.01 |
| (1,2261) | 1:A:25:VAL:HA | 1:A:28:LYS:HE3 | 17 | 0.01 |
| (1,226) | 1:A:18:MET:H | 1:A:18:MET:HG3 | 7 | 0.01 |
| (1,2237) | 1:A:23:THR:HG21 | 1:A:27:SER:HB3 | 17 | 0.01 |
| (1,2237) | 1:A:23:THR:HG22 | 1:A:27:SER:HB3 | 17 | 0.01 |
| (1,2237) | 1:A:23:THR:HG23 | 1:A:27:SER:HB3 | 17 | 0.01 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG21 | 13 | 0.01 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG22 | 13 | 0.01 |
| (1,2192) | 1:B:21:GLN:HE22 | 1:B:25:VAL:HG23 | 13 | 0.01 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG21 | 1 | 0.01 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG22 | 1 | 0.01 |
| (1,2191) | 1:A:21:GLN:HE22 | 1:A:25:VAL:HG23 | 1 | 0.01 |
| (1,2172) | 1:B:25:VAL:HG11 | 1:B:27:SER:H | 5 | 0.01 |
| (1,2172) | 1:B:25:VAL:HG12 | 1:B:27:SER:H | 5 | 0.01 |
| (1,2172) | 1:B:25:VAL:HG13 | 1:B:27:SER:H | 5 | 0.01 |
| (1,2172) | 1:B:25:VAL:HG11 | 1:B:27:SER:H | 8 | 0.01 |
| (1,2172) | 1:B:25:VAL:HG12 | 1:B:27:SER:H | 8 | 0.01 |
| (1,2172) | 1:B:25:VAL:HG13 | 1:B:27:SER:H | 8 | 0.01 |
| (1,2172) | 1:B:25:VAL:HG11 | 1:B:27:SER:H | 11 | 0.01 |
| (1,2172) | 1:B:25:VAL:HG12 | 1:B:27:SER:H | 11 | 0.01 |
| (1,2172) | 1:B:25:VAL:HG13 | 1:B:27:SER:H | 11 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2172) | 1:B:25:VAL:HG11 | 1:B:27:SER:H | 15 | 0.01 |
| (1,2172) | 1:B:25:VAL:HG12 | 1:B:27:SER:H | 15 | 0.01 |
| (1,2172) | 1:B:25:VAL:HG13 | 1:B:27:SER:H | 15 | 0.01 |
| (1,2171) | 1:A:25:VAL:HG11 | 1:A:27:SER:H | 3 | 0.01 |
| (1,2171) | 1:A:25:VAL:HG12 | 1:A:27:SER:H | 3 | 0.01 |
| (1,2171) | 1:A:25:VAL:HG13 | 1:A:27:SER:H | 3 | 0.01 |
| (1,2171) | 1:A:25:VAL:HG11 | 1:A:27:SER:H | 16 | 0.01 |
| (1,2171) | 1:A:25:VAL:HG12 | 1:A:27:SER:H | 16 | 0.01 |
| (1,2171) | 1:A:25:VAL:HG13 | 1:A:27:SER:H | 16 | 0.01 |
| (1,2171) | 1:A:25:VAL:HG11 | 1:A:27:SER:H | 20 | 0.01 |
| (1,2171) | 1:A:25:VAL:HG12 | 1:A:27:SER:H | 20 | 0.01 |
| (1,2171) | 1:A:25:VAL:HG13 | 1:A:27:SER:H | 20 | 0.01 |
| (1,2168) | 1:B:25:VAL:HG11 | 1:B:69:VAL:H | 18 | 0.01 |
| (1,2168) | 1:B:25:VAL:HG12 | 1:B:69:VAL:H | 18 | 0.01 |
| (1,2168) | 1:B:25:VAL:HG13 | 1:B:69:VAL:H | 18 | 0.01 |
| (1,2104) | 1:B:22:ILE:HA | 1:B:22:ILE:HD11 | 6 | 0.01 |
| (1,2104) | 1:B:22:ILE:HA | 1:B:22:ILE:HD12 | 6 | 0.01 |
| (1,2104) | 1:B:22:ILE:HA | 1:B:22:ILE:HD13 | 6 | 0.01 |
| (1,2104) | 1:B:22:ILE:HA | 1:B:22:ILE:HD11 | 12 | 0.01 |
| (1,2104) | 1:B:22:ILE:HA | 1:B:22:ILE:HD12 | 12 | 0.01 |
| (1,2104) | 1:B:22:ILE:HA | 1:B:22:ILE:HD13 | 12 | 0.01 |
| (1,2104) | 1:B:22:ILE:HA | 1:B:22:ILE:HD11 | 13 | 0.01 |
| (1,2104) | 1:B:22:ILE:HA | 1:B:22:ILE:HD12 | 13 | 0.01 |
| (1,2104) | 1:B:22:ILE:HA | 1:B:22:ILE:HD13 | 13 | 0.01 |
| (1,2103) | 1:A:22:ILE:HA | 1:A:22:ILE:HD11 | 8 | 0.01 |
| (1,2103) | 1:A:22:ILE:HA | 1:A:22:ILE:HD12 | 8 | 0.01 |
| (1,2103) | 1:A:22:ILE:HA | 1:A:22:ILE:HD13 | 8 | 0.01 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 3 | 0.01 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 3 | 0.01 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 3 | 0.01 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 5 | 0.01 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 5 | 0.01 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 5 | 0.01 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 9 | 0.01 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 9 | 0.01 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 9 | 0.01 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 14 | 0.01 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 14 | 0.01 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 14 | 0.01 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 17 | 0.01 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 17 | 0.01 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 17 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG21 | 19 | 0.01 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG22 | 19 | 0.01 |
| (1,2069) | 1:B:21:GLN:HG2 | 1:B:22:ILE:HG23 | 19 | 0.01 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG21 | 14 | 0.01 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG22 | 14 | 0.01 |
| (1,2068) | 1:A:21:GLN:HG2 | 1:A:22:ILE:HG23 | 14 | 0.01 |
| (1,2055) | 1:B:20:ASN:H | 1:B:22:ILE:HG13 | 3 | 0.01 |
| (1,2055) | 1:B:20:ASN:H | 1:B:22:ILE:HG13 | 9 | 0.01 |
| (1,2055) | 1:B:20:ASN:H | 1:B:22:ILE:HG13 | 15 | 0.01 |
| (1,2054) | 1:A:20:ASN:H | 1:A:22:ILE:HG13 | 14 | 0.01 |
| (1,2054) | 1:A:20:ASN:H | 1:A:22:ILE:HG13 | 18 | 0.01 |
| (1,2025) | 1:B:22:ILE:HB | 1:B:47:CYS:HG | 4 | 0.01 |
| (1,2025) | 1:B:22:ILE:HB | 1:B:47:CYS:HG | 10 | 0.01 |
| (1,2024) | 1:A:22:ILE:HB | 1:A:47:CYS:HG | 2 | 0.01 |
| (1,2024) | 1:A:22:ILE:HB | 1:A:47:CYS:HG | 8 | 0.01 |
| (1,2017) | 1:B:21:GLN:HE21 | 1:B:22:ILE:HA | 1 | 0.01 |
| (1,2017) | 1:B:21:GLN:HE21 | 1:B:22:ILE:HA | 4 | 0.01 |
| (1,2017) | 1:B:21:GLN:HE21 | 1:B:22:ILE:HA | 5 | 0.01 |
| (1,2017) | 1:B:21:GLN:HE21 | 1:B:22:ILE:HA | 6 | 0.01 |
| (1,2017) | 1:B:21:GLN:HE21 | 1:B:22:ILE:HA | 7 | 0.01 |
| (1,2017) | 1:B:21:GLN:HE21 | 1:B:22:ILE:HA | 16 | 0.01 |
| (1,2016) | 1:A:21:GLN:HE21 | 1:A:22:ILE:HA | 1 | 0.01 |
| (1,2016) | 1:A:21:GLN:HE21 | 1:A:22:ILE:HA | 5 | 0.01 |
| (1,2016) | 1:A:21:GLN:HE21 | 1:A:22:ILE:HA | 8 | 0.01 |
| (1,2016) | 1:A:21:GLN:HE21 | 1:A:22:ILE:HA | 16 | 0.01 |
| (1,2009) | 1:B:21:GLN:HG3 | 1:B:25:VAL:H | 17 | 0.01 |
| (1,2009) | 1:B:21:GLN:HG3 | 1:B:25:VAL:H | 20 | 0.01 |
| (1,2008) | 1:A:21:GLN:HG3 | 1:A:25:VAL:H | 1 | 0.01 |
| (1,1990) | 1:A:21:GLN:HG2 | 1:A:25:VAL:HG21 | 5 | 0.01 |
| (1,1990) | 1:A:21:GLN:HG2 | 1:A:25:VAL:HG22 | 5 | 0.01 |
| (1,1990) | 1:A:21:GLN:HG2 | 1:A:25:VAL:HG23 | 5 | 0.01 |
| (1,1990) | 1:A:21:GLN:HG2 | 1:A:25:VAL:HG21 | 16 | 0.01 |
| (1,1990) | 1:A:21:GLN:HG2 | 1:A:25:VAL:HG22 | 16 | 0.01 |
| (1,1990) | 1:A:21:GLN:HG2 | 1:A:25:VAL:HG23 | 16 | 0.01 |
| (1,1943) | 1:B:18:MET:HE1 | 1:B:70:GLN:H | 14 | 0.01 |
| (1,1943) | 1:B:18:MET:HE2 | 1:B:70:GLN:H | 14 | 0.01 |
| (1,1943) | 1:B:18:MET:HE3 | 1:B:70:GLN:H | 14 | 0.01 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 16 | 0.01 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 16 | 0.01 |
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 16 | 0.01 |
| (1,1927) | 1:B:18:MET:HE1 | 1:B:71:GLY:HA2 | 20 | 0.01 |
| (1,1927) | 1:B:18:MET:HE2 | 1:B:71:GLY:HA2 | 20 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1927) | 1:B:18:MET:HE3 | 1:B:71:GLY:HA2 | 20 | 0.01 |
| (1,1914) | 1:B:17:GLY:H | 1:B:18:MET:HG3 | 13 | 0.01 |
| (1,1909) | 1:A:18:MET:HA | 1:A:21:GLN:HA | 4 | 0.01 |
| (1,1898) | 1:B:16:ASN:HB3 | 1:B:17:GLY:H | 1 | 0.01 |
| (1,1897) | 1:A:16:ASN:HB3 | 1:A:17:GLY:H | 1 | 0.01 |
| (1,1891) | 1:B:15:LYS:HA | 1:B:15:LYS:HE2 | 7 | 0.01 |
| (1,1891) | 1:B:15:LYS:HA | 1:B:15:LYS:HE3 | 7 | 0.01 |
| (1,1881) | 1:B:68:LYS:HE2 | 1:B:69:VAL:HG21 | 10 | 0.01 |
| (1,1881) | 1:B:68:LYS:HE2 | 1:B:69:VAL:HG22 | 10 | 0.01 |
| (1,1881) | 1:B:68:LYS:HE2 | 1:B:69:VAL:HG23 | 10 | 0.01 |
| (1,1881) | 1:B:68:LYS:HE3 | 1:B:69:VAL:HG21 | 10 | 0.01 |
| (1,1881) | 1:B:68:LYS:HE3 | 1:B:69:VAL:HG22 | 10 | 0.01 |
| (1,1881) | 1:B:68:LYS:HE3 | 1:B:69:VAL:HG23 | 10 | 0.01 |
| (1,1880) | 1:A:68:LYS:HE2 | 1:A:69:VAL:HG21 | 5 | 0.01 |
| (1,1880) | 1:A:68:LYS:HE2 | 1:A:69:VAL:HG22 | 5 | 0.01 |
| (1,1880) | 1:A:68:LYS:HE2 | 1:A:69:VAL:HG23 | 5 | 0.01 |
| (1,1880) | 1:A:68:LYS:HE3 | 1:A:69:VAL:HG21 | 5 | 0.01 |
| (1,1880) | 1:A:68:LYS:HE3 | 1:A:69:VAL:HG22 | 5 | 0.01 |
| (1,1880) | 1:A:68:LYS:HE3 | 1:A:69:VAL:HG23 | 5 | 0.01 |
| (1,1880) | 1:A:68:LYS:HE2 | 1:A:69:VAL:HG21 | 20 | 0.01 |
| (1,1880) | 1:A:68:LYS:HE2 | 1:A:69:VAL:HG22 | 20 | 0.01 |
| (1,1880) | 1:A:68:LYS:HE2 | 1:A:69:VAL:HG23 | 20 | 0.01 |
| (1,1880) | 1:A:68:LYS:HE3 | 1:A:69:VAL:HG21 | 20 | 0.01 |
| (1,1880) | 1:A:68:LYS:HE3 | 1:A:69:VAL:HG22 | 20 | 0.01 |
| (1,1880) | 1:A:68:LYS:HE3 | 1:A:69:VAL:HG23 | 20 | 0.01 |
| (1,187) | 1:A:15:LYS:H | 1:A:44:ILE:HA | 18 | 0.01 |
| (1,1863) | 1:B:13:GLU:HB2 | 1:B:15:LYS:HG2 | 15 | 0.01 |
| (1,1863) | 1:B:13:GLU:HB2 | 1:B:15:LYS:HG3 | 15 | 0.01 |
| (1,1847) | 1:B:14:ASP:HB3 | 1:B:43:GLY:HA3 | 17 | 0.01 |
| (1,1838) | 1:A:13:GLU:HG2 | 1:A:44:ILE:HA | 19 | 0.01 |
| (1,1838) | 1:A:13:GLU:HG3 | 1:A:44:ILE:HA | 19 | 0.01 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG11 | 12 | 0.01 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG12 | 12 | 0.01 |
| (1,1825) | 1:B:13:GLU:HG2 | 1:B:69:VAL:HG13 | 12 | 0.01 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG11 | 12 | 0.01 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG12 | 12 | 0.01 |
| (1,1825) | 1:B:13:GLU:HG3 | 1:B:69:VAL:HG13 | 12 | 0.01 |
| (1,182) | 1:B:15:LYS:H | 1:B:18:MET:HG2 | 9 | 0.01 |
| (1,1799) | 1:B:13:GLU:HB3 | 1:B:15:LYS:HD2 | 6 | 0.01 |
| (1,1799) | 1:B:13:GLU:HB3 | 1:B:15:LYS:HD3 | 6 | 0.01 |
| (1,1799) | 1:B:13:GLU:HB3 | 1:B:15:LYS:HD2 | 10 | 0.01 |
| (1,1799) | 1:B:13:GLU:HB3 | 1:B:15:LYS:HD3 | 10 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1798) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HD2 | 2 | 0.01 |
| (1,1798) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HD3 | 2 | 0.01 |
| (1,1796) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HG2 | 6 | 0.01 |
| (1,1796) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HG3 | 6 | 0.01 |
| (1,1796) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HG2 | 16 | 0.01 |
| (1,1796) | 1:A:13:GLU:HB3 | 1:A:15:LYS:HG3 | 16 | 0.01 |
| (1,178) | 1:B:15:LYS:H | 1:B:18:MET:HB2 | 7 | 0.01 |
| (1,177) | 1:A:15:LYS:H | 1:A:18:MET:HB3 | 15 | 0.01 |
| (1,1763) | 1:B:11:VAL:HG11 | 1:B:73:PHE:HB2 | 11 | 0.01 |
| (1,1763) | 1:B:11:VAL:HG12 | 1:B:73:PHE:HB2 | 11 | 0.01 |
| (1,1763) | 1:B:11:VAL:HG13 | 1:B:73:PHE:HB2 | 11 | 0.01 |
| (1,1763) | 1:B:11:VAL:HG11 | 1:B:73:PHE:HB2 | 18 | 0.01 |
| (1,1763) | 1:B:11:VAL:HG12 | 1:B:73:PHE:HB2 | 18 | 0.01 |
| (1,1763) | 1:B:11:VAL:HG13 | 1:B:73:PHE:HB2 | 18 | 0.01 |
| (1,1762) | 1:A:11:VAL:HG11 | 1:A:73:PHE:HB2 | 2 | 0.01 |
| (1,1762) | 1:A:11:VAL:HG12 | 1:A:73:PHE:HB2 | 2 | 0.01 |
| (1,1762) | 1:A:11:VAL:HG13 | 1:A:73:PHE:HB2 | 2 | 0.01 |
| (1,1762) | 1:A:11:VAL:HG11 | 1:A:73:PHE:HB2 | 14 | 0.01 |
| (1,1762) | 1:A:11:VAL:HG12 | 1:A:73:PHE:HB2 | 14 | 0.01 |
| (1,1762) | 1:A:11:VAL:HG13 | 1:A:73:PHE:HB2 | 14 | 0.01 |
| (1,176) | 1:B:13:GLU:HG2 | 1:B:15:LYS:H | 3 | 0.01 |
| (1,176) | 1:B:13:GLU:HG3 | 1:B:15:LYS:H | 3 | 0.01 |
| (1,1748) | 1:A:11:VAL:HG21 | 1:A:40:ALA:HA | 11 | 0.01 |
| (1,1748) | 1:A:11:VAL:HG22 | 1:A:40:ALA:HA | 11 | 0.01 |
| (1,1748) | 1:A:11:VAL:HG23 | 1:A:40:ALA:HA | 11 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG21 | 2 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG22 | 2 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG23 | 2 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG21 | 2 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG22 | 2 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG23 | 2 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG21 | 2 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG22 | 2 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG23 | 2 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG21 | 11 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG22 | 11 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG23 | 11 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG21 | 11 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG22 | 11 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG23 | 11 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG21 | 11 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG22 | 11 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG23 | 11 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG21 | 20 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG22 | 20 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG21 | 1:B:46:THR:HG23 | 20 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG21 | 20 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG22 | 20 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG22 | 1:B:46:THR:HG23 | 20 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG21 | 20 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG22 | 20 | 0.01 |
| (1,1741) | 1:B:11:VAL:HG23 | 1:B:46:THR:HG23 | 20 | 0.01 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG21 | 3 | 0.01 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG22 | 3 | 0.01 |
| (1,1740) | 1:A:11:VAL:HG21 | 1:A:46:THR:HG23 | 3 | 0.01 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG21 | 3 | 0.01 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG22 | 3 | 0.01 |
| (1,1740) | 1:A:11:VAL:HG22 | 1:A:46:THR:HG23 | 3 | 0.01 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG21 | 3 | 0.01 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG22 | 3 | 0.01 |
| (1,1740) | 1:A:11:VAL:HG23 | 1:A:46:THR:HG23 | 3 | 0.01 |
| (1,1731) | 1:B:10:ILE:HD11 | 1:B:49:LEU:H | 5 | 0.01 |
| (1,1731) | 1:B:10:ILE:HD12 | 1:B:49:LEU:H | 5 | 0.01 |
| (1,1731) | 1:B:10:ILE:HD13 | 1:B:49:LEU:H | 5 | 0.01 |
| (1,1730) | 1:A:10:ILE:HD11 | 1:A:49:LEU:H | 8 | 0.01 |
| (1,1730) | 1:A:10:ILE:HD12 | 1:A:49:LEU:H | 8 | 0.01 |
| (1,1730) | 1:A:10:ILE:HD13 | 1:A:49:LEU:H | 8 | 0.01 |
| (1,1721) | 1:B:10:ILE:HD11 | 1:B:11:VAL:H | 14 | 0.01 |
| (1,1721) | 1:B:10:ILE:HD12 | 1:B:11:VAL:H | 14 | 0.01 |
| (1,1721) | 1:B:10:ILE:HD13 | 1:B:11:VAL:H | 14 | 0.01 |
| (1,172) | 1:B:15:LYS:H | 1:B:18:MET:HE1 | 9 | 0.01 |
| (1,172) | 1:B:15:LYS:H | 1:B:18:MET:HE2 | 9 | 0.01 |
| (1,172) | 1:B:15:LYS:H | 1:B:18:MET:HE3 | 9 | 0.01 |
| (1,171) | 1:A:15:LYS:H | 1:A:18:MET:HE1 | 6 | 0.01 |
| (1,171) | 1:A:15:LYS:H | 1:A:18:MET:HE2 | 6 | 0.01 |
| (1,171) | 1:A:15:LYS:H | 1:A:18:MET:HE3 | 6 | 0.01 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD11 | 1 | 0.01 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD12 | 1 | 0.01 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD13 | 1 | 0.01 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD11 | 9 | 0.01 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD12 | 9 | 0.01 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD13 | 9 | 0.01 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD11 | 17 | 0.01 |
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD12 | 17 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1695) | 1:B:8:ILE:HB | 1:B:10:ILE:HD13 | 17 | 0.01 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD11 | 8 | 0.01 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD12 | 8 | 0.01 |
| (1,1694) | 1:A:8:ILE:HB | 1:A:10:ILE:HD13 | 8 | 0.01 |
| (1,164) | 1:A:13:GLU:H | 1:A:73:PHE:H | 8 | 0.01 |
| (1,1631) | 1:B:9:ARG:HD2 | 1:B:11:VAL:HB | 3 | 0.01 |
| (1,1631) | 1:B:9:ARG:HD3 | 1:B:11:VAL:HB | 3 | 0.01 |
| (1,1630) | 1:A:9:ARG:HD2 | 1:A:11:VAL:HB | 5 | 0.01 |
| (1,1630) | 1:A:9:ARG:HD3 | 1:A:11:VAL:HB | 5 | 0.01 |
| (1,1630) | 1:A:9:ARG:HD2 | 1:A:11:VAL:HB | 6 | 0.01 |
| (1,1630) | 1:A:9:ARG:HD3 | 1:A:11:VAL:HB | 6 | 0.01 |
| (1,1630) | 1:A:9:ARG:HD2 | 1:A:11:VAL:HB | 9 | 0.01 |
| (1,1630) | 1:A:9:ARG:HD3 | 1:A:11:VAL:HB | 9 | 0.01 |
| (1,1612) | 1:B:24:GLY:H | 1:B:26:ILE:HD11 | 5 | 0.01 |
| (1,1612) | 1:B:24:GLY:H | 1:B:26:ILE:HD12 | 5 | 0.01 |
| (1,1612) | 1:B:24:GLY:H | 1:B:26:ILE:HD13 | 5 | 0.01 |
| (1,1611) | 1:A:24:GLY:H | 1:A:26:ILE:HD11 | 4 | 0.01 |
| (1,1611) | 1:A:24:GLY:H | 1:A:26:ILE:HD12 | 4 | 0.01 |
| (1,1611) | 1:A:24:GLY:H | 1:A:26:ILE:HD13 | 4 | 0.01 |
| (1,1604) | 1:B:23:THR:HA | 1:B:26:ILE:HD11 | 4 | 0.01 |
| (1,1604) | 1:B:23:THR:HA | 1:B:26:ILE:HD12 | 4 | 0.01 |
| (1,1604) | 1:B:23:THR:HA | 1:B:26:ILE:HD13 | 4 | 0.01 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD21 | 9 | 0.01 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD22 | 9 | 0.01 |
| (1,1589) | 1:A:8:ILE:HD11 | 1:A:62:LEU:HD23 | 9 | 0.01 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD21 | 9 | 0.01 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD22 | 9 | 0.01 |
| (1,1589) | 1:A:8:ILE:HD12 | 1:A:62:LEU:HD23 | 9 | 0.01 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD21 | 9 | 0.01 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD22 | 9 | 0.01 |
| (1,1589) | 1:A:8:ILE:HD13 | 1:A:62:LEU:HD23 | 9 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD2 | 1 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD3 | 1 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD2 | 1 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD3 | 1 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD2 | 1 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD3 | 1 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD2 | 10 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD3 | 10 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD2 | 10 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD3 | 10 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD2 | 10 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD3 | 10 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD2 | 12 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD3 | 12 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD2 | 12 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD3 | 12 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD2 | 12 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD3 | 12 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD2 | 19 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG21 | 1:B:77:ARG:HD3 | 19 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD2 | 19 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG22 | 1:B:77:ARG:HD3 | 19 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD2 | 19 | 0.01 |
| (1,1572) | 1:B:8:ILE:HG23 | 1:B:77:ARG:HD3 | 19 | 0.01 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 7 | 0.01 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 7 | 0.01 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 7 | 0.01 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 7 | 0.01 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 7 | 0.01 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 7 | 0.01 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD2 | 18 | 0.01 |
| (1,1571) | 1:A:8:ILE:HG21 | 1:A:77:ARG:HD3 | 18 | 0.01 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD2 | 18 | 0.01 |
| (1,1571) | 1:A:8:ILE:HG22 | 1:A:77:ARG:HD3 | 18 | 0.01 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD2 | 18 | 0.01 |
| (1,1571) | 1:A:8:ILE:HG23 | 1:A:77:ARG:HD3 | 18 | 0.01 |
| (1,155) | 1:B:13:GLU:H | 1:B:44:ILE:HA | 11 | 0.01 |
| (1,1542) | 1:B:6:ALA:HB1 | 1:B:7:GLY:HA3 | 15 | 0.01 |
| (1,1542) | 1:B:6:ALA:HB2 | 1:B:7:GLY:HA3 | 15 | 0.01 |
| (1,1542) | 1:B:6:ALA:HB3 | 1:B:7:GLY:HA3 | 15 | 0.01 |
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 7 | 0.01 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 7 | 0.01 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 7 | 0.01 |
| (1,1528) | 1:B:5:LEU:HD21 | 1:B:52:PHE:HA | 9 | 0.01 |
| (1,1528) | 1:B:5:LEU:HD22 | 1:B:52:PHE:HA | 9 | 0.01 |
| (1,1528) | 1:B:5:LEU:HD23 | 1:B:52:PHE:HA | 9 | 0.01 |
| (1,1525) | 1:A:5:LEU:HD21 | 1:A:51:ILE:HA | 4 | 0.01 |
| (1,1525) | 1:A:5:LEU:HD22 | 1:A:51:ILE:HA | 4 | 0.01 |
| (1,1525) | 1:A:5:LEU:HD23 | 1:A:51:ILE:HA | 4 | 0.01 |
| (1,148) | 1:A:13:GLU:H | 1:A:13:GLU:HG2 | 7 | 0.01 |
| (1,148) | 1:A:13:GLU:H | 1:A:13:GLU:HG3 | 7 | 0.01 |
| (1,1455) | 1:A:3:ASP:HB2 | 1:A:53:VAL:H | 19 | 0.01 |
| (1,1420) | 1:B:40:ALA:H | 1:B:41:LYS:HD2 | 2 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|---|---|---|---|---|
| (1,1420) | 1:B:40:ALA:H | 1:B:41:LYS:HD3 | 2 | 0.01 |
| (1,1420) | 1:B:40:ALA:H | 1:B:41:LYS:HD2 | 12 | 0.01 |
| (1,1420) | 1:B:40:ALA:H | 1:B:41:LYS:HD3 | 12 | 0.01 |
| (1,1394) | 1:B:81:LEU:HB3 | 1:B:82:GLU:H | 5 | 0.01 |
| (1,1348) | 1:B:77:ARG:H | 1:B:77:ARG:HD2 | 14 | 0.01 |
| (1,1348) | 1:B:77:ARG:H | 1:B:77:ARG:HD3 | 14 | 0.01 |
| (1,1339) | 1:A:76:GLU:HB2 | 1:A:77:ARG:H | 13 | 0.01 |
| (1,1300) | 1:B:74:THR:HG21 | 1:B:75:VAL:H | 17 | 0.01 |
| (1,1300) | 1:B:74:THR:HG22 | 1:B:75:VAL:H | 17 | 0.01 |
| (1,1300) | 1:B:74:THR:HG23 | 1:B:75:VAL:H | 17 | 0.01 |
| (1,1299) | 1:A:74:THR:HG21 | 1:A:75:VAL:H | 7 | 0.01 |
| (1,1299) | 1:A:74:THR:HG22 | 1:A:75:VAL:H | 7 | 0.01 |
| (1,1299) | 1:A:74:THR:HG23 | 1:A:75:VAL:H | 7 | 0.01 |
| (1,1286) | 1:B:12:GLY:HA3 | 1:B:74:THR:H | 7 | 0.01 |
| (1,1242) | 1:B:69:VAL:HG11 | 1:B:71:GLY:H | 12 | 0.01 |
| (1,1242) | 1:B:69:VAL:HG12 | 1:B:71:GLY:H | 12 | 0.01 |
| (1,1242) | 1:B:69:VAL:HG13 | 1:B:71:GLY:H | 12 | 0.01 |
| (1,1242) | 1:B:69:VAL:HG11 | 1:B:71:GLY:H | 20 | 0.01 |
| (1,1242) | 1:B:69:VAL:HG12 | 1:B:71:GLY:H | 20 | 0.01 |
| (1,1242) | 1:B:69:VAL:HG13 | 1:B:71:GLY:H | 20 | 0.01 |
| (1,1241) | 1:A:69:VAL:HG11 | 1:A:71:GLY:H | 20 | 0.01 |
| (1,1241) | 1:A:69:VAL:HG12 | 1:A:71:GLY:H | 20 | 0.01 |
| (1,1241) | 1:A:69:VAL:HG13 | 1:A:71:GLY:H | 20 | 0.01 |
| (1,1226) | 1:B:69:VAL:H | 1:B:70:GLN:H | 8 | 0.01 |
| (1,1226) | 1:B:69:VAL:H | 1:B:70:GLN:H | 16 | 0.01 |
| (1,1226) | 1:B:69:VAL:H | 1:B:70:GLN:H | 17 | 0.01 |
| (1,1225) | 1:A:69:VAL:H | 1:A:70:GLN:H | 10 | 0.01 |
| (1,1222) | 1:B:69:VAL:H | 1:B:72:VAL:H | 2 | 0.01 |
| (1,1221) | 1:A:69:VAL:H | 1:A:72:VAL:H | 16 | 0.01 |
| (1,1176) | 1:B:67:ARG:HE | 1:B:75:VAL:HB | 15 | 0.01 |
| (1,1176) | 1:B:67:ARG:HE | 1:B:75:VAL:HB | 16 | 0.01 |
| (1,1175) | 1:A:67:ARG:HE | 1:A:75:VAL:HB | 15 | 0.01 |
| (1,1165) | 1:A:67:ARG:H | 1:A:67:ARG:HE | 8 | 0.01 |
| (1,1150) | 1:B:67:ARG:H | 1:B:69:VAL:HG21 | 7 | 0.01 |
| (1,1150) | 1:B:67:ARG:H | 1:B:69:VAL:HG22 | 7 | 0.01 |
| (1,1150) | 1:B:67:ARG:H | 1:B:69:VAL:HG23 | 7 | 0.01 |
| (1,1132) | 1:B:62:LEU:HD11 | 1:B:66:LEU:H | 1 | 0.01 |
| (1,1132) | 1:B:62:LEU:HD12 | 1:B:66:LEU:H | 1 | 0.01 |
| (1,1132) | 1:B:62:LEU:HD13 | 1:B:66:LEU:H | 1 | 0.01 |
| (1,1132) | 1:B:62:LEU:HD11 | 1:B:66:LEU:H | 7 | 0.01 |
| (1,1132) | 1:B:62:LEU:HD12 | 1:B:66:LEU:H | 7 | 0.01 |
| (1,1132) | 1:B:62:LEU:HD13 | 1:B:66:LEU:H | 7 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1132) | 1:B:62:LEU:HD11 | 1:B:66:LEU:H | 9 | 0.01 |
| (1,1132) | 1:B:62:LEU:HD12 | 1:B:66:LEU:H | 9 | 0.01 |
| (1,1132) | 1:B:62:LEU:HD13 | 1:B:66:LEU:H | 9 | 0.01 |
| (1,1132) | 1:B:62:LEU:HD11 | 1:B:66:LEU:H | 13 | 0.01 |
| (1,1132) | 1:B:62:LEU:HD12 | 1:B:66:LEU:H | 13 | 0.01 |
| (1,1132) | 1:B:62:LEU:HD13 | 1:B:66:LEU:H | 13 | 0.01 |
| (1,1132) | 1:B:62:LEU:HD11 | 1:B:66:LEU:H | 17 | 0.01 |
| (1,1132) | 1:B:62:LEU:HD12 | 1:B:66:LEU:H | 17 | 0.01 |
| (1,1132) | 1:B:62:LEU:HD13 | 1:B:66:LEU:H | 17 | 0.01 |
| (1,1132) | 1:B:62:LEU:HD11 | 1:B:66:LEU:H | 19 | 0.01 |
| (1,1132) | 1:B:62:LEU:HD12 | 1:B:66:LEU:H | 19 | 0.01 |
| (1,1132) | 1:B:62:LEU:HD13 | 1:B:66:LEU:H | 19 | 0.01 |
| (1,1131) | 1:A:62:LEU:HD11 | 1:A:66:LEU:H | 20 | 0.01 |
| (1,1131) | 1:A:62:LEU:HD12 | 1:A:66:LEU:H | 20 | 0.01 |
| (1,1131) | 1:A:62:LEU:HD13 | 1:A:66:LEU:H | 20 | 0.01 |
| (1,1130) | 1:B:62:LEU:HD11 | 1:B:65:LYS:H | 5 | 0.01 |
| (1,1130) | 1:B:62:LEU:HD12 | 1:B:65:LYS:H | 5 | 0.01 |
| (1,1130) | 1:B:62:LEU:HD13 | 1:B:65:LYS:H | 5 | 0.01 |
| (1,1130) | 1:B:62:LEU:HD11 | 1:B:65:LYS:H | 18 | 0.01 |
| (1,1130) | 1:B:62:LEU:HD12 | 1:B:65:LYS:H | 18 | 0.01 |
| (1,1130) | 1:B:62:LEU:HD13 | 1:B:65:LYS:H | 18 | 0.01 |
| (1,1129) | 1:A:62:LEU:HD11 | 1:A:65:LYS:H | 9 | 0.01 |
| (1,1129) | 1:A:62:LEU:HD12 | 1:A:65:LYS:H | 9 | 0.01 |
| (1,1129) | 1:A:62:LEU:HD13 | 1:A:65:LYS:H | 9 | 0.01 |
| (1,1129) | 1:A:62:LEU:HD11 | 1:A:65:LYS:H | 13 | 0.01 |
| (1,1129) | 1:A:62:LEU:HD12 | 1:A:65:LYS:H | 13 | 0.01 |
| (1,1129) | 1:A:62:LEU:HD13 | 1:A:65:LYS:H | 13 | 0.01 |
| (1,1129) | 1:A:62:LEU:HD11 | 1:A:65:LYS:H | 16 | 0.01 |
| (1,1129) | 1:A:62:LEU:HD12 | 1:A:65:LYS:H | 16 | 0.01 |
| (1,1129) | 1:A:62:LEU:HD13 | 1:A:65:LYS:H | 16 | 0.01 |
| (1,1129) | 1:A:62:LEU:HD11 | 1:A:65:LYS:H | 18 | 0.01 |
| (1,1129) | 1:A:62:LEU:HD12 | 1:A:65:LYS:H | 18 | 0.01 |
| (1,1129) | 1:A:62:LEU:HD13 | 1:A:65:LYS:H | 18 | 0.01 |
| (1,1129) | 1:A:62:LEU:HD11 | 1:A:65:LYS:H | 20 | 0.01 |
| (1,1129) | 1:A:62:LEU:HD12 | 1:A:65:LYS:H | 20 | 0.01 |
| (1,1129) | 1:A:62:LEU:HD13 | 1:A:65:LYS:H | 20 | 0.01 |
| (1,1091) | 1:B:64:ASP:H | 1:B:75:VAL:HG11 | 7 | 0.01 |
| (1,1091) | 1:B:64:ASP:H | 1:B:75:VAL:HG12 | 7 | 0.01 |
| (1,1091) | 1:B:64:ASP:H | 1:B:75:VAL:HG13 | 7 | 0.01 |
| (1,1090) | 1:A:64:ASP:H | 1:A:75:VAL:HG11 | 4 | 0.01 |
| (1,1090) | 1:A:64:ASP:H | 1:A:75:VAL:HG12 | 4 | 0.01 |
| (1,1090) | 1:A:64:ASP:H | 1:A:75:VAL:HG13 | 4 | 0.01 |

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| Key | Atom-1 | Atom-2 | Model | Violation (Å) |
|-----|--------|--------|-------|---------------|
| (1,1090) | 1:A:64:ASP:H | 1:A:75:VAL:HG11 | 18 | 0.01 |
| (1,1090) | 1:A:64:ASP:H | 1:A:75:VAL:HG12 | 18 | 0.01 |
| (1,1090) | 1:A:64:ASP:H | 1:A:75:VAL:HG13 | 18 | 0.01 |
| (1,1067) | 1:B:58:LYS:HZ1 | 1:B:62:LEU:H | 9 | 0.01 |

# 9 Dihedral angle restraints analysis

## 9.1 Dihedral angle restraints summary

| Angle name | Count | % |
|---|---|---|
| PHI | 116 | 50.0 |
| PSI | 116 | 50.0 |
| Total | 232 | 100.0 |

### 9.1.1 Pie chart : Dihedral angle restraints

There are 0 unmapped restraints
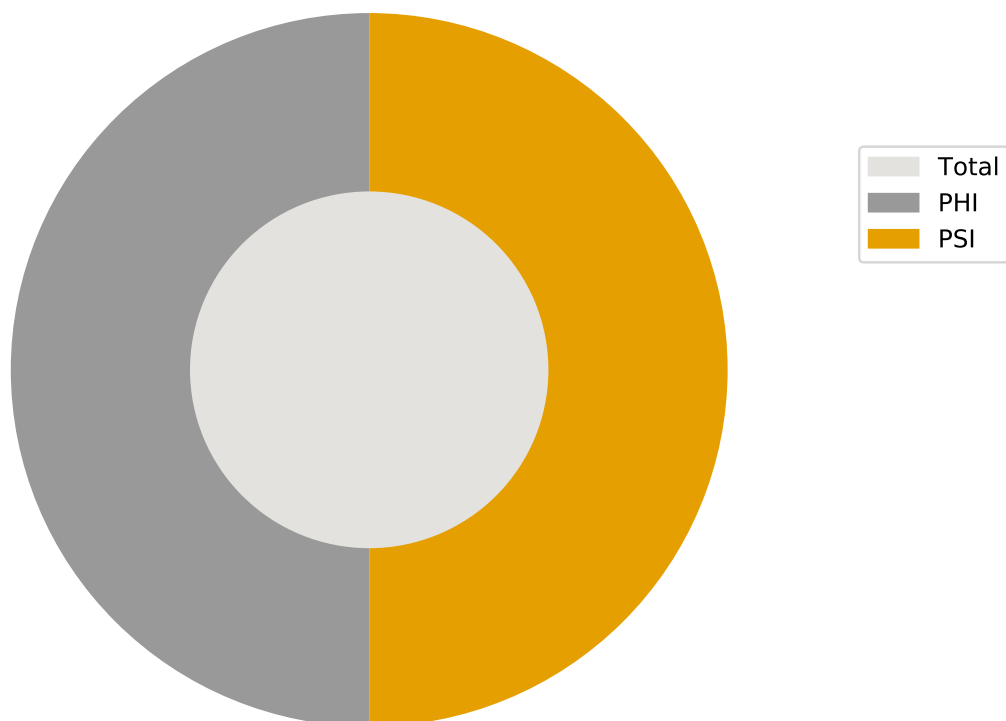


## 9.2 Dihedral angle violations

The following table provides the summary of violated restraints. Restraints that are violated at least in one model are counted as violated.

| Angle name | Count | $\%^1$ | $\%^2$ |
|---|---|---|---|
| PHI | 40 | 34.5 | 37.0 |
| PSI | 68 | 58.6 | 63.0 |

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| Angle name | Count | %[1] | %[2] |
|------------|-------|------|------|
| Total | 108 | 46.6 | 100.0 |

[1]percentage of violated restraints in that particular agnle type, [2]percentage of violation in total violations.

### 9.2.1 Pie chart : Dihedral angle violations
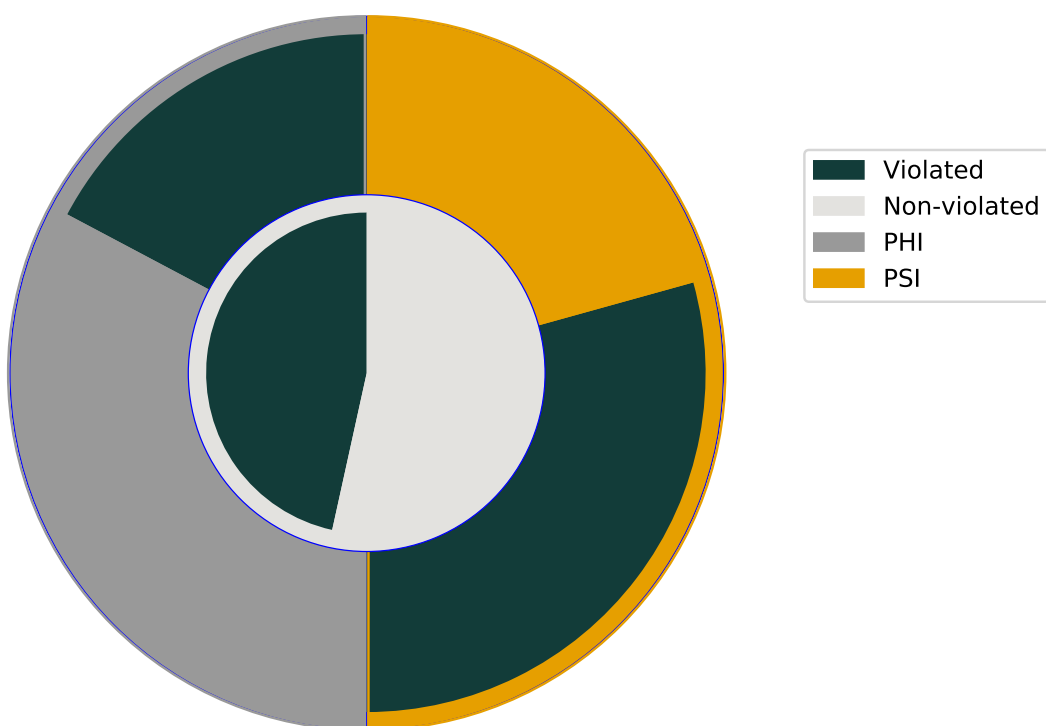


## 9.3 Consistent dihedral angle violations

The following table provides the summary of consistently violated restraints. Restraints that are violated all models are counted as violated.

| Angle name | Count | %[1] | %[2] |
|------------|-------|------|------|
| PHI | 10 | 8.6 | 50.0 |
| PSI | 10 | 8.6 | 50.0 |
| Total | 20 | 8.6 | 100.0 |

[1]percentage of violated restraints in that particular agnle type, [2]percentage of violation in total violations.

### 9.3.1 Pie chart : Consistent dihedral angle violations
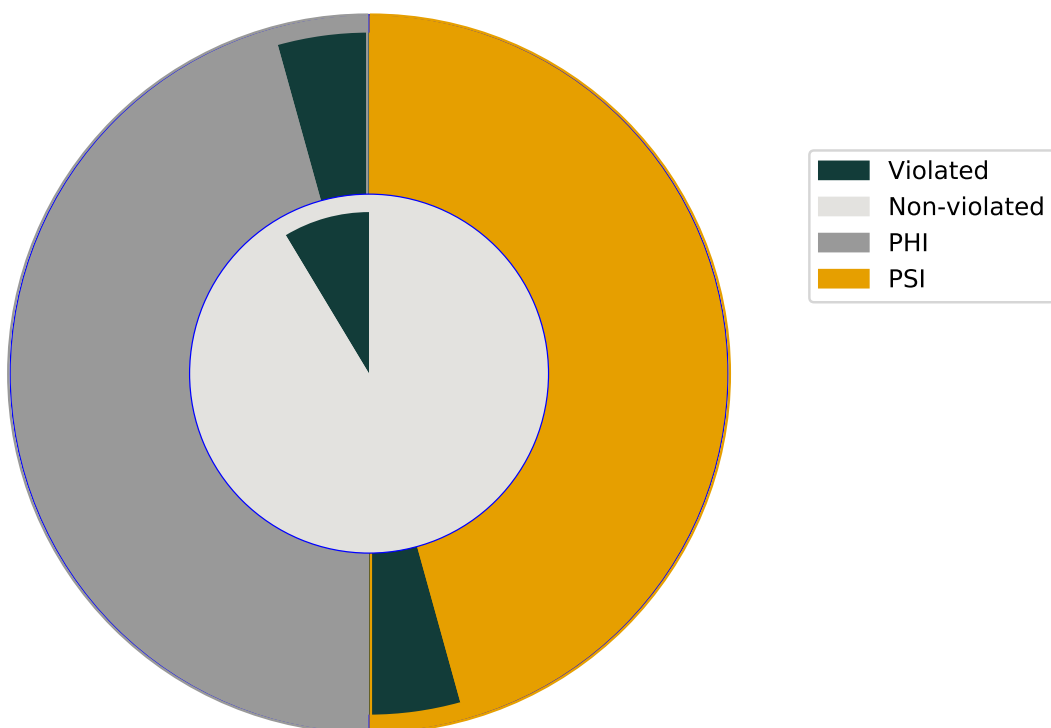


## 9.4 Residual dihedral angle violations

Violation are counted in different bin sizes and listed below

| Range ( ∘ ) | No. of violated restraints per model | Max violation ( ∘ ) |
| --- | --- | --- |
| 0.0-5.0 | 30.4 | 4.64 |
| 5.0-10.0 | 0.5 | 9.93 |
| 10.0-20.0 | 2.4 | 18.2 |
| 20.0-40.0 | 4.6 | 39.94 |
| 40.0-80.0 | 7.7 | 79.58 |
| 80.0< | 4.0 | 110.32 |

## 9.5 Dihedral angle violations in the ensemble

The restraints are grouped based on the number of violated models and listed here.

| No. of violated restraints | | | No. of violated models |
| --- | --- | --- | --- |
| PHI | PSI | Total | |
| 9 | 11 | 20 | 1 |

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| No. of violated restraints | | | No. of violated models |
| --- | --- | --- | --- |
| PHI | PSI | Total | |
| 4 | 10 | 14 | 2 |
| 3 | 3 | 6 | 3 |
| 3 | 2 | 5 | 4 |
| 1 | 7 | 8 | 5 |
| 0 | 0 | 0 | 6 |
| 0 | 4 | 4 | 7 |
| 1 | 2 | 3 | 8 |
| 1 | 0 | 1 | 9 |
| 1 | 0 | 1 | 10 |
| 1 | 1 | 2 | 11 |
| 1 | 2 | 3 | 12 |
| 0 | 2 | 2 | 13 |
| 2 | 3 | 5 | 14 |
| 1 | 1 | 2 | 15 |
| 1 | 2 | 3 | 16 |
| 0 | 2 | 2 | 17 |
| 1 | 5 | 6 | 18 |
| 0 | 1 | 1 | 19 |
| 10 | 10 | 20 | 20 |

### 9.5.1 Bar graph : No. of models vs No. of violations
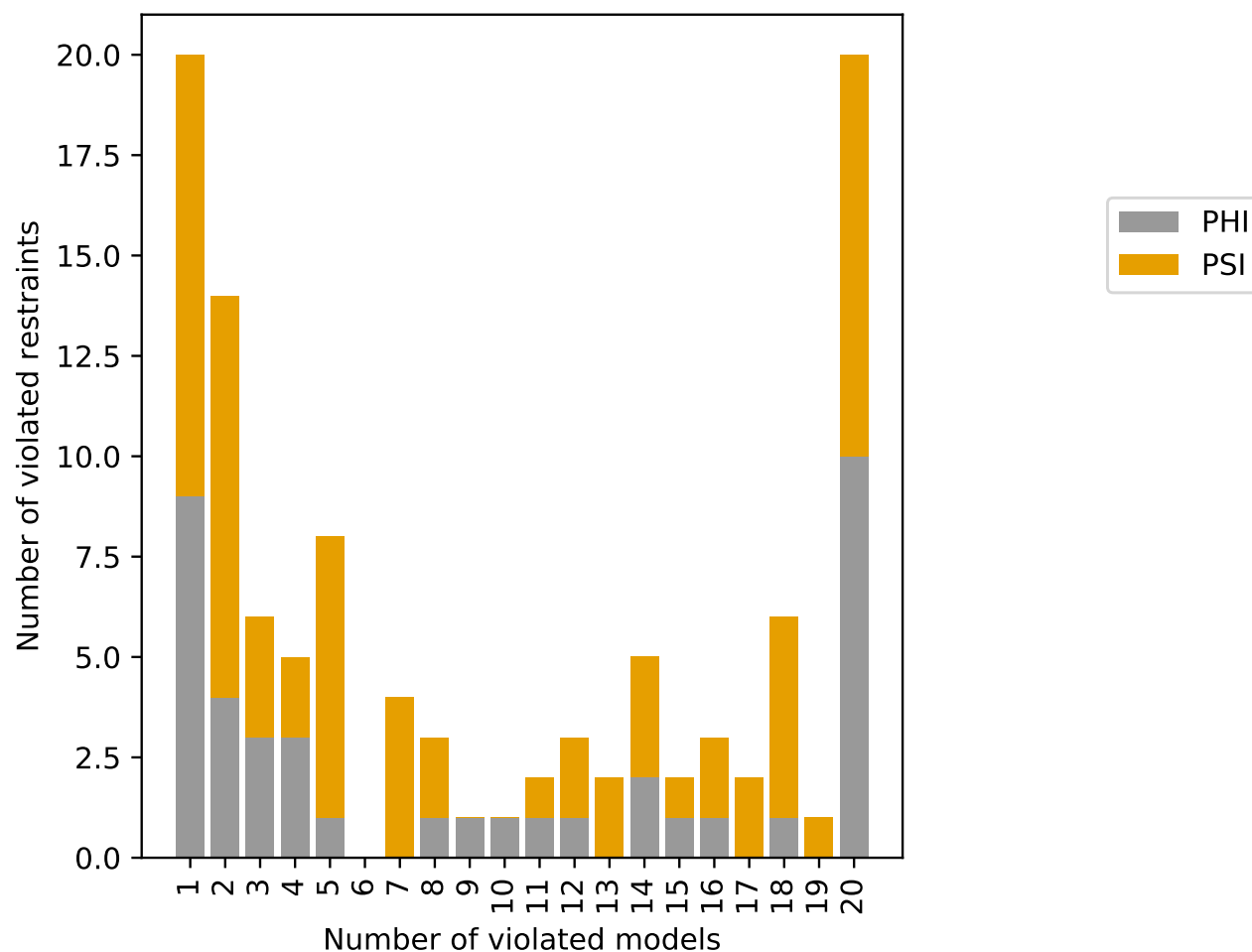


## 9.6 Violations in each model

The following table lists the violation count in each model in the ensemble

| Model ID | No. of violations | | | Mean (Å) | Max (Å) |
| --- | --- | --- | --- | --- | --- |
| | PHI | PSI | Total | | |
| 1 | 21 | 32 | 53 | 18.24 | 104.78 |
| 2 | 19 | 29 | 48 | 19.97 | 97.98 |
| 3 | 17 | 28 | 45 | 22.13 | 109.36 |
| 4 | 18 | 31 | 49 | 19.52 | 103.45 |
| 5 | 19 | 34 | 53 | 19.16 | 101.82 |
| 6 | 17 | 31 | 48 | 18.95 | 105.91 |
| 7 | 16 | 30 | 46 | 18.84 | 100.97 |
| 8 | 21 | 34 | 55 | 16.79 | 110.32 |
| 9 | 19 | 30 | 49 | 21.15 | 104.76 |

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| Model ID | No. of violations | | | Mean (Å) | Max (Å) |
|---|---|---|---|---|---|
| | PHI | PSI | Total | | |
| 10 | 16 | 33 | 49 | 19.67 | 101.76 |
| 11 | 15 | 31 | 46 | 20.88 | 109.45 |
| 12 | 19 | 33 | 52 | 19.54 | 98.09 |
| 13 | 19 | 32 | 51 | 18.48 | 97.34 |
| 14 | 18 | 27 | 45 | 21.4 | 93.65 |
| 15 | 19 | 32 | 51 | 17.51 | 104.1 |
| 16 | 18 | 29 | 47 | 20.44 | 98.66 |
| 17 | 19 | 29 | 48 | 20.4 | 101.04 |
| 18 | 22 | 33 | 55 | 18.17 | 107.94 |
| 19 | 19 | 30 | 49 | 20.21 | 106.17 |
| 20 | 19 | 32 | 51 | 19.11 | 103.4 |

### 9.6.1   Bar graph : Violations in each model
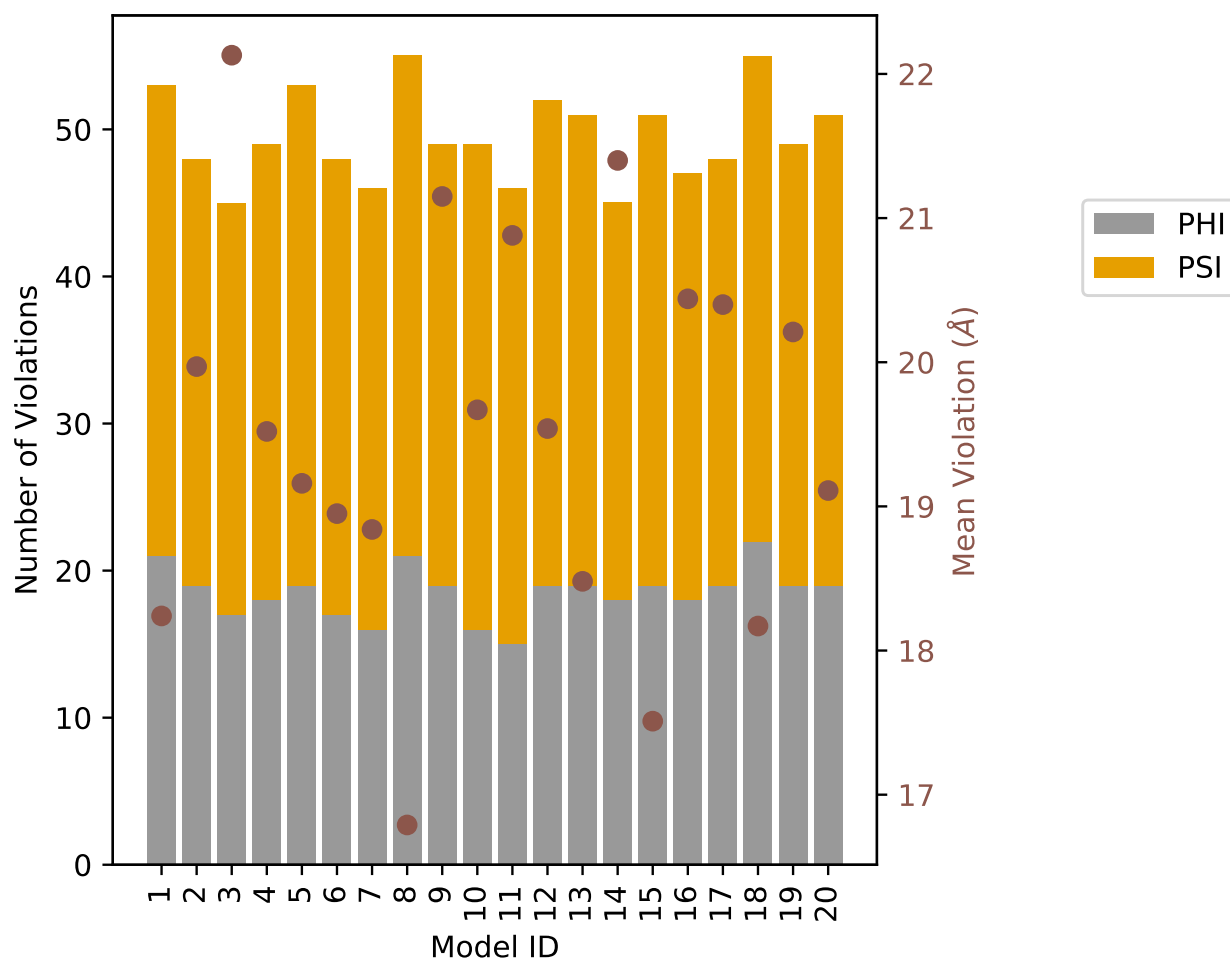
## 9.7    Most violated dihedral angle restraints

### 9.7.1    Histogram : Distribution of mean dihedral angle violations

The following histogram shows the distribution of average violation of each restraint
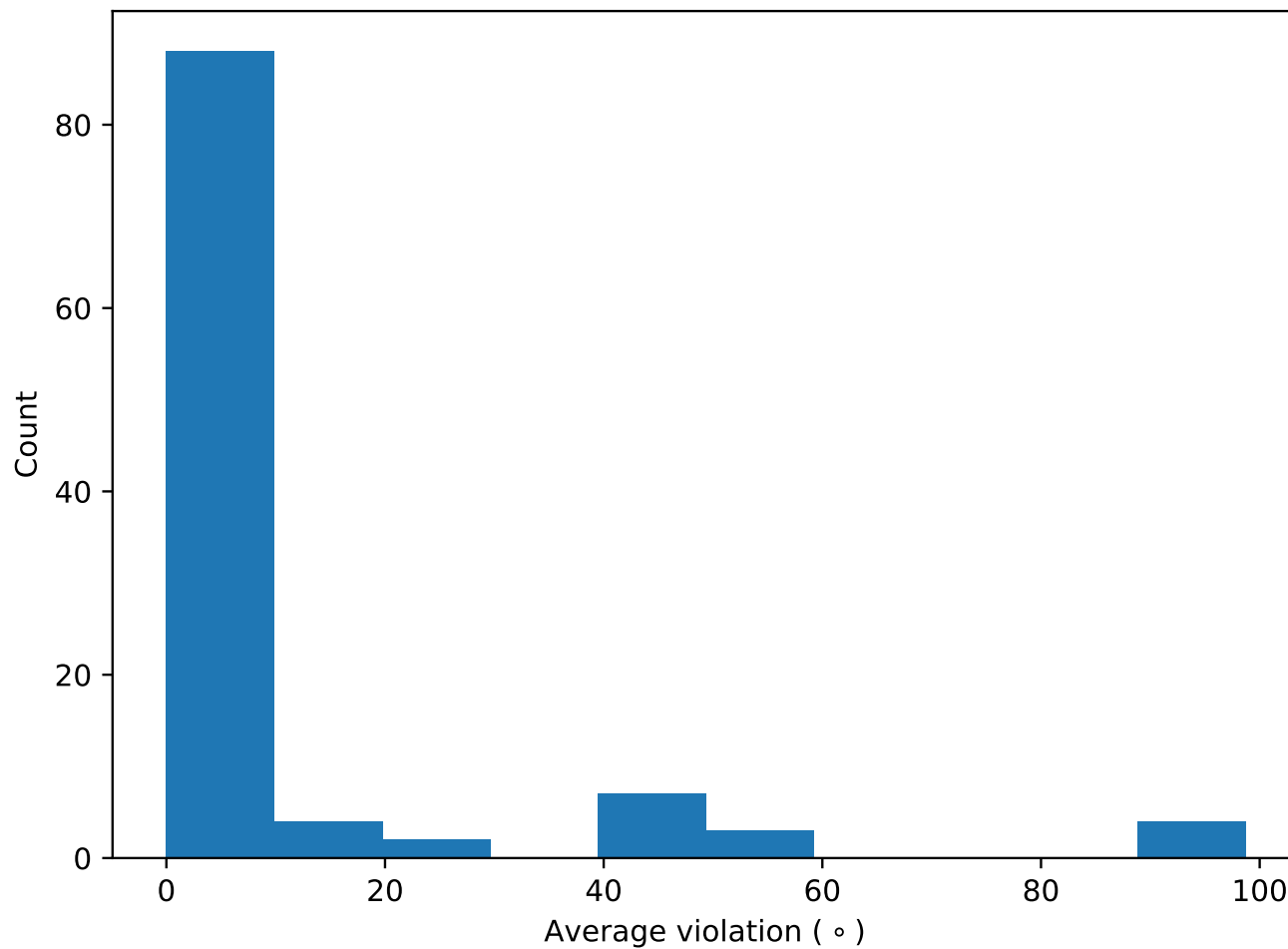


### 9.7.2    Table: Most violated dihedral angle restraints

The following tale lists the average violation of each restraint sorted by number of violated models

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models | Mean ( ∘ ) | Max ( ∘ ) |
|---|---|---|---|---|---|---|---|
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 18 | 46.16 | 69.43 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 19 | 51.38 | 68.8 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 20 | 45.51 | 48.14 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 20 | 42.79 | 48.02 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 20 | 27.54 | 35.74 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 20 | 28.07 | 33.55 |
| (1,22) | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 1:A:16:ASN:N | 14 | 16.22 | 25.52 |
| (1,138) | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1:B:16:ASN:N | 16 | 12.85 | 25.09 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 20 | 11.43 | 15.68 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 20 | 11.82 | 14.38 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models | Mean ( ◦ ) | Max ( ◦ ) |
|---|---|---|---|---|---|---|---|
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 18 | 1.59 | 3.59 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 18 | 1.77 | 3.0 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 20 | 2.06 | 2.99 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 20 | 2.15 | 2.94 |
| (1,140) | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 1:B:19:THR:N | 16 | 1.37 | 2.71 |
| (1,24) | 1:A:18:MET:N | 1:A:18:MET:CA | 1:A:18:MET:C | 1:A:19:THR:N | 12 | 1.73 | 2.59 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 20 | 1.35 | 2.58 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 17 | 1.35 | 2.36 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 18 | 1.23 | 2.25 |
| (1,170) | 1:B:37:VAL:N | 1:B:37:VAL:CA | 1:B:37:VAL:C | 1:B:38:LEU:N | 7 | 0.96 | 2.21 |
| (1,220) | 1:B:67:ARG:N | 1:B:67:ARG:CA | 1:B:67:ARG:C | 1:B:68:LYS:N | 14 | 1.1 | 2.17 |
| (1,42) | 1:A:27:SER:N | 1:A:27:SER:CA | 1:A:27:SER:C | 1:A:28:LYS:N | 15 | 1.05 | 2.14 |
| (1,54) | 1:A:37:VAL:N | 1:A:37:VAL:CA | 1:A:37:VAL:C | 1:A:38:LEU:N | 13 | 0.96 | 2.1 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 20 | 0.77 | 1.93 |
| (1,158) | 1:B:27:SER:N | 1:B:27:SER:CA | 1:B:27:SER:C | 1:B:28:LYS:N | 13 | 1.05 | 1.85 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 18 | 0.74 | 1.66 |
| (1,28) | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 1:A:21:GLN:N | 12 | 0.73 | 1.54 |
| (1,60) | 1:A:40:ALA:N | 1:A:40:ALA:CA | 1:A:40:ALA:C | 1:A:41:LYS:N | 1 | 1.5 | 1.5 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 17 | 0.8 | 1.48 |
| (1,96) | 1:A:63:MET:N | 1:A:63:MET:CA | 1:A:63:MET:C | 1:A:64:ASP:N | 3 | 0.52 | 1.48 |
| (1,128) | 1:B:9:ARG:N | 1:B:9:ARG:CA | 1:B:9:ARG:C | 1:B:10:ILE:N | 7 | 0.79 | 1.4 |
| (1,182) | 1:B:46:THR:N | 1:B:46:THR:CA | 1:B:46:THR:C | 1:B:47:CYS:N | 4 | 0.77 | 1.34 |
| (1,212) | 1:B:63:MET:N | 1:B:63:MET:CA | 1:B:63:MET:C | 1:B:64:ASP:N | 5 | 0.51 | 1.26 |
| (1,204) | 1:B:59:LEU:N | 1:B:59:LEU:CA | 1:B:59:LEU:C | 1:B:60:THR:N | 14 | 0.47 | 1.25 |
| (1,12) | 1:A:9:ARG:N | 1:A:9:ARG:CA | 1:A:9:ARG:C | 1:A:10:ILE:N | 2 | 1.02 | 1.22 |
| (1,196) | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 1:B:54:LYS:N | 5 | 0.66 | 1.21 |
| (1,90) | 1:A:60:THR:N | 1:A:60:THR:CA | 1:A:60:THR:C | 1:A:61:THR:N | 5 | 0.42 | 1.17 |
| (1,110) | 1:A:74:THR:N | 1:A:74:THR:CA | 1:A:74:THR:C | 1:A:75:VAL:N | 2 | 0.76 | 1.16 |
| (1,120) | 1:B:5:LEU:N | 1:B:5:LEU:CA | 1:B:5:LEU:C | 1:B:6:ALA:N | 5 | 0.43 | 1.06 |
| (1,166) | 1:B:35:THR:N | 1:B:35:THR:CA | 1:B:35:THR:C | 1:B:36:ILE:N | 8 | 0.52 | 1.06 |
| (1,206) | 1:B:60:THR:N | 1:B:60:THR:CA | 1:B:60:THR:C | 1:B:61:THR:N | 8 | 0.64 | 1.04 |
| (1,98) | 1:A:64:ASP:N | 1:A:64:ASP:CA | 1:A:64:ASP:C | 1:A:65:LYS:N | 1 | 1.03 | 1.03 |
| (1,66) | 1:A:46:THR:N | 1:A:46:THR:CA | 1:A:46:THR:C | 1:A:47:CYS:N | 5 | 0.46 | 0.98 |
| (1,144) | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 1:B:21:GLN:N | 11 | 0.46 | 0.89 |
| (1,80) | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 1:A:54:LYS:N | 5 | 0.37 | 0.8 |
| (1,50) | 1:A:35:THR:N | 1:A:35:THR:CA | 1:A:35:THR:C | 1:A:36:ILE:N | 7 | 0.31 | 0.79 |
| (1,218) | 1:B:66:LEU:N | 1:B:66:LEU:CA | 1:B:66:LEU:C | 1:B:67:ARG:N | 3 | 0.37 | 0.79 |
| (1,172) | 1:B:38:LEU:N | 1:B:38:LEU:CA | 1:B:38:LEU:C | 1:B:39:ASN:N | 2 | 0.63 | 0.79 |
| (1,4) | 1:A:5:LEU:N | 1:A:5:LEU:CA | 1:A:5:LEU:C | 1:A:6:ALA:N | 7 | 0.42 | 0.77 |
| (1,226) | 1:B:74:THR:N | 1:B:74:THR:CA | 1:B:74:THR:C | 1:B:75:VAL:N | 5 | 0.49 | 0.72 |
| (1,174) | 1:B:39:ASN:N | 1:B:39:ASN:CA | 1:B:39:ASN:C | 1:B:40:ALA:N | 2 | 0.39 | 0.68 |
| (1,224) | 1:B:69:VAL:N | 1:B:69:VAL:CA | 1:B:69:VAL:C | 1:B:70:GLN:N | 2 | 0.46 | 0.63 |
| (1,152) | 1:B:24:GLY:N | 1:B:24:GLY:CA | 1:B:24:GLY:C | 1:B:25:VAL:N | 4 | 0.4 | 0.56 |
| (1,178) | 1:B:44:ILE:N | 1:B:44:ILE:CA | 1:B:44:ILE:C | 1:B:45:PHE:N | 1 | 0.53 | 0.53 |
| (1,116) | 1:A:77:ARG:N | 1:A:77:ARG:CA | 1:A:77:ARG:C | 1:A:78:LEU:N | 1 | 0.47 | 0.47 |
| (1,48) | 1:A:33:ILE:N | 1:A:33:ILE:CA | 1:A:33:ILE:C | 1:A:34:ARG:N | 2 | 0.28 | 0.41 |
| (1,36) | 1:A:24:GLY:N | 1:A:24:GLY:CA | 1:A:24:GLY:C | 1:A:25:VAL:N | 2 | 0.32 | 0.4 |
| (1,114) | 1:A:76:GLU:N | 1:A:76:GLU:CA | 1:A:76:GLU:C | 1:A:77:ARG:N | 2 | 0.3 | 0.4 |
| (1,70) | 1:A:48:ASN:N | 1:A:48:ASN:CA | 1:A:48:ASN:C | 1:A:49:LEU:N | 3 | 0.23 | 0.37 |
| (1,62) | 1:A:44:ILE:N | 1:A:44:ILE:CA | 1:A:44:ILE:C | 1:A:45:PHE:N | 1 | 0.36 | 0.36 |
| (1,214) | 1:B:64:ASP:N | 1:B:64:ASP:CA | 1:B:64:ASP:C | 1:B:65:LYS:N | 1 | 0.36 | 0.36 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models | Mean ( ∘ ) | Max ( ∘ ) |
|---|---|---|---|---|---|---|---|
| (1,102) | 1:A:66:LEU:N | 1:A:66:LEU:CA | 1:A:66:LEU:C | 1:A:67:ARG:N | 2 | 0.15 | 0.24 |
| (1,142) | 1:B:19:THR:N | 1:B:19:THR:CA | 1:B:19:THR:C | 1:B:20:ASN:N | 1 | 0.23 | 0.23 |
| (1,230) | 1:B:76:GLU:N | 1:B:76:GLU:CA | 1:B:76:GLU:C | 1:B:77:ARG:N | 1 | 0.22 | 0.22 |
| (1,186) | 1:B:48:ASN:N | 1:B:48:ASN:CA | 1:B:48:ASN:C | 1:B:49:LEU:N | 2 | 0.15 | 0.16 |
| (1,184) | 1:B:47:CYS:N | 1:B:47:CYS:CA | 1:B:47:CYS:C | 1:B:48:ASN:N | 1 | 0.12 | 0.12 |
| (1,210) | 1:B:62:LEU:N | 1:B:62:LEU:CA | 1:B:62:LEU:C | 1:B:63:MET:N | 1 | 0.1 | 0.1 |
| (1,232) | 1:B:77:ARG:N | 1:B:77:ARG:CA | 1:B:77:ARG:C | 1:B:78:LEU:N | 1 | 0.02 | 0.02 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 20 | 97.79 | 110.32 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 20 | 98.71 | 109.45 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 20 | 89.15 | 97.53 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 20 | 89.98 | 97.28 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 20 | 43.31 | 65.96 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 20 | 41.08 | 63.9 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 20 | 51.54 | 59.94 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 20 | 54.36 | 59.43 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 20 | 45.99 | 55.77 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 20 | 44.8 | 54.8 |
| (1,221) | 1:B:67:ARG:C | 1:B:68:LYS:N | 1:B:68:LYS:CA | 1:B:68:LYS:C | 14 | 0.94 | 2.47 |
| (1,105) | 1:A:67:ARG:C | 1:A:68:LYS:N | 1:A:68:LYS:CA | 1:A:68:LYS:C | 16 | 0.96 | 2.14 |
| (1,55) | 1:A:37:VAL:C | 1:A:38:LEU:N | 1:A:38:LEU:CA | 1:A:38:LEU:C | 4 | 1.3 | 2.06 |
| (1,201) | 1:B:57:ASP:C | 1:B:58:LYS:N | 1:B:58:LYS:CA | 1:B:58:LYS:C | 14 | 0.69 | 1.99 |
| (1,171) | 1:B:37:VAL:C | 1:B:38:LEU:N | 1:B:38:LEU:CA | 1:B:38:LEU:C | 9 | 1.13 | 1.9 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 18 | 0.62 | 1.76 |
| (1,139) | 1:B:17:GLY:C | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 5 | 0.8 | 1.62 |
| (1,23) | 1:A:17:GLY:C | 1:A:18:MET:N | 1:A:18:MET:CA | 1:A:18:MET:C | 3 | 0.7 | 1.21 |
| (1,85) | 1:A:57:ASP:C | 1:A:58:LYS:N | 1:A:58:LYS:CA | 1:A:58:LYS:C | 10 | 0.68 | 1.14 |
| (1,27) | 1:A:19:THR:C | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 11 | 0.41 | 1.08 |
| (1,5) | 1:A:5:LEU:C | 1:A:6:ALA:N | 1:A:6:ALA:CA | 1:A:6:ALA:C | 8 | 0.45 | 1.01 |
| (1,187) | 1:B:48:ASN:C | 1:B:49:LEU:N | 1:B:49:LEU:CA | 1:B:49:LEU:C | 15 | 0.59 | 1.0 |
| (1,33) | 1:A:22:ILE:C | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 4 | 0.49 | 0.94 |
| (1,121) | 1:B:5:LEU:C | 1:B:6:ALA:N | 1:B:6:ALA:CA | 1:B:6:ALA:C | 3 | 0.66 | 0.92 |
| (1,149) | 1:B:22:ILE:C | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 4 | 0.39 | 0.87 |
| (1,143) | 1:B:19:THR:C | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 12 | 0.34 | 0.82 |
| (1,31) | 1:A:21:GLN:C | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 2 | 0.42 | 0.66 |
| (1,87) | 1:A:58:LYS:C | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1 | 0.62 | 0.62 |
| (1,69) | 1:A:47:CYS:C | 1:A:48:ASN:N | 1:A:48:ASN:CA | 1:A:48:ASN:C | 1 | 0.51 | 0.51 |
| (1,57) | 1:A:38:LEU:C | 1:A:39:ASN:N | 1:A:39:ASN:CA | 1:A:39:ASN:C | 2 | 0.29 | 0.5 |
| (1,211) | 1:B:62:LEU:C | 1:B:63:MET:N | 1:B:63:MET:CA | 1:B:63:MET:C | 3 | 0.24 | 0.46 |
| (1,203) | 1:B:58:LYS:C | 1:B:59:LEU:N | 1:B:59:LEU:CA | 1:B:59:LEU:C | 1 | 0.33 | 0.33 |
| (1,59) | 1:A:39:ASN:C | 1:A:40:ALA:N | 1:A:40:ALA:CA | 1:A:40:ALA:C | 1 | 0.26 | 0.26 |
| (1,197) | 1:B:53:VAL:C | 1:B:54:LYS:N | 1:B:54:LYS:CA | 1:B:54:LYS:C | 1 | 0.24 | 0.24 |
| (1,145) | 1:B:20:ASN:C | 1:B:21:GLN:N | 1:B:21:GLN:CA | 1:B:21:GLN:C | 2 | 0.14 | 0.22 |
| (1,185) | 1:B:47:CYS:C | 1:B:48:ASN:N | 1:B:48:ASN:CA | 1:B:48:ASN:C | 2 | 0.14 | 0.18 |
| (1,153) | 1:B:24:GLY:C | 1:B:25:VAL:N | 1:B:25:VAL:CA | 1:B:25:VAL:C | 1 | 0.17 | 0.17 |
| (1,147) | 1:B:21:GLN:C | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1 | 0.14 | 0.14 |
| (1,39) | 1:A:25:VAL:C | 1:A:26:ILE:N | 1:A:26:ILE:CA | 1:A:26:ILE:C | 1 | 0.08 | 0.08 |
| (1,97) | 1:A:63:MET:C | 1:A:64:ASP:N | 1:A:64:ASP:CA | 1:A:64:ASP:C | 1 | 0.01 | 0.01 |

## 9.8 All violated dihedral angleeee restraints

### 9.8.1 Histogram : Distribution of violations

The following histogram shows the distribution of violations in the ensemble.
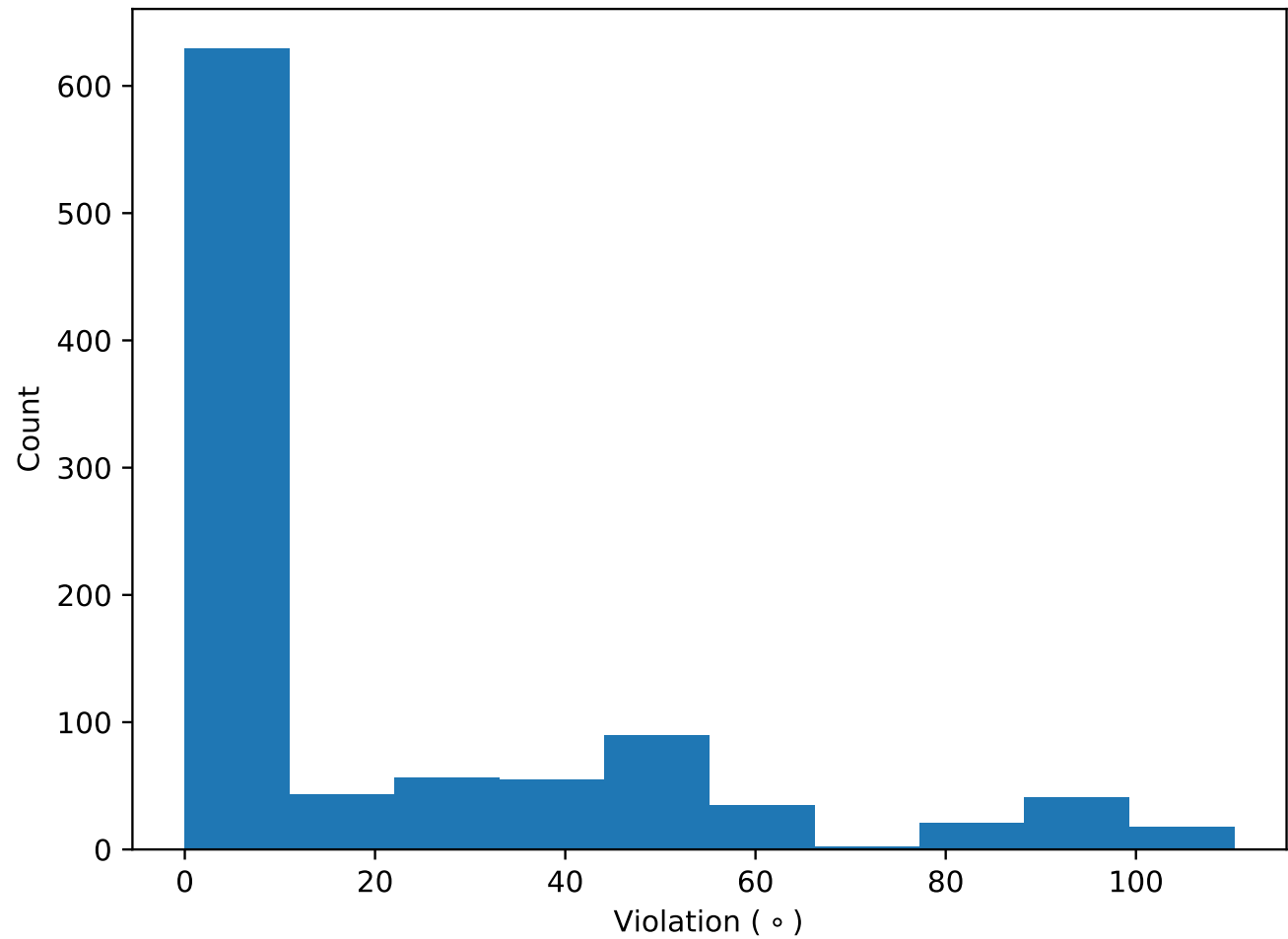


### 9.8.2 Table: All violated dihedral angle restraints

The following table lists the violations in the ensemble sorted by violation value

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ∘ ) |
|---|---|---|---|---|---|---|
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 8 | 110.32 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 11 | 109.45 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 3 | 109.36 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 18 | 107.94 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 19 | 106.17 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 6 | 105.91 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 8 | 105.78 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1 | 104.78 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 9 | 104.76 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 15 | 104.1 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ∘ ) |
|---|---|---|---|---|---|---|
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 4 | 103.45 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 20 | 103.4 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 9 | 102.88 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 20 | 102.67 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 5 | 101.82 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 10 | 101.76 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 17 | 101.04 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 7 | 100.97 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 16 | 98.66 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 17 | 98.54 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 12 | 98.09 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 2 | 97.98 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 6 | 97.53 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 13 | 97.34 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 11 | 97.28 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 10 | 96.71 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 7 | 96.66 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 19 | 96.63 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 6 | 96.55 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 5 | 96.51 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 8 | 96.05 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 15 | 95.77 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 3 | 95.51 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 10 | 95.51 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 13 | 94.51 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 4 | 94.2 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 18 | 94.13 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 2 | 93.76 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 14 | 93.65 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 14 | 93.35 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1 | 93.21 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 14 | 92.72 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 12 | 92.33 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 14 | 92.19 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 12 | 92.18 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 2 | 92.06 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 3 | 91.84 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 17 | 91.52 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1 | 91.29 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 6 | 90.47 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 16 | 90.17 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 9 | 90.05 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 12 | 90.0 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 18 | 89.98 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 16 | 89.55 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 8 | 89.39 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 10 | 89.02 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 5 | 88.8 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 19 | 88.75 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 20 | 88.2 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 11 | 87.93 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ∘ ) |
|---|---|---|---|---|---|---|
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 4 | 87.87 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 15 | 87.45 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 13 | 87.42 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 19 | 87.23 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 13 | 87.05 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 16 | 86.88 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 7 | 86.35 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 4 | 85.97 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 11 | 85.82 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 7 | 85.39 |
| (1,1) | 1:A:3:ASP:C | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 18 | 84.6 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 20 | 84.32 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 15 | 83.2 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1 | 83.14 |
| (1,19) | 1:A:13:GLU:C | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 5 | 82.64 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 3 | 82.14 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 9 | 81.66 |
| (1,135) | 1:B:13:GLU:C | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 17 | 80.79 |
| (1,117) | 1:B:3:ASP:C | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 2 | 79.58 |
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 20 | 69.43 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 6 | 68.8 |
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 3 | 66.02 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 3 | 65.96 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 19 | 63.9 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 12 | 63.57 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 18 | 63.11 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 19 | 62.38 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 17 | 61.48 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 13 | 61.48 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 18 | 60.03 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 5 | 59.94 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 1 | 59.43 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 15 | 59.39 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 17 | 59.37 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 9 | 59.13 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 5 | 58.89 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 3 | 58.62 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 4 | 58.06 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 12 | 57.42 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 19 | 57.3 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 13 | 57.23 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 5 | 56.83 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 7 | 56.74 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 9 | 56.64 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 5 | 56.54 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 2 | 55.93 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 6 | 55.93 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 14 | 55.82 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 18 | 55.79 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 18 | 55.77 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 9 | 55.76 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ° ) |
|---|---|---|---|---|---|---|
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 7 | 55.69 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 16 | 55.54 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 14 | 55.48 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 5 | 55.44 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 16 | 55.28 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 14 | 54.95 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 16 | 54.95 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 3 | 54.93 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 5 | 54.8 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 11 | 54.69 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 9 | 54.65 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 11 | 54.54 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 18 | 54.48 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 2 | 54.4 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 15 | 54.1 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 14 | 54.08 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 19 | 54.07 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 2 | 54.01 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 12 | 53.93 |
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 9 | 53.6 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 13 | 53.58 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 20 | 53.48 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 13 | 53.45 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 6 | 53.35 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 4 | 53.14 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 11 | 53.02 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 17 | 52.88 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 8 | 52.85 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 3 | 52.79 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 8 | 52.79 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 10 | 52.65 |
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 18 | 52.47 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 9 | 52.27 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 19 | 52.17 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 12 | 52.13 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 19 | 51.72 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 12 | 51.63 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 6 | 51.63 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 11 | 51.58 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 9 | 50.87 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 4 | 50.74 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 17 | 50.33 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 14 | 50.07 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 18 | 49.88 |
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 4 | 49.61 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 10 | 49.59 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 3 | 49.44 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 1 | 49.37 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 16 | 49.33 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 14 | 49.02 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 16 | 48.79 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ∘ ) |
|-----|--------|--------|--------|--------|-------|-----------------|
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 16 | 48.14 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 11 | 48.02 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1 | 47.91 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 6 | 47.88 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 10 | 47.84 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 9 | 47.83 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 12 | 47.79 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 13 | 47.78 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 10 | 47.73 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 6 | 47.44 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 12 | 47.1 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 9 | 47.05 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 19 | 46.85 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 11 | 46.77 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 20 | 46.69 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 15 | 46.56 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 2 | 46.54 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 8 | 46.53 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 4 | 46.47 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 8 | 46.42 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1 | 46.37 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 1 | 46.36 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 5 | 46.33 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 20 | 46.23 |
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 13 | 46.19 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 7 | 46.18 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 14 | 46.13 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 7 | 46.12 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 20 | 46.05 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 17 | 45.91 |
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 17 | 45.91 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 19 | 45.84 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 12 | 45.74 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 12 | 45.4 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 17 | 45.38 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 14 | 45.24 |
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 14 | 45.2 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 4 | 45.16 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 2 | 45.02 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 5 | 44.95 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 15 | 44.9 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 10 | 44.79 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 2 | 44.53 |
| (1,195) | 1:B:52:PHE:C | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 4 | 44.3 |
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 16 | 44.13 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 2 | 44.12 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 8 | 44.06 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 13 | 43.72 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 1 | 43.68 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 10 | 43.65 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 11 | 43.53 |

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*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ∘ ) |
|---|---|---|---|---|---|---|
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 4 | 43.41 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 8 | 43.39 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 20 | 43.28 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 3 | 43.2 |
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 15 | 42.82 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 20 | 42.7 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 1 | 42.37 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 15 | 42.06 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 20 | 41.94 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 7 | 41.87 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 11 | 41.51 |
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 12 | 41.47 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 20 | 40.88 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 18 | 40.73 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 16 | 40.68 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 18 | 40.29 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 17 | 40.16 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 9 | 40.16 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 6 | 40.04 |
| (1,8) | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1:A:8:ILE:N | 7 | 39.94 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 17 | 39.84 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 14 | 39.8 |
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 11 | 39.74 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 7 | 39.71 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 4 | 39.43 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 15 | 39.23 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 20 | 39.1 |
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 1 | 38.96 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 5 | 38.73 |
| (1,79) | 1:A:52:PHE:C | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 17 | 38.57 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 10 | 38.25 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 18 | 37.75 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 1 | 37.39 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 10 | 37.13 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 7 | 36.98 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 16 | 36.84 |
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 5 | 36.82 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 15 | 36.76 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 13 | 36.06 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 17 | 35.74 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 8 | 35.58 |
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 19 | 35.31 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 13 | 34.73 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 10 | 34.43 |
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 2 | 33.85 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 2 | 33.67 |
| (1,136) | 1:B:14:ASP:N | 1:B:14:ASP:CA | 1:B:14:ASP:C | 1:B:15:LYS:N | 10 | 33.62 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 2 | 33.55 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 4 | 32.71 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 15 | 32.39 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 19 | 31.88 |

*Continued on next page...*

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ∘ ) |
|---|---|---|---|---|---|---|
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 5 | 31.51 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 11 | 31.27 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 3 | 31.12 |
| (1,7) | 1:A:6:ALA:C | 1:A:7:GLY:N | 1:A:7:GLY:CA | 1:A:7:GLY:C | 1 | 30.93 |
| (1,124) | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 1:B:8:ILE:N | 3 | 30.86 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 3 | 30.82 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 10 | 30.71 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 3 | 30.66 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 9 | 30.5 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 10 | 30.5 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 20 | 30.24 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 19 | 30.11 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 17 | 30.09 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 13 | 30.05 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 16 | 29.86 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 20 | 29.84 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 15 | 29.62 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 18 | 29.44 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 15 | 29.31 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 12 | 29.23 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 2 | 29.19 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 8 | 28.96 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 4 | 28.72 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 4 | 28.45 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 18 | 27.63 |
| (1,123) | 1:B:6:ALA:C | 1:B:7:GLY:N | 1:B:7:GLY:CA | 1:B:7:GLY:C | 8 | 27.6 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 7 | 27.52 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 9 | 27.45 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 16 | 27.33 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 7 | 27.32 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 11 | 27.19 |
| (1,20) | 1:A:14:ASP:N | 1:A:14:ASP:CA | 1:A:14:ASP:C | 1:A:15:LYS:N | 3 | 26.96 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 11 | 26.92 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 1 | 26.71 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 1 | 26.66 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 6 | 26.13 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 16 | 26.04 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 15 | 25.97 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 5 | 25.83 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 8 | 25.78 |
| (1,22) | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 1:A:16:ASN:N | 8 | 25.52 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 6 | 25.47 |
| (1,22) | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 1:A:16:ASN:N | 3 | 25.12 |
| (1,138) | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1:B:16:ASN:N | 1 | 25.09 |
| (1,22) | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 1:A:16:ASN:N | 2 | 24.56 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 13 | 23.6 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 2 | 23.58 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 12 | 23.57 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 8 | 23.5 |
| (1,138) | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1:B:16:ASN:N | 6 | 22.96 |
| (1,22) | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 1:A:16:ASN:N | 10 | 22.66 |

*Continued on next page...*

*Continued from previous page...*

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ◦ ) |
|-----|--------|--------|--------|--------|-------|-----------------|
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 13 | 22.65 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 14 | 22.39 |
| (1,22) | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 1:A:16:ASN:N | 1 | 22.06 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 6 | 21.82 |
| (1,118) | 1:B:4:PHE:N | 1:B:4:PHE:CA | 1:B:4:PHE:C | 1:B:5:LEU:N | 14 | 20.92 |
| (1,2) | 1:A:4:PHE:N | 1:A:4:PHE:CA | 1:A:4:PHE:C | 1:A:5:LEU:N | 19 | 20.66 |
| (1,138) | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1:B:16:ASN:N | 2 | 20.49 |
| (1,22) | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 1:A:16:ASN:N | 7 | 20.2 |
| (1,138) | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1:B:16:ASN:N | 5 | 20.04 |
| (1,22) | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 1:A:16:ASN:N | 16 | 18.2 |
| (1,138) | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1:B:16:ASN:N | 19 | 17.94 |
| (1,138) | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1:B:16:ASN:N | 12 | 17.17 |
| (1,138) | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1:B:16:ASN:N | 17 | 16.57 |
| (1,22) | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 1:A:16:ASN:N | 9 | 16.28 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 20 | 15.68 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 11 | 14.69 |
| (1,138) | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1:B:16:ASN:N | 10 | 14.49 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 11 | 14.38 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 5 | 14.1 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 14 | 13.69 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 3 | 13.66 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 6 | 13.65 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 8 | 13.62 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 9 | 13.6 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 7 | 13.57 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 12 | 13.41 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 15 | 13.22 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 10 | 12.9 |
| (1,138) | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1:B:16:ASN:N | 16 | 12.71 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 2 | 12.62 |
| (1,22) | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 1:A:16:ASN:N | 12 | 12.59 |
| (1,138) | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1:B:16:ASN:N | 9 | 12.55 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 8 | 12.51 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 2 | 12.47 |
| (1,22) | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 1:A:16:ASN:N | 4 | 12.43 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 13 | 12.27 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 3 | 12.25 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 20 | 12.16 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 4 | 12.1 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 1 | 11.82 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 7 | 11.65 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 5 | 11.36 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 17 | 11.21 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 17 | 11.19 |
| (1,138) | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1:B:16:ASN:N | 8 | 11.11 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 9 | 11.04 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 18 | 11.02 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 16 | 10.98 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 4 | 10.86 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 19 | 10.79 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 14 | 10.59 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ∘ ) |
|-----|--------|--------|--------|--------|-------|-----------------|
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 10 | 10.57 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 13 | 10.41 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 16 | 10.32 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 18 | 10.29 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 12 | 10.24 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 6 | 9.93 |
| (1,22) | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 1:A:16:ASN:N | 13 | 8.21 |
| (1,22) | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 1:A:16:ASN:N | 11 | 7.7 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 19 | 7.56 |
| (1,138) | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1:B:16:ASN:N | 20 | 6.3 |
| (1,22) | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 1:A:16:ASN:N | 6 | 6.25 |
| (1,138) | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1:B:16:ASN:N | 13 | 6.06 |
| (1,21) | 1:A:14:ASP:C | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 7 | 6.05 |
| (1,22) | 1:A:15:LYS:N | 1:A:15:LYS:CA | 1:A:15:LYS:C | 1:A:16:ASN:N | 5 | 5.35 |
| (1,137) | 1:B:14:ASP:C | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 6 | 4.64 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 18 | 3.59 |
| (1,76) | 1:A:51:ILE:N | 1:A:51:ILE:CA | 1:A:51:ILE:C | 1:A:52:PHE:N | 1 | 3.53 |
| (1,192) | 1:B:51:ILE:N | 1:B:51:ILE:CA | 1:B:51:ILE:C | 1:B:52:PHE:N | 15 | 3.07 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 5 | 3.0 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 10 | 2.99 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 17 | 2.98 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 18 | 2.94 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 11 | 2.76 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 4 | 2.72 |
| (1,140) | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 1:B:19:THR:N | 8 | 2.71 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 9 | 2.69 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 2 | 2.67 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 2 | 2.65 |
| (1,24) | 1:A:18:MET:N | 1:A:18:MET:CA | 1:A:18:MET:C | 1:A:19:THR:N | 9 | 2.59 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 16 | 2.58 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 9 | 2.57 |
| (1,140) | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 1:B:19:THR:N | 12 | 2.56 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 10 | 2.55 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 20 | 2.49 |
| (1,221) | 1:B:67:ARG:C | 1:B:68:LYS:N | 1:B:68:LYS:CA | 1:B:68:LYS:C | 9 | 2.47 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 4 | 2.45 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 12 | 2.43 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 19 | 2.43 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 17 | 2.43 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 8 | 2.42 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 3 | 2.41 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 5 | 2.4 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 12 | 2.4 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 20 | 2.4 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 13 | 2.39 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 14 | 2.37 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 7 | 2.37 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 13 | 2.36 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 1 | 2.34 |
| (1,24) | 1:A:18:MET:N | 1:A:18:MET:CA | 1:A:18:MET:C | 1:A:19:THR:N | 7 | 2.33 |
| (1,221) | 1:B:67:ARG:C | 1:B:68:LYS:N | 1:B:68:LYS:CA | 1:B:68:LYS:C | 14 | 2.32 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ○ ) |
|-----|--------|--------|--------|--------|-------|-----------------|
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 7 | 2.32 |
| (1,140) | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 1:B:19:THR:N | 5 | 2.3 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 3 | 2.3 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 12 | 2.28 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 5 | 2.27 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 6 | 2.25 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 20 | 2.23 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 20 | 2.22 |
| (1,170) | 1:B:37:VAL:N | 1:B:37:VAL:CA | 1:B:37:VAL:C | 1:B:38:LEU:N | 14 | 2.21 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 16 | 2.18 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 1 | 2.18 |
| (1,220) | 1:B:67:ARG:N | 1:B:67:ARG:CA | 1:B:67:ARG:C | 1:B:68:LYS:N | 9 | 2.17 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 10 | 2.17 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 7 | 2.16 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 15 | 2.15 |
| (1,42) | 1:A:27:SER:N | 1:A:27:SER:CA | 1:A:27:SER:C | 1:A:28:LYS:N | 15 | 2.14 |
| (1,105) | 1:A:67:ARG:C | 1:A:68:LYS:N | 1:A:68:LYS:CA | 1:A:68:LYS:C | 5 | 2.14 |
| (1,24) | 1:A:18:MET:N | 1:A:18:MET:CA | 1:A:18:MET:C | 1:A:19:THR:N | 3 | 2.13 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 5 | 2.11 |
| (1,54) | 1:A:37:VAL:N | 1:A:37:VAL:CA | 1:A:37:VAL:C | 1:A:38:LEU:N | 1 | 2.1 |
| (1,42) | 1:A:27:SER:N | 1:A:27:SER:CA | 1:A:27:SER:C | 1:A:28:LYS:N | 13 | 2.1 |
| (1,24) | 1:A:18:MET:N | 1:A:18:MET:CA | 1:A:18:MET:C | 1:A:19:THR:N | 10 | 2.1 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 11 | 2.1 |
| (1,140) | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 1:B:19:THR:N | 9 | 2.1 |
| (1,220) | 1:B:67:ARG:N | 1:B:67:ARG:CA | 1:B:67:ARG:C | 1:B:68:LYS:N | 7 | 2.08 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 9 | 2.08 |
| (1,55) | 1:A:37:VAL:C | 1:A:38:LEU:N | 1:A:38:LEU:CA | 1:A:38:LEU:C | 8 | 2.06 |
| (1,54) | 1:A:37:VAL:N | 1:A:37:VAL:CA | 1:A:37:VAL:C | 1:A:38:LEU:N | 10 | 2.06 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 8 | 2.06 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 18 | 2.06 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 1 | 2.05 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 3 | 2.05 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 19 | 2.05 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 13 | 2.03 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 20 | 2.0 |
| (1,201) | 1:B:57:ASP:C | 1:B:58:LYS:N | 1:B:58:LYS:CA | 1:B:58:LYS:C | 14 | 1.99 |
| (1,105) | 1:A:67:ARG:C | 1:A:68:LYS:N | 1:A:68:LYS:CA | 1:A:68:LYS:C | 13 | 1.98 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 4 | 1.97 |
| (1,220) | 1:B:67:ARG:N | 1:B:67:ARG:CA | 1:B:67:ARG:C | 1:B:68:LYS:N | 1 | 1.97 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 13 | 1.97 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 20 | 1.97 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 4 | 1.93 |
| (1,24) | 1:A:18:MET:N | 1:A:18:MET:CA | 1:A:18:MET:C | 1:A:19:THR:N | 12 | 1.92 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 2 | 1.92 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 16 | 1.91 |
| (1,221) | 1:B:67:ARG:C | 1:B:68:LYS:N | 1:B:68:LYS:CA | 1:B:68:LYS:C | 1 | 1.91 |
| (1,171) | 1:B:37:VAL:C | 1:B:38:LEU:N | 1:B:38:LEU:CA | 1:B:38:LEU:C | 13 | 1.9 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 1 | 1.9 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 6 | 1.88 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 4 | 1.87 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 17 | 1.86 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ∘ ) |
|---|---|---|---|---|---|---|
| (1,158) | 1:B:27:SER:N | 1:B:27:SER:CA | 1:B:27:SER:C | 1:B:28:LYS:N | 18 | 1.85 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 2 | 1.84 |
| (1,158) | 1:B:27:SER:N | 1:B:27:SER:CA | 1:B:27:SER:C | 1:B:28:LYS:N | 11 | 1.84 |
| (1,158) | 1:B:27:SER:N | 1:B:27:SER:CA | 1:B:27:SER:C | 1:B:28:LYS:N | 16 | 1.84 |
| (1,138) | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1:B:16:ASN:N | 18 | 1.83 |
| (1,42) | 1:A:27:SER:N | 1:A:27:SER:CA | 1:A:27:SER:C | 1:A:28:LYS:N | 1 | 1.82 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 11 | 1.82 |
| (1,221) | 1:B:67:ARG:C | 1:B:68:LYS:N | 1:B:68:LYS:CA | 1:B:68:LYS:C | 7 | 1.79 |
| (1,24) | 1:A:18:MET:N | 1:A:18:MET:CA | 1:A:18:MET:C | 1:A:19:THR:N | 8 | 1.77 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 6 | 1.76 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 17 | 1.75 |
| (1,24) | 1:A:18:MET:N | 1:A:18:MET:CA | 1:A:18:MET:C | 1:A:19:THR:N | 1 | 1.74 |
| (1,220) | 1:B:67:ARG:N | 1:B:67:ARG:CA | 1:B:67:ARG:C | 1:B:68:LYS:N | 14 | 1.74 |
| (1,24) | 1:A:18:MET:N | 1:A:18:MET:CA | 1:A:18:MET:C | 1:A:19:THR:N | 11 | 1.72 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 6 | 1.71 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 12 | 1.71 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 8 | 1.69 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 19 | 1.69 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 10 | 1.69 |
| (1,105) | 1:A:67:ARG:C | 1:A:68:LYS:N | 1:A:68:LYS:CA | 1:A:68:LYS:C | 3 | 1.69 |
| (1,201) | 1:B:57:ASP:C | 1:B:58:LYS:N | 1:B:58:LYS:CA | 1:B:58:LYS:C | 2 | 1.68 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 16 | 1.68 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 18 | 1.67 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 12 | 1.67 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 2 | 1.66 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 14 | 1.66 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 15 | 1.66 |
| (1,24) | 1:A:18:MET:N | 1:A:18:MET:CA | 1:A:18:MET:C | 1:A:19:THR:N | 14 | 1.64 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 1 | 1.64 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 17 | 1.64 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 18 | 1.64 |
| (1,105) | 1:A:67:ARG:C | 1:A:68:LYS:N | 1:A:68:LYS:CA | 1:A:68:LYS:C | 10 | 1.63 |
| (1,139) | 1:B:17:GLY:C | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 6 | 1.62 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 14 | 1.61 |
| (1,171) | 1:B:37:VAL:C | 1:B:38:LEU:N | 1:B:38:LEU:CA | 1:B:38:LEU:C | 16 | 1.59 |
| (1,158) | 1:B:27:SER:N | 1:B:27:SER:CA | 1:B:27:SER:C | 1:B:28:LYS:N | 14 | 1.59 |
| (1,55) | 1:A:37:VAL:C | 1:A:38:LEU:N | 1:A:38:LEU:CA | 1:A:38:LEU:C | 11 | 1.58 |
| (1,42) | 1:A:27:SER:N | 1:A:27:SER:CA | 1:A:27:SER:C | 1:A:28:LYS:N | 18 | 1.57 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 4 | 1.57 |
| (1,28) | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 1:A:21:GLN:N | 20 | 1.54 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 16 | 1.54 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 15 | 1.52 |
| (1,60) | 1:A:40:ALA:N | 1:A:40:ALA:CA | 1:A:40:ALA:C | 1:A:41:LYS:N | 7 | 1.5 |
| (1,170) | 1:B:37:VAL:N | 1:B:37:VAL:CA | 1:B:37:VAL:C | 1:B:38:LEU:N | 1 | 1.5 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 3 | 1.49 |
| (1,96) | 1:A:63:MET:N | 1:A:63:MET:CA | 1:A:63:MET:C | 1:A:64:ASP:N | 1 | 1.48 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 4 | 1.48 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 12 | 1.48 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 14 | 1.42 |
| (1,42) | 1:A:27:SER:N | 1:A:27:SER:CA | 1:A:27:SER:C | 1:A:28:LYS:N | 8 | 1.42 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 7 | 1.42 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ∘ ) |
|-----|--------|--------|--------|--------|-------|-----------------|
| (1,140) | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 1:B:19:THR:N | 1 | 1.42 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 10 | 1.41 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 9 | 1.4 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 8 | 1.4 |
| (1,128) | 1:B:9:ARG:N | 1:B:9:ARG:CA | 1:B:9:ARG:C | 1:B:10:ILE:N | 20 | 1.4 |
| (1,105) | 1:A:67:ARG:C | 1:A:68:LYS:N | 1:A:68:LYS:CA | 1:A:68:LYS:C | 2 | 1.4 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 8 | 1.4 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 15 | 1.39 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 2 | 1.38 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 16 | 1.38 |
| (1,28) | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 1:A:21:GLN:N | 4 | 1.37 |
| (1,171) | 1:B:37:VAL:C | 1:B:38:LEU:N | 1:B:38:LEU:CA | 1:B:38:LEU:C | 12 | 1.35 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 4 | 1.35 |
| (1,182) | 1:B:46:THR:N | 1:B:46:THR:CA | 1:B:46:THR:C | 1:B:47:CYS:N | 8 | 1.34 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 14 | 1.33 |
| (1,28) | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 1:A:21:GLN:N | 6 | 1.32 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 16 | 1.31 |
| (1,140) | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 1:B:19:THR:N | 10 | 1.31 |
| (1,140) | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 1:B:19:THR:N | 19 | 1.31 |
| (1,105) | 1:A:67:ARG:C | 1:A:68:LYS:N | 1:A:68:LYS:CA | 1:A:68:LYS:C | 1 | 1.29 |
| (1,220) | 1:B:67:ARG:N | 1:B:67:ARG:CA | 1:B:67:ARG:C | 1:B:68:LYS:N | 11 | 1.27 |
| (1,140) | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 1:B:19:THR:N | 20 | 1.27 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 6 | 1.27 |
| (1,54) | 1:A:37:VAL:N | 1:A:37:VAL:CA | 1:A:37:VAL:C | 1:A:38:LEU:N | 5 | 1.26 |
| (1,212) | 1:B:63:MET:N | 1:B:63:MET:CA | 1:B:63:MET:C | 1:B:64:ASP:N | 19 | 1.26 |
| (1,148) | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 1:B:23:THR:N | 7 | 1.26 |
| (1,220) | 1:B:67:ARG:N | 1:B:67:ARG:CA | 1:B:67:ARG:C | 1:B:68:LYS:N | 8 | 1.25 |
| (1,204) | 1:B:59:LEU:N | 1:B:59:LEU:CA | 1:B:59:LEU:C | 1:B:60:THR:N | 20 | 1.25 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 20 | 1.25 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 14 | 1.24 |
| (1,158) | 1:B:27:SER:N | 1:B:27:SER:CA | 1:B:27:SER:C | 1:B:28:LYS:N | 3 | 1.23 |
| (1,158) | 1:B:27:SER:N | 1:B:27:SER:CA | 1:B:27:SER:C | 1:B:28:LYS:N | 20 | 1.23 |
| (1,140) | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 1:B:19:THR:N | 2 | 1.23 |
| (1,12) | 1:A:9:ARG:N | 1:A:9:ARG:CA | 1:A:9:ARG:C | 1:A:10:ILE:N | 13 | 1.22 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 17 | 1.21 |
| (1,23) | 1:A:17:GLY:C | 1:A:18:MET:N | 1:A:18:MET:CA | 1:A:18:MET:C | 5 | 1.21 |
| (1,196) | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 1:B:54:LYS:N | 12 | 1.21 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 11 | 1.2 |
| (1,171) | 1:B:37:VAL:C | 1:B:38:LEU:N | 1:B:38:LEU:CA | 1:B:38:LEU:C | 4 | 1.2 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 10 | 1.2 |
| (1,54) | 1:A:37:VAL:N | 1:A:37:VAL:CA | 1:A:37:VAL:C | 1:A:38:LEU:N | 6 | 1.18 |
| (1,105) | 1:A:67:ARG:C | 1:A:68:LYS:N | 1:A:68:LYS:CA | 1:A:68:LYS:C | 16 | 1.18 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 1 | 1.18 |
| (1,90) | 1:A:60:THR:N | 1:A:60:THR:CA | 1:A:60:THR:C | 1:A:61:THR:N | 3 | 1.17 |
| (1,140) | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 1:B:19:THR:N | 16 | 1.16 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 3 | 1.16 |
| (1,110) | 1:A:74:THR:N | 1:A:74:THR:CA | 1:A:74:THR:C | 1:A:75:VAL:N | 14 | 1.16 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 4 | 1.15 |
| (1,171) | 1:B:37:VAL:C | 1:B:38:LEU:N | 1:B:38:LEU:CA | 1:B:38:LEU:C | 5 | 1.15 |
| (1,85) | 1:A:57:ASP:C | 1:A:58:LYS:N | 1:A:58:LYS:CA | 1:A:58:LYS:C | 8 | 1.14 |
| (1,85) | 1:A:57:ASP:C | 1:A:58:LYS:N | 1:A:58:LYS:CA | 1:A:58:LYS:C | 11 | 1.14 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ∘ ) |
|---|---|---|---|---|---|---|
| (1,24) | 1:A:18:MET:N | 1:A:18:MET:CA | 1:A:18:MET:C | 1:A:19:THR:N | 19 | 1.14 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 1 | 1.12 |
| (1,55) | 1:A:37:VAL:C | 1:A:38:LEU:N | 1:A:38:LEU:CA | 1:A:38:LEU:C | 9 | 1.12 |
| (1,170) | 1:B:37:VAL:N | 1:B:37:VAL:CA | 1:B:37:VAL:C | 1:B:38:LEU:N | 20 | 1.12 |
| (1,158) | 1:B:27:SER:N | 1:B:27:SER:CA | 1:B:27:SER:C | 1:B:28:LYS:N | 10 | 1.12 |
| (1,42) | 1:A:27:SER:N | 1:A:27:SER:CA | 1:A:27:SER:C | 1:A:28:LYS:N | 12 | 1.11 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 13 | 1.11 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 2 | 1.11 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 5 | 1.09 |
| (1,27) | 1:A:19:THR:C | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 20 | 1.08 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 7 | 1.08 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 18 | 1.07 |
| (1,32) | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 1:A:23:THR:N | 15 | 1.06 |
| (1,166) | 1:B:35:THR:N | 1:B:35:THR:CA | 1:B:35:THR:C | 1:B:36:ILE:N | 4 | 1.06 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 5 | 1.06 |
| (1,120) | 1:B:5:LEU:N | 1:B:5:LEU:CA | 1:B:5:LEU:C | 1:B:6:ALA:N | 17 | 1.06 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 9 | 1.05 |
| (1,105) | 1:A:67:ARG:C | 1:A:68:LYS:N | 1:A:68:LYS:CA | 1:A:68:LYS:C | 18 | 1.05 |
| (1,206) | 1:B:60:THR:N | 1:B:60:THR:CA | 1:B:60:THR:C | 1:B:61:THR:N | 15 | 1.04 |
| (1,140) | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 1:B:19:THR:N | 18 | 1.04 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 13 | 1.04 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 17 | 1.04 |
| (1,98) | 1:A:64:ASP:N | 1:A:64:ASP:CA | 1:A:64:ASP:C | 1:A:65:LYS:N | 18 | 1.03 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 12 | 1.03 |
| (1,201) | 1:B:57:ASP:C | 1:B:58:LYS:N | 1:B:58:LYS:CA | 1:B:58:LYS:C | 3 | 1.03 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 8 | 1.02 |
| (1,128) | 1:B:9:ARG:N | 1:B:9:ARG:CA | 1:B:9:ARG:C | 1:B:10:ILE:N | 19 | 1.02 |
| (1,5) | 1:A:5:LEU:C | 1:A:6:ALA:N | 1:A:6:ALA:CA | 1:A:6:ALA:C | 18 | 1.01 |
| (1,5) | 1:A:5:LEU:C | 1:A:6:ALA:N | 1:A:6:ALA:CA | 1:A:6:ALA:C | 20 | 1.01 |
| (1,220) | 1:B:67:ARG:N | 1:B:67:ARG:CA | 1:B:67:ARG:C | 1:B:68:LYS:N | 13 | 1.01 |
| (1,139) | 1:B:17:GLY:C | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 2 | 1.01 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 18 | 1.0 |
| (1,187) | 1:B:48:ASN:C | 1:B:49:LEU:N | 1:B:49:LEU:CA | 1:B:49:LEU:C | 18 | 1.0 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 18 | 1.0 |
| (1,139) | 1:B:17:GLY:C | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 18 | 0.99 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 10 | 0.98 |
| (1,66) | 1:A:46:THR:N | 1:A:46:THR:CA | 1:A:46:THR:C | 1:A:47:CYS:N | 13 | 0.98 |
| (1,42) | 1:A:27:SER:N | 1:A:27:SER:CA | 1:A:27:SER:C | 1:A:28:LYS:N | 16 | 0.98 |
| (1,42) | 1:A:27:SER:N | 1:A:27:SER:CA | 1:A:27:SER:C | 1:A:28:LYS:N | 19 | 0.98 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 8 | 0.98 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 15 | 0.97 |
| (1,24) | 1:A:18:MET:N | 1:A:18:MET:CA | 1:A:18:MET:C | 1:A:19:THR:N | 18 | 0.97 |
| (1,204) | 1:B:59:LEU:N | 1:B:59:LEU:CA | 1:B:59:LEU:C | 1:B:60:THR:N | 11 | 0.97 |
| (1,140) | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 1:B:19:THR:N | 13 | 0.97 |
| (1,85) | 1:A:57:ASP:C | 1:A:58:LYS:N | 1:A:58:LYS:CA | 1:A:58:LYS:C | 15 | 0.96 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 4 | 0.96 |
| (1,201) | 1:B:57:ASP:C | 1:B:58:LYS:N | 1:B:58:LYS:CA | 1:B:58:LYS:C | 18 | 0.96 |
| (1,158) | 1:B:27:SER:N | 1:B:27:SER:CA | 1:B:27:SER:C | 1:B:28:LYS:N | 17 | 0.96 |
| (1,128) | 1:B:9:ARG:N | 1:B:9:ARG:CA | 1:B:9:ARG:C | 1:B:10:ILE:N | 15 | 0.96 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 3 | 0.95 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 7 | 0.94 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ◦ ) |
|---|---|---|---|---|---|---|
| (1,33) | 1:A:22:ILE:C | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 20 | 0.94 |
| (1,220) | 1:B:67:ARG:N | 1:B:67:ARG:CA | 1:B:67:ARG:C | 1:B:68:LYS:N | 15 | 0.94 |
| (1,204) | 1:B:59:LEU:N | 1:B:59:LEU:CA | 1:B:59:LEU:C | 1:B:60:THR:N | 12 | 0.93 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 20 | 0.92 |
| (1,54) | 1:A:37:VAL:N | 1:A:37:VAL:CA | 1:A:37:VAL:C | 1:A:38:LEU:N | 15 | 0.92 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 11 | 0.92 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 8 | 0.92 |
| (1,121) | 1:B:5:LEU:C | 1:B:6:ALA:N | 1:B:6:ALA:CA | 1:B:6:ALA:C | 4 | 0.92 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 10 | 0.91 |
| (1,170) | 1:B:37:VAL:N | 1:B:37:VAL:CA | 1:B:37:VAL:C | 1:B:38:LEU:N | 11 | 0.91 |
| (1,140) | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 1:B:19:THR:N | 6 | 0.91 |
| (1,85) | 1:A:57:ASP:C | 1:A:58:LYS:N | 1:A:58:LYS:CA | 1:A:58:LYS:C | 7 | 0.9 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 5 | 0.9 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 7 | 0.89 |
| (1,187) | 1:B:48:ASN:C | 1:B:49:LEU:N | 1:B:49:LEU:CA | 1:B:49:LEU:C | 1 | 0.89 |
| (1,144) | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 1:B:21:GLN:N | 3 | 0.89 |
| (1,187) | 1:B:48:ASN:C | 1:B:49:LEU:N | 1:B:49:LEU:CA | 1:B:49:LEU:C | 17 | 0.88 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 1 | 0.88 |
| (1,85) | 1:A:57:ASP:C | 1:A:58:LYS:N | 1:A:58:LYS:CA | 1:A:58:LYS:C | 10 | 0.87 |
| (1,221) | 1:B:67:ARG:C | 1:B:68:LYS:N | 1:B:68:LYS:CA | 1:B:68:LYS:C | 12 | 0.87 |
| (1,206) | 1:B:60:THR:N | 1:B:60:THR:CA | 1:B:60:THR:C | 1:B:61:THR:N | 14 | 0.87 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 6 | 0.87 |
| (1,149) | 1:B:22:ILE:C | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 17 | 0.87 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 16 | 0.86 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 13 | 0.86 |
| (1,201) | 1:B:57:ASP:C | 1:B:58:LYS:N | 1:B:58:LYS:CA | 1:B:58:LYS:C | 7 | 0.86 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 7 | 0.86 |
| (1,221) | 1:B:67:ARG:C | 1:B:68:LYS:N | 1:B:68:LYS:CA | 1:B:68:LYS:C | 11 | 0.85 |
| (1,204) | 1:B:59:LEU:N | 1:B:59:LEU:CA | 1:B:59:LEU:C | 1:B:60:THR:N | 6 | 0.85 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 19 | 0.85 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 17 | 0.84 |
| (1,12) | 1:A:9:ARG:N | 1:A:9:ARG:CA | 1:A:9:ARG:C | 1:A:10:ILE:N | 12 | 0.83 |
| (1,105) | 1:A:67:ARG:C | 1:A:68:LYS:N | 1:A:68:LYS:CA | 1:A:68:LYS:C | 12 | 0.83 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 8 | 0.82 |
| (1,171) | 1:B:37:VAL:C | 1:B:38:LEU:N | 1:B:38:LEU:CA | 1:B:38:LEU:C | 9 | 0.82 |
| (1,143) | 1:B:19:THR:C | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 6 | 0.82 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 19 | 0.81 |
| (1,187) | 1:B:48:ASN:C | 1:B:49:LEU:N | 1:B:49:LEU:CA | 1:B:49:LEU:C | 10 | 0.81 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 4 | 0.8 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 12 | 0.8 |
| (1,80) | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 1:A:54:LYS:N | 18 | 0.8 |
| (1,187) | 1:B:48:ASN:C | 1:B:49:LEU:N | 1:B:49:LEU:CA | 1:B:49:LEU:C | 16 | 0.8 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 16 | 0.79 |
| (1,54) | 1:A:37:VAL:N | 1:A:37:VAL:CA | 1:A:37:VAL:C | 1:A:38:LEU:N | 7 | 0.79 |
| (1,50) | 1:A:35:THR:N | 1:A:35:THR:CA | 1:A:35:THR:C | 1:A:36:ILE:N | 13 | 0.79 |
| (1,218) | 1:B:66:LEU:N | 1:B:66:LEU:CA | 1:B:66:LEU:C | 1:B:67:ARG:N | 3 | 0.79 |
| (1,212) | 1:B:63:MET:N | 1:B:63:MET:CA | 1:B:63:MET:C | 1:B:64:ASP:N | 8 | 0.79 |
| (1,206) | 1:B:60:THR:N | 1:B:60:THR:CA | 1:B:60:THR:C | 1:B:61:THR:N | 2 | 0.79 |
| (1,172) | 1:B:38:LEU:N | 1:B:38:LEU:CA | 1:B:38:LEU:C | 1:B:39:ASN:N | 19 | 0.79 |
| (1,171) | 1:B:37:VAL:C | 1:B:38:LEU:N | 1:B:38:LEU:CA | 1:B:38:LEU:C | 2 | 0.79 |
| (1,171) | 1:B:37:VAL:C | 1:B:38:LEU:N | 1:B:38:LEU:CA | 1:B:38:LEU:C | 19 | 0.79 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ∘ ) |
|---|---|---|---|---|---|---|
| (1,206) | 1:B:60:THR:N | 1:B:60:THR:CA | 1:B:60:THR:C | 1:B:61:THR:N | 11 | 0.78 |
| (1,144) | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 1:B:21:GLN:N | 1 | 0.78 |
| (1,4) | 1:A:5:LEU:N | 1:A:5:LEU:CA | 1:A:5:LEU:C | 1:A:6:ALA:N | 12 | 0.77 |
| (1,206) | 1:B:60:THR:N | 1:B:60:THR:CA | 1:B:60:THR:C | 1:B:61:THR:N | 18 | 0.77 |
| (1,140) | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 1:B:19:THR:N | 4 | 0.77 |
| (1,54) | 1:A:37:VAL:N | 1:A:37:VAL:CA | 1:A:37:VAL:C | 1:A:38:LEU:N | 19 | 0.76 |
| (1,24) | 1:A:18:MET:N | 1:A:18:MET:CA | 1:A:18:MET:C | 1:A:19:THR:N | 5 | 0.76 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 10 | 0.76 |
| (1,66) | 1:A:46:THR:N | 1:A:46:THR:CA | 1:A:46:THR:C | 1:A:47:CYS:N | 6 | 0.75 |
| (1,54) | 1:A:37:VAL:N | 1:A:37:VAL:CA | 1:A:37:VAL:C | 1:A:38:LEU:N | 16 | 0.75 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 10 | 0.75 |
| (1,196) | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 1:B:54:LYS:N | 11 | 0.75 |
| (1,196) | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 1:B:54:LYS:N | 19 | 0.75 |
| (1,28) | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 1:A:21:GLN:N | 19 | 0.74 |
| (1,128) | 1:B:9:ARG:N | 1:B:9:ARG:CA | 1:B:9:ARG:C | 1:B:10:ILE:N | 6 | 0.74 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 13 | 0.73 |
| (1,42) | 1:A:27:SER:N | 1:A:27:SER:CA | 1:A:27:SER:C | 1:A:28:LYS:N | 5 | 0.73 |
| (1,28) | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 1:A:21:GLN:N | 15 | 0.73 |
| (1,105) | 1:A:67:ARG:C | 1:A:68:LYS:N | 1:A:68:LYS:CA | 1:A:68:LYS:C | 20 | 0.73 |
| (1,27) | 1:A:19:THR:C | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 6 | 0.72 |
| (1,226) | 1:B:74:THR:N | 1:B:74:THR:CA | 1:B:74:THR:C | 1:B:75:VAL:N | 17 | 0.72 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 19 | 0.71 |
| (1,220) | 1:B:67:ARG:N | 1:B:67:ARG:CA | 1:B:67:ARG:C | 1:B:68:LYS:N | 4 | 0.71 |
| (1,182) | 1:B:46:THR:N | 1:B:46:THR:CA | 1:B:46:THR:C | 1:B:47:CYS:N | 10 | 0.71 |
| (1,28) | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 1:A:21:GLN:N | 2 | 0.7 |
| (1,158) | 1:B:27:SER:N | 1:B:27:SER:CA | 1:B:27:SER:C | 1:B:28:LYS:N | 8 | 0.7 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 15 | 0.7 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 19 | 0.69 |
| (1,226) | 1:B:74:THR:N | 1:B:74:THR:CA | 1:B:74:THR:C | 1:B:75:VAL:N | 12 | 0.69 |
| (1,187) | 1:B:48:ASN:C | 1:B:49:LEU:N | 1:B:49:LEU:CA | 1:B:49:LEU:C | 4 | 0.69 |
| (1,187) | 1:B:48:ASN:C | 1:B:49:LEU:N | 1:B:49:LEU:CA | 1:B:49:LEU:C | 9 | 0.69 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 12 | 0.69 |
| (1,54) | 1:A:37:VAL:N | 1:A:37:VAL:CA | 1:A:37:VAL:C | 1:A:38:LEU:N | 3 | 0.68 |
| (1,42) | 1:A:27:SER:N | 1:A:27:SER:CA | 1:A:27:SER:C | 1:A:28:LYS:N | 10 | 0.68 |
| (1,28) | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 1:A:21:GLN:N | 5 | 0.68 |
| (1,221) | 1:B:67:ARG:C | 1:B:68:LYS:N | 1:B:68:LYS:CA | 1:B:68:LYS:C | 15 | 0.68 |
| (1,174) | 1:B:39:ASN:N | 1:B:39:ASN:CA | 1:B:39:ASN:C | 1:B:40:ALA:N | 4 | 0.68 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 3 | 0.68 |
| (1,226) | 1:B:74:THR:N | 1:B:74:THR:CA | 1:B:74:THR:C | 1:B:75:VAL:N | 4 | 0.67 |
| (1,187) | 1:B:48:ASN:C | 1:B:49:LEU:N | 1:B:49:LEU:CA | 1:B:49:LEU:C | 5 | 0.67 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 13 | 0.67 |
| (1,54) | 1:A:37:VAL:N | 1:A:37:VAL:CA | 1:A:37:VAL:C | 1:A:38:LEU:N | 17 | 0.66 |
| (1,42) | 1:A:27:SER:N | 1:A:27:SER:CA | 1:A:27:SER:C | 1:A:28:LYS:N | 9 | 0.66 |
| (1,31) | 1:A:21:GLN:C | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 20 | 0.66 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 5 | 0.66 |
| (1,182) | 1:B:46:THR:N | 1:B:46:THR:CA | 1:B:46:THR:C | 1:B:47:CYS:N | 15 | 0.66 |
| (1,166) | 1:B:35:THR:N | 1:B:35:THR:CA | 1:B:35:THR:C | 1:B:36:ILE:N | 2 | 0.66 |
| (1,128) | 1:B:9:ARG:N | 1:B:9:ARG:CA | 1:B:9:ARG:C | 1:B:10:ILE:N | 18 | 0.66 |
| (1,33) | 1:A:22:ILE:C | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 19 | 0.64 |
| (1,220) | 1:B:67:ARG:N | 1:B:67:ARG:CA | 1:B:67:ARG:C | 1:B:68:LYS:N | 12 | 0.64 |
| (1,166) | 1:B:35:THR:N | 1:B:35:THR:CA | 1:B:35:THR:C | 1:B:36:ILE:N | 9 | 0.64 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ○ ) |
|---|---|---|---|---|---|---|
| (1,28) | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 1:A:21:GLN:N | 3 | 0.63 |
| (1,224) | 1:B:69:VAL:N | 1:B:69:VAL:CA | 1:B:69:VAL:C | 1:B:70:GLN:N | 14 | 0.63 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 20 | 0.63 |
| (1,144) | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 1:B:21:GLN:N | 7 | 0.63 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 14 | 0.63 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 15 | 0.62 |
| (1,87) | 1:A:58:LYS:C | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 16 | 0.62 |
| (1,54) | 1:A:37:VAL:N | 1:A:37:VAL:CA | 1:A:37:VAL:C | 1:A:38:LEU:N | 2 | 0.62 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 5 | 0.62 |
| (1,166) | 1:B:35:THR:N | 1:B:35:THR:CA | 1:B:35:THR:C | 1:B:36:ILE:N | 11 | 0.61 |
| (1,120) | 1:B:5:LEU:N | 1:B:5:LEU:CA | 1:B:5:LEU:C | 1:B:6:ALA:N | 16 | 0.61 |
| (1,201) | 1:B:57:ASP:C | 1:B:58:LYS:N | 1:B:58:LYS:CA | 1:B:58:LYS:C | 4 | 0.6 |
| (1,187) | 1:B:48:ASN:C | 1:B:49:LEU:N | 1:B:49:LEU:CA | 1:B:49:LEU:C | 8 | 0.6 |
| (1,171) | 1:B:37:VAL:C | 1:B:38:LEU:N | 1:B:38:LEU:CA | 1:B:38:LEU:C | 17 | 0.6 |
| (1,85) | 1:A:57:ASP:C | 1:A:58:LYS:N | 1:A:58:LYS:CA | 1:A:58:LYS:C | 18 | 0.59 |
| (1,4) | 1:A:5:LEU:N | 1:A:5:LEU:CA | 1:A:5:LEU:C | 1:A:6:ALA:N | 13 | 0.59 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 16 | 0.59 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 15 | 0.59 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 1 | 0.58 |
| (1,220) | 1:B:67:ARG:N | 1:B:67:ARG:CA | 1:B:67:ARG:C | 1:B:68:LYS:N | 6 | 0.58 |
| (1,121) | 1:B:5:LEU:C | 1:B:6:ALA:N | 1:B:6:ALA:CA | 1:B:6:ALA:C | 8 | 0.58 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 6 | 0.56 |
| (1,27) | 1:A:19:THR:C | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 13 | 0.56 |
| (1,152) | 1:B:24:GLY:N | 1:B:24:GLY:CA | 1:B:24:GLY:C | 1:B:25:VAL:N | 15 | 0.56 |
| (1,144) | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 1:B:21:GLN:N | 11 | 0.56 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 3 | 0.55 |
| (1,28) | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 1:A:21:GLN:N | 1 | 0.54 |
| (1,166) | 1:B:35:THR:N | 1:B:35:THR:CA | 1:B:35:THR:C | 1:B:36:ILE:N | 14 | 0.54 |
| (1,178) | 1:B:44:ILE:N | 1:B:44:ILE:CA | 1:B:44:ILE:C | 1:B:45:PHE:N | 12 | 0.53 |
| (1,143) | 1:B:19:THR:C | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 1 | 0.53 |
| (1,90) | 1:A:60:THR:N | 1:A:60:THR:CA | 1:A:60:THR:C | 1:A:61:THR:N | 4 | 0.52 |
| (1,187) | 1:B:48:ASN:C | 1:B:49:LEU:N | 1:B:49:LEU:CA | 1:B:49:LEU:C | 7 | 0.52 |
| (1,144) | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 1:B:21:GLN:N | 20 | 0.52 |
| (1,105) | 1:A:67:ARG:C | 1:A:68:LYS:N | 1:A:68:LYS:CA | 1:A:68:LYS:C | 14 | 0.52 |
| (1,69) | 1:A:47:CYS:C | 1:A:48:ASN:N | 1:A:48:ASN:CA | 1:A:48:ASN:C | 2 | 0.51 |
| (1,4) | 1:A:5:LEU:N | 1:A:5:LEU:CA | 1:A:5:LEU:C | 1:A:6:ALA:N | 1 | 0.51 |
| (1,221) | 1:B:67:ARG:C | 1:B:68:LYS:N | 1:B:68:LYS:CA | 1:B:68:LYS:C | 2 | 0.51 |
| (1,220) | 1:B:67:ARG:N | 1:B:67:ARG:CA | 1:B:67:ARG:C | 1:B:68:LYS:N | 20 | 0.51 |
| (1,143) | 1:B:19:THR:C | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 9 | 0.51 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 19 | 0.51 |
| (1,57) | 1:A:38:LEU:C | 1:A:39:ASN:N | 1:A:39:ASN:CA | 1:A:39:ASN:C | 18 | 0.5 |
| (1,23) | 1:A:17:GLY:C | 1:A:18:MET:N | 1:A:18:MET:CA | 1:A:18:MET:C | 6 | 0.5 |
| (1,201) | 1:B:57:ASP:C | 1:B:58:LYS:N | 1:B:58:LYS:CA | 1:B:58:LYS:C | 9 | 0.5 |
| (1,80) | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 1:A:54:LYS:N | 1 | 0.49 |
| (1,143) | 1:B:19:THR:C | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 12 | 0.49 |
| (1,140) | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 1:B:19:THR:N | 15 | 0.49 |
| (1,121) | 1:B:5:LEU:C | 1:B:6:ALA:N | 1:B:6:ALA:CA | 1:B:6:ALA:C | 1 | 0.49 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 8 | 0.48 |
| (1,221) | 1:B:67:ARG:C | 1:B:68:LYS:N | 1:B:68:LYS:CA | 1:B:68:LYS:C | 19 | 0.48 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 2 | 0.47 |
| (1,4) | 1:A:5:LEU:N | 1:A:5:LEU:CA | 1:A:5:LEU:C | 1:A:6:ALA:N | 17 | 0.47 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ∘ ) |
|---|---|---|---|---|---|---|
| (1,170) | 1:B:37:VAL:N | 1:B:37:VAL:CA | 1:B:37:VAL:C | 1:B:38:LEU:N | 18 | 0.47 |
| (1,116) | 1:A:77:ARG:N | 1:A:77:ARG:CA | 1:A:77:ARG:C | 1:A:78:LEU:N | 8 | 0.47 |
| (1,211) | 1:B:62:LEU:C | 1:B:63:MET:N | 1:B:63:MET:CA | 1:B:63:MET:C | 19 | 0.46 |
| (1,204) | 1:B:59:LEU:N | 1:B:59:LEU:CA | 1:B:59:LEU:C | 1:B:60:THR:N | 2 | 0.46 |
| (1,172) | 1:B:38:LEU:N | 1:B:38:LEU:CA | 1:B:38:LEU:C | 1:B:39:ASN:N | 10 | 0.46 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 11 | 0.46 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 3 | 0.45 |
| (1,5) | 1:A:5:LEU:C | 1:A:6:ALA:N | 1:A:6:ALA:CA | 1:A:6:ALA:C | 17 | 0.45 |
| (1,220) | 1:B:67:ARG:N | 1:B:67:ARG:CA | 1:B:67:ARG:C | 1:B:68:LYS:N | 10 | 0.45 |
| (1,206) | 1:B:60:THR:N | 1:B:60:THR:CA | 1:B:60:THR:C | 1:B:61:THR:N | 4 | 0.45 |
| (1,158) | 1:B:27:SER:N | 1:B:27:SER:CA | 1:B:27:SER:C | 1:B:28:LYS:N | 2 | 0.45 |
| (1,143) | 1:B:19:THR:C | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 3 | 0.45 |
| (1,55) | 1:A:37:VAL:C | 1:A:38:LEU:N | 1:A:38:LEU:CA | 1:A:38:LEU:C | 13 | 0.44 |
| (1,42) | 1:A:27:SER:N | 1:A:27:SER:CA | 1:A:27:SER:C | 1:A:28:LYS:N | 11 | 0.44 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 13 | 0.44 |
| (1,27) | 1:A:19:THR:C | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 19 | 0.44 |
| (1,158) | 1:B:27:SER:N | 1:B:27:SER:CA | 1:B:27:SER:C | 1:B:28:LYS:N | 15 | 0.44 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 16 | 0.43 |
| (1,201) | 1:B:57:ASP:C | 1:B:58:LYS:N | 1:B:58:LYS:CA | 1:B:58:LYS:C | 15 | 0.43 |
| (1,187) | 1:B:48:ASN:C | 1:B:49:LEU:N | 1:B:49:LEU:CA | 1:B:49:LEU:C | 14 | 0.43 |
| (1,143) | 1:B:19:THR:C | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 2 | 0.43 |
| (1,143) | 1:B:19:THR:C | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 7 | 0.43 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 5 | 0.42 |
| (1,50) | 1:A:35:THR:N | 1:A:35:THR:CA | 1:A:35:THR:C | 1:A:36:ILE:N | 1 | 0.42 |
| (1,204) | 1:B:59:LEU:N | 1:B:59:LEU:CA | 1:B:59:LEU:C | 1:B:60:THR:N | 10 | 0.42 |
| (1,187) | 1:B:48:ASN:C | 1:B:49:LEU:N | 1:B:49:LEU:CA | 1:B:49:LEU:C | 20 | 0.42 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 9 | 0.42 |
| (1,48) | 1:A:33:ILE:N | 1:A:33:ILE:CA | 1:A:33:ILE:C | 1:A:34:ARG:N | 7 | 0.41 |
| (1,144) | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 1:B:21:GLN:N | 17 | 0.41 |
| (1,128) | 1:B:9:ARG:N | 1:B:9:ARG:CA | 1:B:9:ARG:C | 1:B:10:ILE:N | 8 | 0.41 |
| (1,50) | 1:A:35:THR:N | 1:A:35:THR:CA | 1:A:35:THR:C | 1:A:36:ILE:N | 8 | 0.4 |
| (1,42) | 1:A:27:SER:N | 1:A:27:SER:CA | 1:A:27:SER:C | 1:A:28:LYS:N | 7 | 0.4 |
| (1,36) | 1:A:24:GLY:N | 1:A:24:GLY:CA | 1:A:24:GLY:C | 1:A:25:VAL:N | 11 | 0.4 |
| (1,23) | 1:A:17:GLY:C | 1:A:18:MET:N | 1:A:18:MET:CA | 1:A:18:MET:C | 13 | 0.4 |
| (1,221) | 1:B:67:ARG:C | 1:B:68:LYS:N | 1:B:68:LYS:CA | 1:B:68:LYS:C | 3 | 0.4 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 11 | 0.4 |
| (1,114) | 1:A:76:GLU:N | 1:A:76:GLU:CA | 1:A:76:GLU:C | 1:A:77:ARG:N | 8 | 0.4 |
| (1,105) | 1:A:67:ARG:C | 1:A:68:LYS:N | 1:A:68:LYS:CA | 1:A:68:LYS:C | 6 | 0.4 |
| (1,85) | 1:A:57:ASP:C | 1:A:58:LYS:N | 1:A:58:LYS:CA | 1:A:58:LYS:C | 2 | 0.39 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 12 | 0.39 |
| (1,54) | 1:A:37:VAL:N | 1:A:37:VAL:CA | 1:A:37:VAL:C | 1:A:38:LEU:N | 20 | 0.39 |
| (1,5) | 1:A:5:LEU:C | 1:A:6:ALA:N | 1:A:6:ALA:CA | 1:A:6:ALA:C | 1 | 0.39 |
| (1,27) | 1:A:19:THR:C | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 3 | 0.39 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 7 | 0.39 |
| (1,27) | 1:A:19:THR:C | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 14 | 0.38 |
| (1,152) | 1:B:24:GLY:N | 1:B:24:GLY:CA | 1:B:24:GLY:C | 1:B:25:VAL:N | 5 | 0.38 |
| (1,130) | 1:B:10:ILE:N | 1:B:10:ILE:CA | 1:B:10:ILE:C | 1:B:11:VAL:N | 6 | 0.38 |
| (1,85) | 1:A:57:ASP:C | 1:A:58:LYS:N | 1:A:58:LYS:CA | 1:A:58:LYS:C | 16 | 0.37 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 14 | 0.37 |
| (1,70) | 1:A:48:ASN:N | 1:A:48:ASN:CA | 1:A:48:ASN:C | 1:A:49:LEU:N | 12 | 0.37 |
| (1,42) | 1:A:27:SER:N | 1:A:27:SER:CA | 1:A:27:SER:C | 1:A:28:LYS:N | 6 | 0.37 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ∘ ) |
|-----|--------|--------|--------|--------|-------|-----------------|
| (1,201) | 1:B:57:ASP:C | 1:B:58:LYS:N | 1:B:58:LYS:CA | 1:B:58:LYS:C | 1 | 0.37 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 17 | 0.36 |
| (1,62) | 1:A:44:ILE:N | 1:A:44:ILE:CA | 1:A:44:ILE:C | 1:A:45:PHE:N | 20 | 0.36 |
| (1,214) | 1:B:64:ASP:N | 1:B:64:ASP:CA | 1:B:64:ASP:C | 1:B:65:LYS:N | 3 | 0.36 |
| (1,204) | 1:B:59:LEU:N | 1:B:59:LEU:CA | 1:B:59:LEU:C | 1:B:60:THR:N | 19 | 0.36 |
| (1,182) | 1:B:46:THR:N | 1:B:46:THR:CA | 1:B:46:THR:C | 1:B:47:CYS:N | 13 | 0.36 |
| (1,139) | 1:B:17:GLY:C | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 13 | 0.36 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 8 | 0.36 |
| (1,110) | 1:A:74:THR:N | 1:A:74:THR:CA | 1:A:74:THR:C | 1:A:75:VAL:N | 17 | 0.36 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 6 | 0.35 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 7 | 0.35 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 9 | 0.35 |
| (1,204) | 1:B:59:LEU:N | 1:B:59:LEU:CA | 1:B:59:LEU:C | 1:B:60:THR:N | 7 | 0.35 |
| (1,166) | 1:B:35:THR:N | 1:B:35:THR:CA | 1:B:35:THR:C | 1:B:36:ILE:N | 19 | 0.35 |
| (1,149) | 1:B:22:ILE:C | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 9 | 0.35 |
| (1,221) | 1:B:67:ARG:C | 1:B:68:LYS:N | 1:B:68:LYS:CA | 1:B:68:LYS:C | 18 | 0.34 |
| (1,152) | 1:B:24:GLY:N | 1:B:24:GLY:CA | 1:B:24:GLY:C | 1:B:25:VAL:N | 3 | 0.34 |
| (1,140) | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 1:B:19:THR:N | 11 | 0.34 |
| (1,27) | 1:A:19:THR:C | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 1 | 0.33 |
| (1,212) | 1:B:63:MET:N | 1:B:63:MET:CA | 1:B:63:MET:C | 1:B:64:ASP:N | 9 | 0.33 |
| (1,203) | 1:B:58:LYS:C | 1:B:59:LEU:N | 1:B:59:LEU:CA | 1:B:59:LEU:C | 6 | 0.33 |
| (1,144) | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 1:B:21:GLN:N | 5 | 0.33 |
| (1,85) | 1:A:57:ASP:C | 1:A:58:LYS:N | 1:A:58:LYS:CA | 1:A:58:LYS:C | 12 | 0.32 |
| (1,27) | 1:A:19:THR:C | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 5 | 0.32 |
| (1,221) | 1:B:67:ARG:C | 1:B:68:LYS:N | 1:B:68:LYS:CA | 1:B:68:LYS:C | 8 | 0.32 |
| (1,149) | 1:B:22:ILE:C | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 8 | 0.32 |
| (1,128) | 1:B:9:ARG:N | 1:B:9:ARG:CA | 1:B:9:ARG:C | 1:B:10:ILE:N | 2 | 0.32 |
| (1,54) | 1:A:37:VAL:N | 1:A:37:VAL:CA | 1:A:37:VAL:C | 1:A:38:LEU:N | 4 | 0.31 |
| (1,204) | 1:B:59:LEU:N | 1:B:59:LEU:CA | 1:B:59:LEU:C | 1:B:60:THR:N | 5 | 0.31 |
| (1,170) | 1:B:37:VAL:N | 1:B:37:VAL:CA | 1:B:37:VAL:C | 1:B:38:LEU:N | 7 | 0.31 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 11 | 0.31 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 9 | 0.3 |
| (1,80) | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 1:A:54:LYS:N | 10 | 0.3 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 1 | 0.3 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 14 | 0.3 |
| (1,33) | 1:A:22:ILE:C | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 9 | 0.3 |
| (1,28) | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 1:A:21:GLN:N | 10 | 0.3 |
| (1,196) | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 1:B:54:LYS:N | 2 | 0.3 |
| (1,152) | 1:B:24:GLY:N | 1:B:24:GLY:CA | 1:B:24:GLY:C | 1:B:25:VAL:N | 18 | 0.3 |
| (1,144) | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 1:B:21:GLN:N | 6 | 0.3 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 19 | 0.29 |
| (1,42) | 1:A:27:SER:N | 1:A:27:SER:CA | 1:A:27:SER:C | 1:A:28:LYS:N | 14 | 0.28 |
| (1,224) | 1:B:69:VAL:N | 1:B:69:VAL:CA | 1:B:69:VAL:C | 1:B:70:GLN:N | 7 | 0.28 |
| (1,201) | 1:B:57:ASP:C | 1:B:58:LYS:N | 1:B:58:LYS:CA | 1:B:58:LYS:C | 10 | 0.28 |
| (1,201) | 1:B:57:ASP:C | 1:B:58:LYS:N | 1:B:58:LYS:CA | 1:B:58:LYS:C | 19 | 0.28 |
| (1,66) | 1:A:46:THR:N | 1:A:46:THR:CA | 1:A:46:THR:C | 1:A:47:CYS:N | 17 | 0.27 |
| (1,4) | 1:A:5:LEU:N | 1:A:5:LEU:CA | 1:A:5:LEU:C | 1:A:6:ALA:N | 8 | 0.27 |
| (1,196) | 1:B:53:VAL:N | 1:B:53:VAL:CA | 1:B:53:VAL:C | 1:B:54:LYS:N | 5 | 0.27 |
| (1,187) | 1:B:48:ASN:C | 1:B:49:LEU:N | 1:B:49:LEU:CA | 1:B:49:LEU:C | 15 | 0.27 |
| (1,105) | 1:A:67:ARG:C | 1:A:68:LYS:N | 1:A:68:LYS:CA | 1:A:68:LYS:C | 8 | 0.27 |
| (1,59) | 1:A:39:ASN:C | 1:A:40:ALA:N | 1:A:40:ALA:CA | 1:A:40:ALA:C | 10 | 0.26 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ∘ ) |
|---|---|---|---|---|---|---|
| (1,50) | 1:A:35:THR:N | 1:A:35:THR:CA | 1:A:35:THR:C | 1:A:36:ILE:N | 9 | 0.26 |
| (1,201) | 1:B:57:ASP:C | 1:B:58:LYS:N | 1:B:58:LYS:CA | 1:B:58:LYS:C | 12 | 0.26 |
| (1,144) | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 1:B:21:GLN:N | 4 | 0.26 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 20 | 0.25 |
| (1,211) | 1:B:62:LEU:C | 1:B:63:MET:N | 1:B:63:MET:CA | 1:B:63:MET:C | 16 | 0.25 |
| (1,206) | 1:B:60:THR:N | 1:B:60:THR:CA | 1:B:60:THR:C | 1:B:61:THR:N | 7 | 0.25 |
| (1,158) | 1:B:27:SER:N | 1:B:27:SER:CA | 1:B:27:SER:C | 1:B:28:LYS:N | 9 | 0.25 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 5 | 0.24 |
| (1,50) | 1:A:35:THR:N | 1:A:35:THR:CA | 1:A:35:THR:C | 1:A:36:ILE:N | 18 | 0.24 |
| (1,204) | 1:B:59:LEU:N | 1:B:59:LEU:CA | 1:B:59:LEU:C | 1:B:60:THR:N | 13 | 0.24 |
| (1,197) | 1:B:53:VAL:C | 1:B:54:LYS:N | 1:B:54:LYS:CA | 1:B:54:LYS:C | 4 | 0.24 |
| (1,143) | 1:B:19:THR:C | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 17 | 0.24 |
| (1,102) | 1:A:66:LEU:N | 1:A:66:LEU:CA | 1:A:66:LEU:C | 1:A:67:ARG:N | 5 | 0.24 |
| (1,70) | 1:A:48:ASN:N | 1:A:48:ASN:CA | 1:A:48:ASN:C | 1:A:49:LEU:N | 15 | 0.23 |
| (1,66) | 1:A:46:THR:N | 1:A:46:THR:CA | 1:A:46:THR:C | 1:A:47:CYS:N | 4 | 0.23 |
| (1,36) | 1:A:24:GLY:N | 1:A:24:GLY:CA | 1:A:24:GLY:C | 1:A:25:VAL:N | 9 | 0.23 |
| (1,226) | 1:B:74:THR:N | 1:B:74:THR:CA | 1:B:74:THR:C | 1:B:75:VAL:N | 6 | 0.23 |
| (1,201) | 1:B:57:ASP:C | 1:B:58:LYS:N | 1:B:58:LYS:CA | 1:B:58:LYS:C | 5 | 0.23 |
| (1,142) | 1:B:19:THR:N | 1:B:19:THR:CA | 1:B:19:THR:C | 1:B:20:ASN:N | 20 | 0.23 |
| (1,5) | 1:A:5:LEU:C | 1:A:6:ALA:N | 1:A:6:ALA:CA | 1:A:6:ALA:C | 15 | 0.22 |
| (1,230) | 1:B:76:GLU:N | 1:B:76:GLU:CA | 1:B:76:GLU:C | 1:B:77:ARG:N | 6 | 0.22 |
| (1,170) | 1:B:37:VAL:N | 1:B:37:VAL:CA | 1:B:37:VAL:C | 1:B:38:LEU:N | 8 | 0.22 |
| (1,166) | 1:B:35:THR:N | 1:B:35:THR:CA | 1:B:35:THR:C | 1:B:36:ILE:N | 13 | 0.22 |
| (1,150) | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 1:B:24:GLY:N | 18 | 0.22 |
| (1,145) | 1:B:20:ASN:C | 1:B:21:GLN:N | 1:B:21:GLN:CA | 1:B:21:GLN:C | 13 | 0.22 |
| (1,120) | 1:B:5:LEU:N | 1:B:5:LEU:CA | 1:B:5:LEU:C | 1:B:6:ALA:N | 20 | 0.22 |
| (1,112) | 1:A:75:VAL:N | 1:A:75:VAL:CA | 1:A:75:VAL:C | 1:A:76:GLU:N | 9 | 0.22 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 11 | 0.21 |
| (1,5) | 1:A:5:LEU:C | 1:A:6:ALA:N | 1:A:6:ALA:CA | 1:A:6:ALA:C | 8 | 0.21 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 15 | 0.21 |
| (1,218) | 1:B:66:LEU:N | 1:B:66:LEU:CA | 1:B:66:LEU:C | 1:B:67:ARG:N | 5 | 0.21 |
| (1,120) | 1:B:5:LEU:N | 1:B:5:LEU:CA | 1:B:5:LEU:C | 1:B:6:ALA:N | 1 | 0.21 |
| (1,158) | 1:B:27:SER:N | 1:B:27:SER:CA | 1:B:27:SER:C | 1:B:28:LYS:N | 19 | 0.2 |
| (1,144) | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 1:B:21:GLN:N | 16 | 0.2 |
| (1,80) | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 1:A:54:LYS:N | 2 | 0.19 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 13 | 0.19 |
| (1,4) | 1:A:5:LEU:N | 1:A:5:LEU:CA | 1:A:5:LEU:C | 1:A:6:ALA:N | 16 | 0.19 |
| (1,221) | 1:B:67:ARG:C | 1:B:68:LYS:N | 1:B:68:LYS:CA | 1:B:68:LYS:C | 13 | 0.19 |
| (1,114) | 1:A:76:GLU:N | 1:A:76:GLU:CA | 1:A:76:GLU:C | 1:A:77:ARG:N | 18 | 0.19 |
| (1,31) | 1:A:21:GLN:C | 1:A:22:ILE:N | 1:A:22:ILE:CA | 1:A:22:ILE:C | 19 | 0.18 |
| (1,206) | 1:B:60:THR:N | 1:B:60:THR:CA | 1:B:60:THR:C | 1:B:61:THR:N | 19 | 0.18 |
| (1,185) | 1:B:47:CYS:C | 1:B:48:ASN:N | 1:B:48:ASN:CA | 1:B:48:ASN:C | 20 | 0.18 |
| (1,5) | 1:A:5:LEU:C | 1:A:6:ALA:N | 1:A:6:ALA:CA | 1:A:6:ALA:C | 9 | 0.17 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 2 | 0.17 |
| (1,153) | 1:B:24:GLY:C | 1:B:25:VAL:N | 1:B:25:VAL:CA | 1:B:25:VAL:C | 14 | 0.17 |
| (1,144) | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 1:B:21:GLN:N | 9 | 0.17 |
| (1,90) | 1:A:60:THR:N | 1:A:60:THR:CA | 1:A:60:THR:C | 1:A:61:THR:N | 20 | 0.16 |
| (1,226) | 1:B:74:THR:N | 1:B:74:THR:CA | 1:B:74:THR:C | 1:B:75:VAL:N | 18 | 0.16 |
| (1,201) | 1:B:57:ASP:C | 1:B:58:LYS:N | 1:B:58:LYS:CA | 1:B:58:LYS:C | 11 | 0.16 |
| (1,186) | 1:B:48:ASN:N | 1:B:48:ASN:CA | 1:B:48:ASN:C | 1:B:49:LEU:N | 10 | 0.16 |
| (1,90) | 1:A:60:THR:N | 1:A:60:THR:CA | 1:A:60:THR:C | 1:A:61:THR:N | 17 | 0.15 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ∘ ) |
|-----|--------|--------|--------|--------|-------|-----------------|
| (1,48) | 1:A:33:ILE:N | 1:A:33:ILE:CA | 1:A:33:ILE:C | 1:A:34:ARG:N | 11 | 0.15 |
| (1,4) | 1:A:5:LEU:N | 1:A:5:LEU:CA | 1:A:5:LEU:C | 1:A:6:ALA:N | 20 | 0.15 |
| (1,28) | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 1:A:21:GLN:N | 17 | 0.15 |
| (1,204) | 1:B:59:LEU:N | 1:B:59:LEU:CA | 1:B:59:LEU:C | 1:B:60:THR:N | 3 | 0.15 |
| (1,204) | 1:B:59:LEU:N | 1:B:59:LEU:CA | 1:B:59:LEU:C | 1:B:60:THR:N | 15 | 0.15 |
| (1,186) | 1:B:48:ASN:N | 1:B:48:ASN:CA | 1:B:48:ASN:C | 1:B:49:LEU:N | 18 | 0.15 |
| (1,88) | 1:A:59:LEU:N | 1:A:59:LEU:CA | 1:A:59:LEU:C | 1:A:60:THR:N | 3 | 0.14 |
| (1,27) | 1:A:19:THR:C | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 8 | 0.14 |
| (1,187) | 1:B:48:ASN:C | 1:B:49:LEU:N | 1:B:49:LEU:CA | 1:B:49:LEU:C | 3 | 0.14 |
| (1,147) | 1:B:21:GLN:C | 1:B:22:ILE:N | 1:B:22:ILE:CA | 1:B:22:ILE:C | 17 | 0.14 |
| (1,138) | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1:B:16:ASN:N | 15 | 0.14 |
| (1,85) | 1:A:57:ASP:C | 1:A:58:LYS:N | 1:A:58:LYS:CA | 1:A:58:LYS:C | 4 | 0.13 |
| (1,228) | 1:B:75:VAL:N | 1:B:75:VAL:CA | 1:B:75:VAL:C | 1:B:76:GLU:N | 12 | 0.13 |
| (1,204) | 1:B:59:LEU:N | 1:B:59:LEU:CA | 1:B:59:LEU:C | 1:B:60:THR:N | 17 | 0.13 |
| (1,34) | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1:A:24:GLY:N | 2 | 0.12 |
| (1,184) | 1:B:47:CYS:N | 1:B:47:CYS:CA | 1:B:47:CYS:C | 1:B:48:ASN:N | 5 | 0.12 |
| (1,105) | 1:A:67:ARG:C | 1:A:68:LYS:N | 1:A:68:LYS:CA | 1:A:68:LYS:C | 17 | 0.12 |
| (1,90) | 1:A:60:THR:N | 1:A:60:THR:CA | 1:A:60:THR:C | 1:A:61:THR:N | 16 | 0.11 |
| (1,218) | 1:B:66:LEU:N | 1:B:66:LEU:CA | 1:B:66:LEU:C | 1:B:67:ARG:N | 15 | 0.11 |
| (1,105) | 1:A:67:ARG:C | 1:A:68:LYS:N | 1:A:68:LYS:CA | 1:A:68:LYS:C | 15 | 0.11 |
| (1,5) | 1:A:5:LEU:C | 1:A:6:ALA:N | 1:A:6:ALA:CA | 1:A:6:ALA:C | 16 | 0.1 |
| (1,33) | 1:A:22:ILE:C | 1:A:23:THR:N | 1:A:23:THR:CA | 1:A:23:THR:C | 1 | 0.1 |
| (1,220) | 1:B:67:ARG:N | 1:B:67:ARG:CA | 1:B:67:ARG:C | 1:B:68:LYS:N | 5 | 0.1 |
| (1,210) | 1:B:62:LEU:N | 1:B:62:LEU:CA | 1:B:62:LEU:C | 1:B:63:MET:N | 6 | 0.1 |
| (1,143) | 1:B:19:THR:C | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 5 | 0.1 |
| (1,14) | 1:A:10:ILE:N | 1:A:10:ILE:CA | 1:A:10:ILE:C | 1:A:11:VAL:N | 14 | 0.1 |
| (1,138) | 1:B:15:LYS:N | 1:B:15:LYS:CA | 1:B:15:LYS:C | 1:B:16:ASN:N | 4 | 0.1 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 18 | 0.09 |
| (1,57) | 1:A:38:LEU:C | 1:A:39:ASN:N | 1:A:39:ASN:CA | 1:A:39:ASN:C | 1 | 0.09 |
| (1,185) | 1:B:47:CYS:C | 1:B:48:ASN:N | 1:B:48:ASN:CA | 1:B:48:ASN:C | 18 | 0.09 |
| (1,174) | 1:B:39:ASN:N | 1:B:39:ASN:CA | 1:B:39:ASN:C | 1:B:40:ALA:N | 10 | 0.09 |
| (1,105) | 1:A:67:ARG:C | 1:A:68:LYS:N | 1:A:68:LYS:CA | 1:A:68:LYS:C | 19 | 0.09 |
| (1,70) | 1:A:48:ASN:N | 1:A:48:ASN:CA | 1:A:48:ASN:C | 1:A:49:LEU:N | 16 | 0.08 |
| (1,50) | 1:A:35:THR:N | 1:A:35:THR:CA | 1:A:35:THR:C | 1:A:36:ILE:N | 17 | 0.08 |
| (1,39) | 1:A:25:VAL:C | 1:A:26:ILE:N | 1:A:26:ILE:CA | 1:A:26:ILE:C | 17 | 0.08 |
| (1,212) | 1:B:63:MET:N | 1:B:63:MET:CA | 1:B:63:MET:C | 1:B:64:ASP:N | 10 | 0.08 |
| (1,28) | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 1:A:21:GLN:N | 8 | 0.07 |
| (1,212) | 1:B:63:MET:N | 1:B:63:MET:CA | 1:B:63:MET:C | 1:B:64:ASP:N | 14 | 0.07 |
| (1,96) | 1:A:63:MET:N | 1:A:63:MET:CA | 1:A:63:MET:C | 1:A:64:ASP:N | 13 | 0.06 |
| (1,71) | 1:A:48:ASN:C | 1:A:49:LEU:N | 1:A:49:LEU:CA | 1:A:49:LEU:C | 15 | 0.06 |
| (1,66) | 1:A:46:THR:N | 1:A:46:THR:CA | 1:A:46:THR:C | 1:A:47:CYS:N | 7 | 0.06 |
| (1,27) | 1:A:19:THR:C | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 4 | 0.06 |
| (1,27) | 1:A:19:THR:C | 1:A:20:ASN:N | 1:A:20:ASN:CA | 1:A:20:ASN:C | 12 | 0.06 |
| (1,145) | 1:B:20:ASN:C | 1:B:21:GLN:N | 1:B:21:GLN:CA | 1:B:21:GLN:C | 8 | 0.06 |
| (1,120) | 1:B:5:LEU:N | 1:B:5:LEU:CA | 1:B:5:LEU:C | 1:B:6:ALA:N | 13 | 0.06 |
| (1,102) | 1:A:66:LEU:N | 1:A:66:LEU:CA | 1:A:66:LEU:C | 1:A:67:ARG:N | 9 | 0.06 |
| (1,80) | 1:A:53:VAL:N | 1:A:53:VAL:CA | 1:A:53:VAL:C | 1:A:54:LYS:N | 5 | 0.05 |
| (1,221) | 1:B:67:ARG:C | 1:B:68:LYS:N | 1:B:68:LYS:CA | 1:B:68:LYS:C | 5 | 0.05 |
| (1,187) | 1:B:48:ASN:C | 1:B:49:LEU:N | 1:B:49:LEU:CA | 1:B:49:LEU:C | 12 | 0.04 |
| (1,166) | 1:B:35:THR:N | 1:B:35:THR:CA | 1:B:35:THR:C | 1:B:36:ILE:N | 12 | 0.04 |
| (1,143) | 1:B:19:THR:C | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 15 | 0.04 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model | Violation ( ∘ ) |
|---|---|---|---|---|---|---|
| (1,143) | 1:B:19:THR:C | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 20 | 0.04 |
| (1,104) | 1:A:67:ARG:N | 1:A:67:ARG:CA | 1:A:67:ARG:C | 1:A:68:LYS:N | 6 | 0.04 |
| (1,204) | 1:B:59:LEU:N | 1:B:59:LEU:CA | 1:B:59:LEU:C | 1:B:60:THR:N | 18 | 0.03 |
| (1,139) | 1:B:17:GLY:C | 1:B:18:MET:N | 1:B:18:MET:CA | 1:B:18:MET:C | 15 | 0.03 |
| (1,96) | 1:A:63:MET:N | 1:A:63:MET:CA | 1:A:63:MET:C | 1:A:64:ASP:N | 12 | 0.02 |
| (1,232) | 1:B:77:ARG:N | 1:B:77:ARG:CA | 1:B:77:ARG:C | 1:B:78:LEU:N | 8 | 0.02 |
| (1,211) | 1:B:62:LEU:C | 1:B:63:MET:N | 1:B:63:MET:CA | 1:B:63:MET:C | 18 | 0.02 |
| (1,149) | 1:B:22:ILE:C | 1:B:23:THR:N | 1:B:23:THR:CA | 1:B:23:THR:C | 18 | 0.02 |
| (1,143) | 1:B:19:THR:C | 1:B:20:ASN:N | 1:B:20:ASN:CA | 1:B:20:ASN:C | 11 | 0.02 |
| (1,97) | 1:A:63:MET:C | 1:A:64:ASP:N | 1:A:64:ASP:CA | 1:A:64:ASP:C | 14 | 0.01 |
| (1,50) | 1:A:35:THR:N | 1:A:35:THR:CA | 1:A:35:THR:C | 1:A:36:ILE:N | 6 | 0.01 |