



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2PNG
Title : Type I rat fatty acid synthase acyl carrier protein (ACP) domain
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Deposited on : 2007-04-24

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

| | | |
|--------------------------------|---|--|
| Cyrange | : | Kirchner and Güntert (2011) |
| NmrClust | : | Kelley et al. (1996) |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20171227.v01 (using entries in the PDB archive December 27th 2017) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | 2.6.dev1 |
| BMRB Restraints Analysis | : | v1.2 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.6.dev1 |

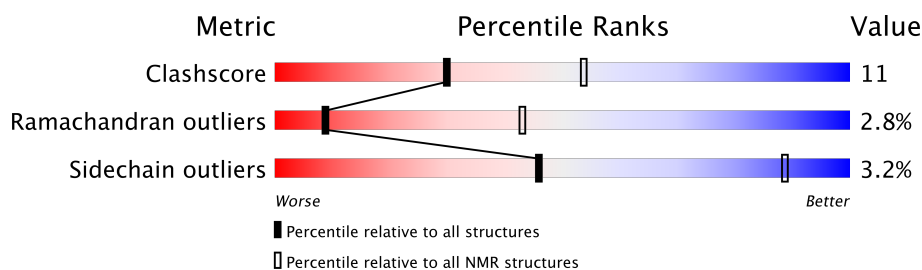
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 53%.

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 | 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 $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 89 | <div> <div></div> <div>60%</div> <div>16%</div> <div>25%</div> </div> |

2 Ensemble composition and analysis

This entry contains 30 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:8-A:74 (67) | 0.52 | 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 3 clusters and 1 single-model cluster was found.

| Cluster number | Models |
|-----------------------|--|
| 1 | 1, 2, 3, 4, 5, 6, 8, 9, 10, 12, 17, 19, 20, 21, 22, 25, 26, 27, 28, 29 |
| 2 | 7, 11, 13, 16, 24, 30 |
| 3 | 14, 15, 23 |
| Single-model clusters | 18 |

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1386 atoms, of which 708 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Fatty acid synthase (EC 2.3.1.85).

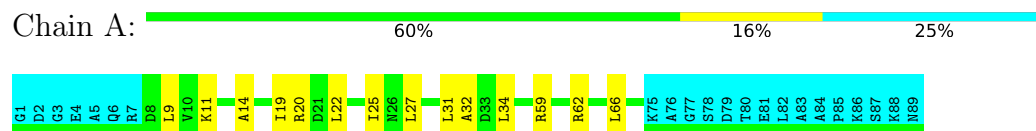
| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1 | A | 89 | Total | C | H | N | O | S | 0 |
| | | | 1386 | 416 | 708 | 125 | 135 | 2 | |

4 Residue-property plots [i](#)

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.

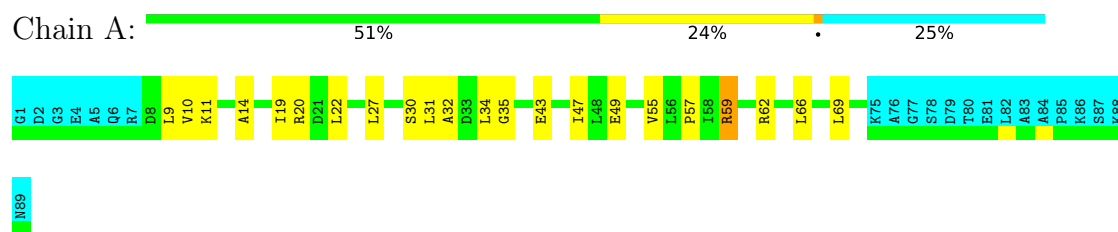
- Molecule 1: Fatty acid synthase (EC 2.3.1.85)



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: Fatty acid synthase (EC 2.3.1.85)



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 30 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification | Version |
|---------------|--------------------|---------|
| CNS | refinement | 1.1 |
| Aria | structure solution | 1.2 |

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) | 2png_nmr.cif |
| Number of chemical shift lists | 1 |
| Total number of shifts | 980 |
| Number of shifts mapped to atoms | 558 |
| Number of unparsed shifts | 156 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 266 |
| Assignment completeness (well-defined parts) | 53% |

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1 | A | 0.0±0.0 | 0.6±0.7 |
| All | All | 0 | 19 |

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1 | A | 45 | ARG | Sidechain | 6 |
| 1 | A | 59 | ARG | Sidechain | 5 |
| 1 | A | 67 | ARG | Sidechain | 5 |
| 1 | A | 20 | ARG | Sidechain | 2 |
| 1 | A | 62 | ARG | Sidechain | 1 |

6.2 Too-close contacts [i](#)

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 | 522 | 556 | 554 | 12±3 |
| All | All | 15660 | 16680 | 16620 | 352 |

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 11.

5 of 122 unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:8:ASP:HB2 | 1:A:11:LYS:HG2 | 0.89 | 1.45 | 13 | 6 |
| 1:A:31:LEU:HD12 | 1:A:34:LEU:HD12 | 0.79 | 1.54 | 4 | 9 |
| 1:A:32:ALA:HB2 | 1:A:62:ARG:HG2 | 0.79 | 1.53 | 24 | 8 |
| 1:A:27:LEU:HD22 | 1:A:67:ARG:HG2 | 0.72 | 1.62 | 10 | 2 |
| 1:A:22:LEU:HG | 1:A:27:LEU:HD21 | 0.72 | 1.62 | 14 | 6 |

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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 | 67/89 (75%) | 56±2 (84±3%) | 9±2 (13±3%) | 2±1 (3±2%) | 9 | 43 |
| All | All | 2010/2670 (75%) | 1687 (84%) | 266 (13%) | 57 (3%) | 9 | 43 |

5 of 13 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 20 | ARG | 22 |
| 1 | A | 35 | GLY | 10 |
| 1 | A | 38 | SER | 8 |
| 1 | A | 37 | ASP | 5 |
| 1 | A | 41 | GLY | 2 |

6.3.2 Protein sidechains [i](#)

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 | 59/74 (80%) | 57±1 (97±2%) | 2±1 (3±2%) | 46 | 89 |
| All | All | 1770/2220 (80%) | 1713 (97%) | 57 (3%) | 46 | 89 |

5 of 12 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 | A | 59 | ARG | 18 |
| 1 | A | 11 | LYS | 10 |
| 1 | A | 63 | GLN | 9 |
| 1 | A | 66 | LEU | 8 |
| 1 | A | 34 | LEU | 3 |

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 53% for the well-defined parts and 51% for the entire structure.

7.1 Chemical shift list 1

File name: 2png_nmr.cif

Chemical shift list name: *nef_chemical_shift_list_*

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 | 980 |
| Number of shifts mapped to atoms | 558 |
| Number of unparsed shifts | 156 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 266 |
| 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 156) occurrences are reported below.

| Shift ID | Chain | Res | Type | Atom | Shift Data | | |
|----------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 9 | A | 4 | GLU | HG% | 2.208 | 0.000 | 1 |
| 17 | A | 5 | ALA | HB% | 1.348 | 0.000 | 1 |
| 18 | A | 5 | ALA | HB% | 1.348 | 0.000 | 1 |
| 40 | A | 7 | ARG | HD% | 3.121 | 0.000 | 1 |
| 42 | A | 7 | ARG | HG% | 1.599 | 0.000 | 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 266) occurrences are reported below.

| Chain | Res | Type | Atom | Shift Data | | |
|-------|-----|------|------|------------|-------------|-----------|
| | | | | Value | Uncertainty | Ambiguity |
| A | 9 | LEU | HD1% | 0.577 | 0.0 | 1 |
| A | 13 | VAL | HG2% | 0.986 | 0.0 | 1 |

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| Chain | Res | Type | Atom | Shift Data | | |
|-------|-----|------|------|------------|-------------|-----------|
| | | | | Value | Uncertainty | Ambiguity |
| A | 60 | GLU | HBy | 1.915 | 0.0 | 2 |
| A | 86 | LYS | HG% | 1.457 | 0.0 | 1 |
| A | 16 | ILE | HG1y | 1.224 | 0.0 | 2 |

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 87 | -0.36 ± 0.08 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 80 | -0.10 ± 0.09 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 0 | — | None (insufficient data) |
| ^{15}N | 84 | -0.18 ± 0.37 | None needed (< 0.5 ppm) |

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 53%, i.e. 444 atoms were assigned a chemical shift out of a possible 844. 16 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone | 260/333 (78%) | 128/133 (96%) | 67/134 (50%) | 65/66 (98%) |
| Sidechain | 184/495 (37%) | 29/285 (10%) | 152/186 (82%) | 3/24 (12%) |
| Aromatic | 0/16 (0%) | 0/8 (0%) | 0/4 (0%) | 0/4 (0%) |
| Overall | 444/844 (53%) | 157/426 (37%) | 219/324 (68%) | 68/94 (72%) |

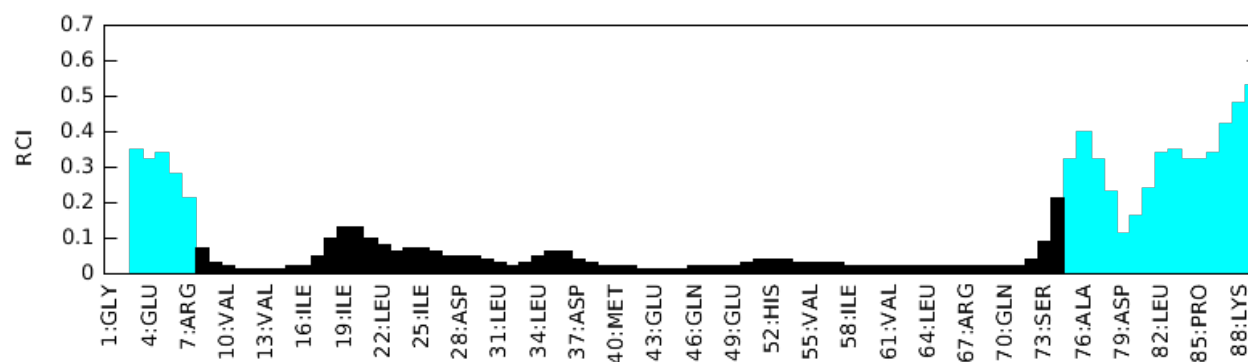
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *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:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

| Description | Value |
|---|-------|
| Total distance restraints | 1732 |
| Intra-residue ($ i-j =0$) | 697 |
| Sequential ($ i-j =1$) | 396 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 425 |
| Long range ($ i-j \geq 5$) | 214 |
| Inter-chain | 0 |
| Total dihedral-angle restraints | 0 |
| Total hydrogen bond restraints | 0 |
| Total disulfide bond restraints | 0 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 0.8 |
| Number of long range restraints per residue | 0.1 |

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

| Bins (Å) | Average number of violations per model | Max (Å) |
|------------------|--|---------|
| 0.1-0.2 (Small) | 8.8 | 0.2 |
| 0.2-0.5 (Medium) | 7.7 | 0.5 |
| >0.5 (Large) | 11.5 | 3.01 |

8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis

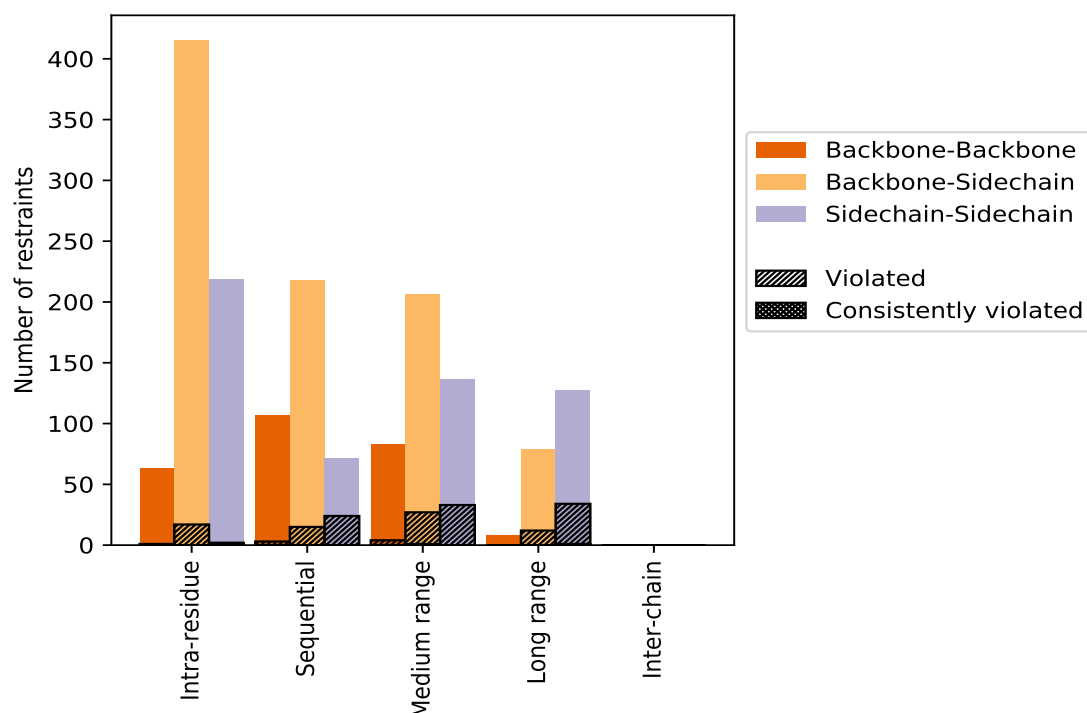
9.1 Summary of distance violations

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

| Restrains type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue ($i-j =0$) | 697 | 40.2 | 20 | 2.9 | 1.2 | 1 | 0.1 | 0.1 |
| Backbone-Backbone | 63 | 3.6 | 1 | 1.6 | 0.1 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 415 | 24.0 | 17 | 4.1 | 1.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 219 | 12.6 | 2 | 0.9 | 0.1 | 1 | 0.5 | 0.1 |
| Sequential ($i-j =1$) | 396 | 22.9 | 42 | 10.6 | 2.4 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 107 | 6.2 | 3 | 2.8 | 0.2 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 218 | 12.6 | 15 | 6.9 | 0.9 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 71 | 4.1 | 24 | 33.8 | 1.4 | 0 | 0.0 | 0.0 |
| Medium range ($i-j >1$ & $i-j <5$) | 425 | 24.5 | 64 | 15.1 | 3.7 | 1 | 0.2 | 0.1 |
| Backbone-Backbone | 83 | 4.8 | 4 | 4.8 | 0.2 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 206 | 11.9 | 27 | 13.1 | 1.6 | 1 | 0.5 | 0.1 |
| Sidechain-Sidechain | 136 | 7.9 | 33 | 24.3 | 1.9 | 0 | 0.0 | 0.0 |
| Long range ($i-j \geq 5$) | 214 | 12.4 | 46 | 21.5 | 2.7 | 1 | 0.5 | 0.1 |
| Backbone-Backbone | 8 | 0.5 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 79 | 4.6 | 12 | 15.2 | 0.7 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 127 | 7.3 | 34 | 26.8 | 2.0 | 1 | 0.8 | 0.1 |
| Inter-chain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 1732 | 100.0 | 172 | 9.9 | 9.9 | 3 | 0.2 | 0.2 |
| Backbone-Backbone | 261 | 15.1 | 8 | 3.1 | 0.5 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 918 | 53.0 | 71 | 7.7 | 4.1 | 1 | 0.1 | 0.1 |
| Sidechain-Sidechain | 553 | 31.9 | 93 | 16.8 | 5.4 | 2 | 0.4 | 0.1 |

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

9.2 Distance violation statistics for each model

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | |
| 1 | 2 | 7 | 12 | 8 | 0 | 29 | 0.6 | 1.58 | 0.41 |
| 2 | 2 | 5 | 15 | 6 | 0 | 28 | 0.71 | 3.01 | 0.64 |
| 3 | 3 | 6 | 10 | 12 | 0 | 31 | 0.5 | 1.56 | 0.41 |
| 4 | 1 | 2 | 4 | 7 | 0 | 14 | 0.49 | 1.72 | 0.52 |
| 5 | 4 | 4 | 11 | 13 | 0 | 32 | 0.52 | 1.62 | 0.36 |
| 6 | 3 | 1 | 12 | 9 | 0 | 25 | 0.43 | 1.56 | 0.41 |
| 7 | 3 | 5 | 10 | 11 | 0 | 29 | 0.4 | 1.39 | 0.33 |
| 8 | 4 | 7 | 9 | 5 | 0 | 25 | 0.47 | 1.62 | 0.38 |
| 9 | 2 | 4 | 6 | 6 | 0 | 18 | 0.41 | 1.64 | 0.46 |
| 10 | 2 | 1 | 9 | 4 | 0 | 16 | 0.58 | 1.51 | 0.43 |
| 11 | 2 | 3 | 9 | 9 | 0 | 23 | 0.52 | 1.62 | 0.35 |
| 12 | 4 | 6 | 9 | 7 | 0 | 26 | 0.4 | 1.52 | 0.34 |

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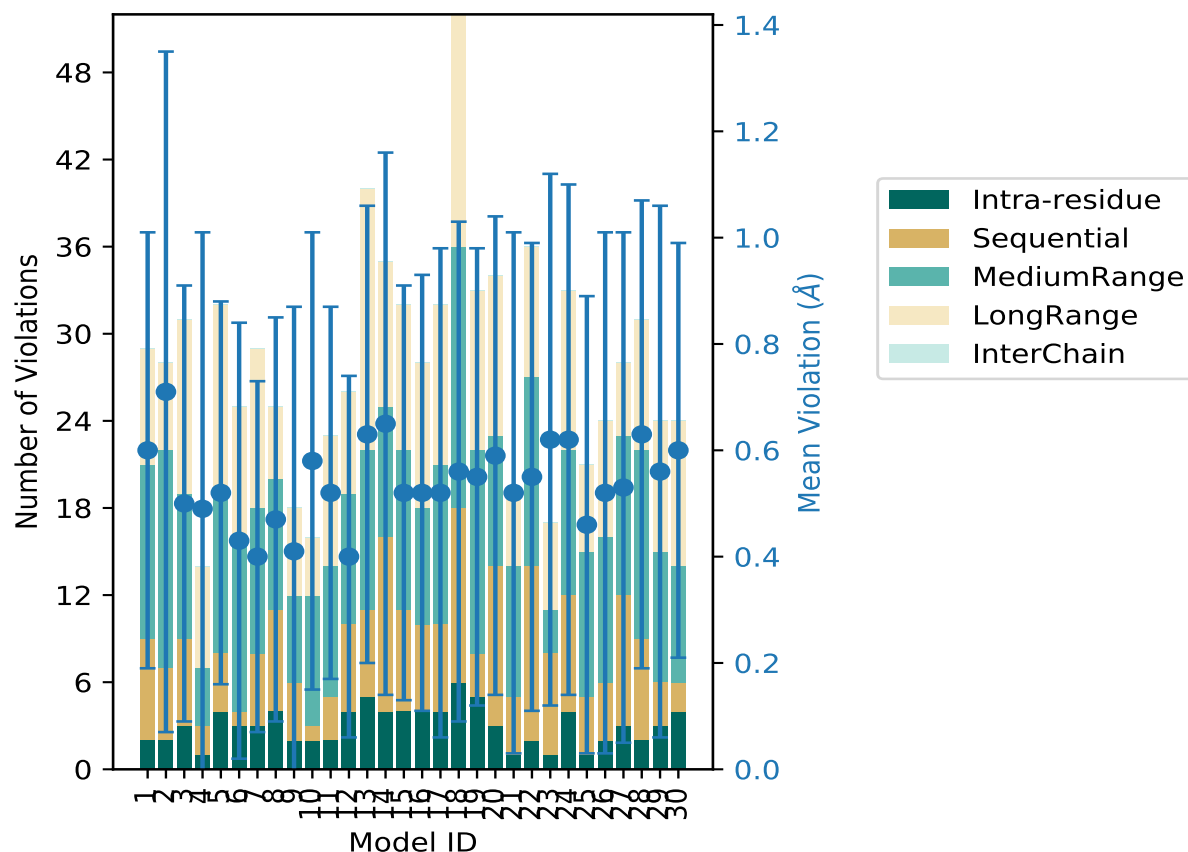
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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | |
| 13 | 5 | 6 | 11 | 18 | 0 | 40 | 0.63 | 1.87 | 0.43 |
| 14 | 4 | 12 | 9 | 10 | 0 | 35 | 0.65 | 2.01 | 0.51 |
| 15 | 4 | 7 | 11 | 10 | 0 | 32 | 0.52 | 1.65 | 0.39 |
| 16 | 4 | 6 | 8 | 10 | 0 | 28 | 0.52 | 1.66 | 0.41 |
| 17 | 4 | 6 | 11 | 11 | 0 | 32 | 0.52 | 1.89 | 0.46 |
| 18 | 6 | 12 | 18 | 16 | 0 | 52 | 0.56 | 1.88 | 0.47 |
| 19 | 5 | 3 | 14 | 11 | 0 | 33 | 0.55 | 1.72 | 0.43 |
| 20 | 3 | 11 | 9 | 11 | 0 | 34 | 0.59 | 1.51 | 0.45 |
| 21 | 1 | 4 | 9 | 5 | 0 | 19 | 0.52 | 1.82 | 0.49 |
| 22 | 2 | 12 | 13 | 9 | 0 | 36 | 0.55 | 1.67 | 0.44 |
| 23 | 1 | 7 | 3 | 6 | 0 | 17 | 0.62 | 1.71 | 0.5 |
| 24 | 4 | 8 | 10 | 11 | 0 | 33 | 0.62 | 2.1 | 0.48 |
| 25 | 1 | 4 | 10 | 6 | 0 | 21 | 0.46 | 1.59 | 0.43 |
| 26 | 2 | 4 | 10 | 8 | 0 | 24 | 0.52 | 1.96 | 0.49 |
| 27 | 3 | 9 | 11 | 5 | 0 | 28 | 0.53 | 1.98 | 0.48 |
| 28 | 2 | 7 | 13 | 9 | 0 | 31 | 0.63 | 1.72 | 0.44 |
| 29 | 3 | 3 | 9 | 9 | 0 | 24 | 0.56 | 1.72 | 0.5 |
| 30 | 4 | 2 | 8 | 10 | 0 | 24 | 0.6 | 1.57 | 0.39 |

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model



The mean and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1560(IR:677, SQ:354, MR:361, LR:168, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 7 | 14 | 25 | 12 | 0 | 58 | 1 | 3.3 |
| 4 | 7 | 9 | 6 | 0 | 26 | 2 | 6.7 |
| 3 | 7 | 7 | 5 | 0 | 22 | 3 | 10.0 |
| 0 | 5 | 2 | 3 | 0 | 10 | 4 | 13.3 |
| 1 | 0 | 4 | 0 | 0 | 5 | 5 | 16.7 |
| 2 | 1 | 0 | 6 | 0 | 9 | 6 | 20.0 |
| 1 | 1 | 2 | 1 | 0 | 5 | 7 | 23.3 |
| 0 | 1 | 4 | 1 | 0 | 6 | 8 | 26.7 |

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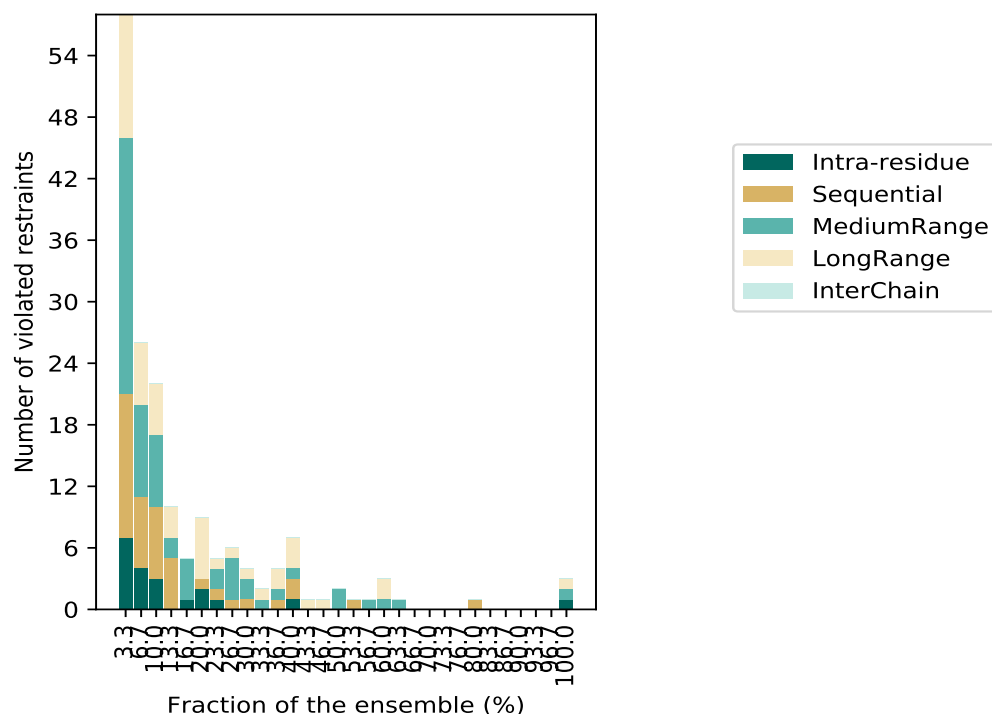
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| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 0 | 1 | 2 | 1 | 0 | 4 | 9 | 30.0 |
| 0 | 0 | 1 | 1 | 0 | 2 | 10 | 33.3 |
| 0 | 1 | 1 | 2 | 0 | 4 | 11 | 36.7 |
| 1 | 2 | 1 | 3 | 0 | 7 | 12 | 40.0 |
| 0 | 0 | 0 | 1 | 0 | 1 | 13 | 43.3 |
| 0 | 0 | 0 | 1 | 0 | 1 | 14 | 46.7 |
| 0 | 0 | 2 | 0 | 0 | 2 | 15 | 50.0 |
| 0 | 1 | 0 | 0 | 0 | 1 | 16 | 53.3 |
| 0 | 0 | 1 | 0 | 0 | 1 | 17 | 56.7 |
| 0 | 0 | 1 | 2 | 0 | 3 | 18 | 60.0 |
| 0 | 0 | 1 | 0 | 0 | 1 | 19 | 63.3 |
| 0 | 0 | 0 | 0 | 0 | 0 | 20 | 66.7 |
| 0 | 0 | 0 | 0 | 0 | 0 | 21 | 70.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 22 | 73.3 |
| 0 | 0 | 0 | 0 | 0 | 0 | 23 | 76.7 |
| 0 | 1 | 0 | 0 | 0 | 1 | 24 | 80.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 25 | 83.3 |
| 0 | 0 | 0 | 0 | 0 | 0 | 26 | 86.7 |
| 0 | 0 | 0 | 0 | 0 | 0 | 27 | 90.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 28 | 93.3 |
| 0 | 0 | 0 | 0 | 0 | 0 | 29 | 96.7 |
| 1 | 0 | 1 | 1 | 0 | 3 | 30 | 100.0 |

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

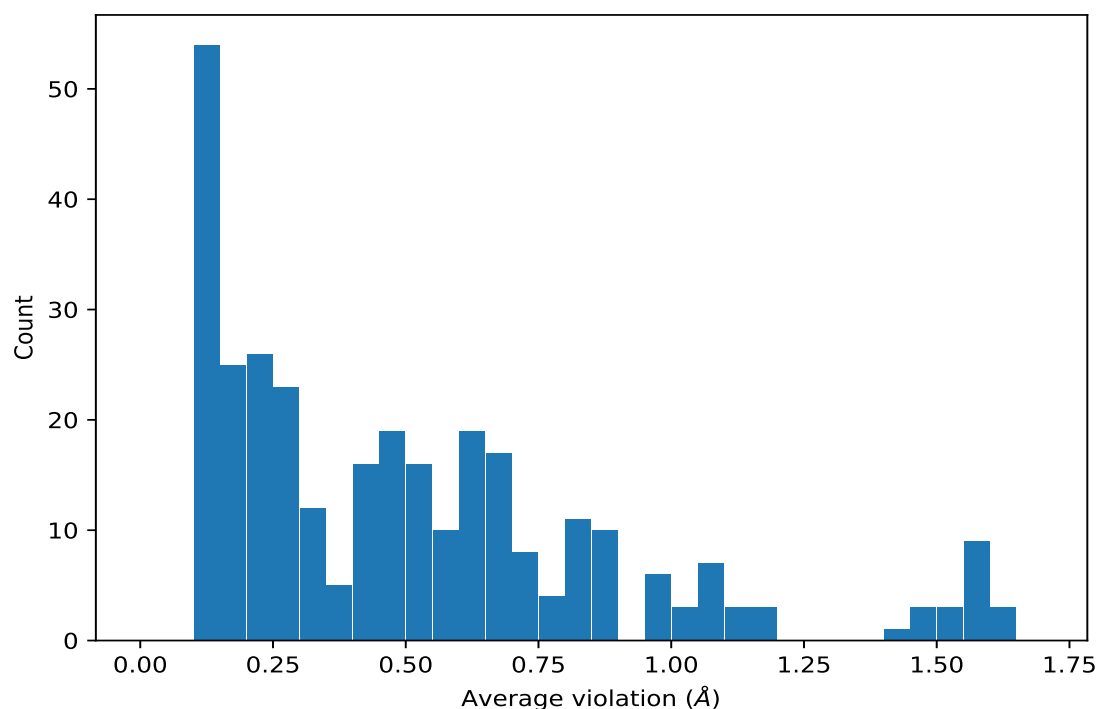
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of the absolute value of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 30 | 0.2 | 0.01 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 30 | 1.46 | 0.35 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 30 | 1.46 | 0.35 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 30 | 1.46 | 0.35 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 30 | 0.86 | 0.32 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 24 | 1.01 | 0.59 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 24 | 1.01 | 0.59 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 24 | 1.01 | 0.59 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 19 | 0.42 | 0.17 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 19 | 0.42 | 0.17 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 18 | 0.84 | 0.41 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 18 | 0.23 | 0.2 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 18 | 0.23 | 0.2 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 18 | 0.23 | 0.2 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 18 | 1.05 | 0.42 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 17 | 0.23 | 0.09 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 17 | 0.23 | 0.09 |
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 17 | 0.23 | 0.09 |
| (1,1248) | 1:A:61:VAL:HA | 1:A:62:ARG:HB3 | 16 | 0.56 | 0.05 |
| (1,813) | 1:A:65:THR:HG21 | 1:A:69:LEU:H | 15 | 0.14 | 0.02 |
| (1,813) | 1:A:65:THR:HG22 | 1:A:69:LEU:H | 15 | 0.14 | 0.02 |
| (1,813) | 1:A:65:THR:HG23 | 1:A:69:LEU:H | 15 | 0.14 | 0.02 |
| (1,1638) | 1:A:57:PRO:HB3 | 1:A:59:ARG:HB2 | 15 | 0.76 | 0.35 |
| (1,972) | 1:A:27:LEU:HD21 | 1:A:70:GLN:HE21 | 14 | 0.64 | 0.34 |
| (1,972) | 1:A:27:LEU:HD22 | 1:A:70:GLN:HE21 | 14 | 0.64 | 0.34 |
| (1,972) | 1:A:27:LEU:HD23 | 1:A:70:GLN:HE21 | 14 | 0.64 | 0.34 |
| (1,239) | 1:A:31:LEU:HD11 | 1:A:62:ARG:HG3 | 13 | 0.66 | 0.27 |
| (1,239) | 1:A:31:LEU:HD12 | 1:A:62:ARG:HG3 | 13 | 0.66 | 0.27 |
| (1,239) | 1:A:31:LEU:HD13 | 1:A:62:ARG:HG3 | 13 | 0.66 | 0.27 |
| (1,177) | 1:A:22:LEU:HD11 | 1:A:24:GLY:HA2 | 12 | 0.47 | 0.2 |
| (1,177) | 1:A:22:LEU:HD12 | 1:A:24:GLY:HA2 | 12 | 0.47 | 0.2 |
| (1,177) | 1:A:22:LEU:HD13 | 1:A:24:GLY:HA2 | 12 | 0.47 | 0.2 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD2 | 12 | 0.32 | 0.14 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD3 | 12 | 0.32 | 0.14 |
| (1,1554) | 1:A:34:LEU:HD21 | 1:A:26:ASN:HB3 | 12 | 1.07 | 0.58 |
| (1,1554) | 1:A:34:LEU:HD22 | 1:A:26:ASN:HB3 | 12 | 1.07 | 0.58 |
| (1,1554) | 1:A:34:LEU:HD23 | 1:A:26:ASN:HB3 | 12 | 1.07 | 0.58 |
| (1,1369) | 1:A:71:GLU:HG2 | 1:A:72:MET:H | 12 | 0.41 | 0.22 |
| (1,1302) | 1:A:64:LEU:HB3 | 1:A:31:LEU:HB3 | 12 | 0.69 | 0.28 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB1 | 12 | 0.16 | 0.04 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB2 | 12 | 0.16 | 0.04 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB3 | 12 | 0.16 | 0.04 |
| (1,1019) | 1:A:34:LEU:HD21 | 1:A:34:LEU:HA | 12 | 0.45 | 0.06 |
| (1,1019) | 1:A:34:LEU:HD22 | 1:A:34:LEU:HA | 12 | 0.45 | 0.06 |
| (1,1019) | 1:A:34:LEU:HD23 | 1:A:34:LEU:HA | 12 | 0.45 | 0.06 |
| (1,85) | 1:A:24:GLY:H | 1:A:23:ALA:HA | 11 | 0.14 | 0.03 |
| (1,85) | 1:A:24:GLY:H | 1:A:25:ILE:HA | 11 | 0.14 | 0.03 |
| (1,394) | 1:A:19:ILE:HG21 | 1:A:25:ILE:HG13 | 11 | 0.35 | 0.18 |
| (1,394) | 1:A:19:ILE:HG22 | 1:A:25:ILE:HG13 | 11 | 0.35 | 0.18 |
| (1,394) | 1:A:19:ILE:HG23 | 1:A:25:ILE:HG13 | 11 | 0.35 | 0.18 |
| (1,1593) | 1:A:34:LEU:HD21 | 1:A:29:SER:HA | 11 | 0.98 | 0.31 |
| (1,1593) | 1:A:34:LEU:HD22 | 1:A:29:SER:HA | 11 | 0.98 | 0.31 |
| (1,1593) | 1:A:34:LEU:HD23 | 1:A:29:SER:HA | 11 | 0.98 | 0.31 |
| (1,1491) | 1:A:42:VAL:HG21 | 1:A:46:GLN:HG2 | 11 | 0.33 | 0.13 |
| (1,1491) | 1:A:42:VAL:HG22 | 1:A:46:GLN:HG2 | 11 | 0.33 | 0.13 |
| (1,1491) | 1:A:42:VAL:HG23 | 1:A:46:GLN:HG2 | 11 | 0.33 | 0.13 |
| (1,1037) | 1:A:36:LEU:HB3 | 1:A:40:MET:HA | 10 | 0.13 | 0.03 |
| (1,1018) | 1:A:34:LEU:HD21 | 1:A:29:SER:HB2 | 10 | 0.25 | 0.06 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|
| (1,1018) | 1:A:34:LEU:HD22 | 1:A:29:SER:HB2 | 10 | 0.25 | 0.06 |
| (1,1018) | 1:A:34:LEU:HD23 | 1:A:29:SER:HB2 | 10 | 0.25 | 0.06 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD21 | 9 | 0.27 | 0.05 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD22 | 9 | 0.27 | 0.05 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD23 | 9 | 0.27 | 0.05 |
| (1,60) | 1:A:47:ILE:HG21 | 1:A:74:SER:HB2 | 9 | 0.58 | 0.22 |
| (1,60) | 1:A:47:ILE:HG22 | 1:A:74:SER:HB2 | 9 | 0.58 | 0.22 |
| (1,60) | 1:A:47:ILE:HG23 | 1:A:74:SER:HB2 | 9 | 0.58 | 0.22 |
| (1,60) | 1:A:58:ILE:HG21 | 1:A:31:LEU:HA | 9 | 0.58 | 0.22 |
| (1,60) | 1:A:58:ILE:HG22 | 1:A:31:LEU:HA | 9 | 0.58 | 0.22 |
| (1,60) | 1:A:58:ILE:HG23 | 1:A:31:LEU:HA | 9 | 0.58 | 0.22 |
| (1,444) | 1:A:47:ILE:HA | 1:A:50:ARG:HB3 | 9 | 1.4 | 0.22 |
| (1,1017) | 1:A:34:LEU:HD21 | 1:A:31:LEU:HA | 9 | 0.12 | 0.01 |
| (1,1017) | 1:A:34:LEU:HD22 | 1:A:31:LEU:HA | 9 | 0.12 | 0.01 |
| (1,1017) | 1:A:34:LEU:HD23 | 1:A:31:LEU:HA | 9 | 0.12 | 0.01 |
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB2 | 8 | 0.4 | 0.26 |
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB3 | 8 | 0.4 | 0.26 |
| (1,1642) | 1:A:9:LEU:HD11 | 1:A:6:GLN:HE21 | 8 | 0.65 | 0.32 |
| (1,1642) | 1:A:9:LEU:HD12 | 1:A:6:GLN:HE21 | 8 | 0.65 | 0.32 |
| (1,1642) | 1:A:9:LEU:HD13 | 1:A:6:GLN:HE21 | 8 | 0.65 | 0.32 |
| (1,1592) | 1:A:34:LEU:HD21 | 1:A:30:SER:H | 8 | 0.61 | 0.17 |
| (1,1592) | 1:A:34:LEU:HD22 | 1:A:30:SER:H | 8 | 0.61 | 0.17 |
| (1,1592) | 1:A:34:LEU:HD23 | 1:A:30:SER:H | 8 | 0.61 | 0.17 |
| (1,1584) | 1:A:59:ARG:HG3 | 1:A:58:ILE:H | 8 | 0.22 | 0.08 |
| (1,1484) | 1:A:14:ALA:HB1 | 1:A:19:ILE:HB | 8 | 0.13 | 0.01 |
| (1,1484) | 1:A:14:ALA:HB2 | 1:A:19:ILE:HB | 8 | 0.13 | 0.01 |
| (1,1484) | 1:A:14:ALA:HB3 | 1:A:19:ILE:HB | 8 | 0.13 | 0.01 |
| (1,1327) | 1:A:68:LYS:HD2 | 1:A:71:GLU:HB2 | 8 | 0.27 | 0.23 |
| (1,1327) | 1:A:68:LYS:HD3 | 1:A:71:GLU:HB2 | 8 | 0.27 | 0.23 |
| (1,244) | 1:A:31:LEU:HD21 | 1:A:64:LEU:HG | 7 | 0.84 | 0.02 |
| (1,244) | 1:A:31:LEU:HD22 | 1:A:64:LEU:HG | 7 | 0.84 | 0.02 |
| (1,244) | 1:A:31:LEU:HD23 | 1:A:64:LEU:HG | 7 | 0.84 | 0.02 |
| (1,240) | 1:A:31:LEU:HD11 | 1:A:34:LEU:HB2 | 7 | 0.52 | 0.15 |
| (1,240) | 1:A:31:LEU:HD12 | 1:A:34:LEU:HB2 | 7 | 0.52 | 0.15 |
| (1,240) | 1:A:31:LEU:HD13 | 1:A:34:LEU:HB2 | 7 | 0.52 | 0.15 |
| (1,233) | 1:A:31:LEU:HD11 | 1:A:31:LEU:HA | 7 | 0.75 | 0.03 |
| (1,233) | 1:A:31:LEU:HD12 | 1:A:31:LEU:HA | 7 | 0.75 | 0.03 |
| (1,233) | 1:A:31:LEU:HD13 | 1:A:31:LEU:HA | 7 | 0.75 | 0.03 |
| (1,1163) | 1:A:54:LEU:HD11 | 1:A:51:GLU:HB2 | 7 | 1.51 | 0.57 |
| (1,1163) | 1:A:54:LEU:HD12 | 1:A:51:GLU:HB2 | 7 | 1.51 | 0.57 |
| (1,1163) | 1:A:54:LEU:HD13 | 1:A:51:GLU:HB2 | 7 | 1.51 | 0.57 |
| (1,1028) | 1:A:34:LEU:HD21 | 1:A:33:ASP:H | 7 | 0.24 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|
| (1,1028) | 1:A:34:LEU:HD22 | 1:A:33:ASP:H | 7 | 0.24 | 0.11 |
| (1,1028) | 1:A:34:LEU:HD23 | 1:A:33:ASP:H | 7 | 0.24 | 0.11 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD11 | 6 | 0.85 | 0.12 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD12 | 6 | 0.85 | 0.12 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD13 | 6 | 0.85 | 0.12 |
| (1,779) | 1:A:52:HIS:HB2 | 1:A:6:GLN:HE21 | 6 | 0.67 | 0.36 |
| (1,719) | 1:A:63:GLN:HB2 | 1:A:63:GLN:HE21 | 6 | 0.81 | 0.04 |
| (1,704) | 1:A:59:ARG:HB2 | 1:A:59:ARG:H | 6 | 0.14 | 0.02 |
| (1,502) | 1:A:19:ILE:HD11 | 1:A:25:ILE:HG13 | 6 | 0.43 | 0.29 |
| (1,502) | 1:A:19:ILE:HD12 | 1:A:25:ILE:HG13 | 6 | 0.43 | 0.29 |
| (1,502) | 1:A:19:ILE:HD13 | 1:A:25:ILE:HG13 | 6 | 0.43 | 0.29 |
| (1,294) | 1:A:17:LEU:HD11 | 1:A:36:LEU:HB2 | 6 | 0.28 | 0.11 |
| (1,294) | 1:A:17:LEU:HD12 | 1:A:36:LEU:HB2 | 6 | 0.28 | 0.11 |
| (1,294) | 1:A:17:LEU:HD13 | 1:A:36:LEU:HB2 | 6 | 0.28 | 0.11 |
| (1,294) | 1:A:17:LEU:HD21 | 1:A:36:LEU:HB2 | 6 | 0.28 | 0.11 |
| (1,294) | 1:A:17:LEU:HD22 | 1:A:36:LEU:HB2 | 6 | 0.28 | 0.11 |
| (1,294) | 1:A:17:LEU:HD23 | 1:A:36:LEU:HB2 | 6 | 0.28 | 0.11 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD21 | 6 | 0.88 | 0.29 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD22 | 6 | 0.88 | 0.29 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD23 | 6 | 0.88 | 0.29 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD11 | 6 | 0.88 | 0.29 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD12 | 6 | 0.88 | 0.29 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD13 | 6 | 0.88 | 0.29 |
| (1,1303) | 1:A:64:LEU:HB2 | 1:A:31:LEU:HB3 | 6 | 0.35 | 0.11 |
| (1,1263) | 1:A:61:VAL:HG11 | 1:A:62:ARG:HB3 | 6 | 0.2 | 0.08 |
| (1,1263) | 1:A:61:VAL:HG12 | 1:A:62:ARG:HB3 | 6 | 0.2 | 0.08 |
| (1,1263) | 1:A:61:VAL:HG13 | 1:A:62:ARG:HB3 | 6 | 0.2 | 0.08 |
| (1,700) | 1:A:59:ARG:HA | 1:A:62:ARG:HD2 | 5 | 0.52 | 0.28 |
| (1,662) | 1:A:49:GLU:HA | 1:A:46:GLN:HA | 5 | 0.14 | 0.02 |
| (1,549) | 1:A:72:MET:HB2 | 1:A:72:MET:H | 5 | 0.2 | 0.06 |
| (1,499) | 1:A:47:ILE:HD11 | 1:A:43:GLU:HG2 | 5 | 0.6 | 0.12 |
| (1,499) | 1:A:47:ILE:HD12 | 1:A:43:GLU:HG2 | 5 | 0.6 | 0.12 |
| (1,499) | 1:A:47:ILE:HD13 | 1:A:43:GLU:HG2 | 5 | 0.6 | 0.12 |
| (1,18) | 1:A:71:GLU:HA | 1:A:74:SER:H | 5 | 0.14 | 0.03 |
| (1,18) | 1:A:71:GLU:HA | 1:A:69:LEU:H | 5 | 0.14 | 0.03 |
| (1,798) | 1:A:51:GLU:HG2 | 1:A:50:ARG:HG2 | 4 | 0.42 | 0.11 |
| (1,798) | 1:A:51:GLU:HG3 | 1:A:50:ARG:HG2 | 4 | 0.42 | 0.11 |
| (1,787) | 1:A:51:GLU:HB3 | 1:A:6:GLN:HE21 | 4 | 0.31 | 0.06 |
| (1,668) | 1:A:49:GLU:HG2 | 1:A:46:GLN:HA | 4 | 0.37 | 0.2 |
| (1,412) | 1:A:45:ARG:HD2 | 1:A:58:ILE:HA | 4 | 0.71 | 0.05 |
| (1,412) | 1:A:45:ARG:HD3 | 1:A:58:ILE:HA | 4 | 0.71 | 0.05 |
| (1,316) | 1:A:40:MET:HB2 | 1:A:39:LEU:HD21 | 4 | 0.42 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|
| (1,316) | 1:A:40:MET:HB2 | 1:A:39:LEU:HD22 | 4 | 0.42 | 0.16 |
| (1,316) | 1:A:40:MET:HB2 | 1:A:39:LEU:HD23 | 4 | 0.42 | 0.16 |
| (1,315) | 1:A:40:MET:HB3 | 1:A:39:LEU:HD21 | 4 | 0.74 | 0.26 |
| (1,315) | 1:A:40:MET:HB3 | 1:A:39:LEU:HD22 | 4 | 0.74 | 0.26 |
| (1,315) | 1:A:40:MET:HB3 | 1:A:39:LEU:HD23 | 4 | 0.74 | 0.26 |
| (1,1555) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB3 | 4 | 1.06 | 0.36 |
| (1,1555) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB3 | 4 | 1.06 | 0.36 |
| (1,1555) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB3 | 4 | 1.06 | 0.36 |
| (1,1548) | 1:A:19:ILE:HG21 | 1:A:21:ASP:HB2 | 4 | 0.26 | 0.08 |
| (1,1548) | 1:A:19:ILE:HG22 | 1:A:21:ASP:HB2 | 4 | 0.26 | 0.08 |
| (1,1548) | 1:A:19:ILE:HG23 | 1:A:21:ASP:HB2 | 4 | 0.26 | 0.08 |
| (1,111) | 1:A:55:VAL:HG21 | 1:A:49:GLU:HG3 | 4 | 0.65 | 0.25 |
| (1,111) | 1:A:55:VAL:HG22 | 1:A:49:GLU:HG3 | 4 | 0.65 | 0.25 |
| (1,111) | 1:A:55:VAL:HG23 | 1:A:49:GLU:HG3 | 4 | 0.65 | 0.25 |
| (1,1099) | 1:A:40:MET:HG3 | 1:A:39:LEU:HD21 | 4 | 0.67 | 0.32 |
| (1,1099) | 1:A:40:MET:HG3 | 1:A:39:LEU:HD22 | 4 | 0.67 | 0.32 |
| (1,1099) | 1:A:40:MET:HG3 | 1:A:39:LEU:HD23 | 4 | 0.67 | 0.32 |
| (1,900) | 1:A:47:ILE:HG21 | 1:A:48:LEU:HD11 | 3 | 1.59 | 0.18 |
| (1,900) | 1:A:47:ILE:HG21 | 1:A:48:LEU:HD12 | 3 | 1.59 | 0.18 |
| (1,900) | 1:A:47:ILE:HG21 | 1:A:48:LEU:HD13 | 3 | 1.59 | 0.18 |
| (1,900) | 1:A:47:ILE:HG22 | 1:A:48:LEU:HD11 | 3 | 1.59 | 0.18 |
| (1,900) | 1:A:47:ILE:HG22 | 1:A:48:LEU:HD12 | 3 | 1.59 | 0.18 |
| (1,900) | 1:A:47:ILE:HG22 | 1:A:48:LEU:HD13 | 3 | 1.59 | 0.18 |
| (1,900) | 1:A:47:ILE:HG23 | 1:A:48:LEU:HD11 | 3 | 1.59 | 0.18 |
| (1,900) | 1:A:47:ILE:HG23 | 1:A:48:LEU:HD12 | 3 | 1.59 | 0.18 |
| (1,900) | 1:A:47:ILE:HG23 | 1:A:48:LEU:HD13 | 3 | 1.59 | 0.18 |
| (1,72) | 1:A:48:LEU:HD11 | 1:A:6:GLN:HE21 | 3 | 0.54 | 0.38 |
| (1,72) | 1:A:48:LEU:HD12 | 1:A:6:GLN:HE21 | 3 | 0.54 | 0.38 |
| (1,72) | 1:A:48:LEU:HD13 | 1:A:6:GLN:HE21 | 3 | 0.54 | 0.38 |
| (1,72) | 1:A:9:LEU:HD21 | 1:A:6:GLN:HE21 | 3 | 0.54 | 0.38 |
| (1,72) | 1:A:9:LEU:HD22 | 1:A:6:GLN:HE21 | 3 | 0.54 | 0.38 |
| (1,72) | 1:A:9:LEU:HD23 | 1:A:6:GLN:HE21 | 3 | 0.54 | 0.38 |
| (1,593) | 1:A:66:LEU:HD11 | 1:A:66:LEU:HA | 3 | 0.42 | 0.02 |
| (1,593) | 1:A:66:LEU:HD12 | 1:A:66:LEU:HA | 3 | 0.42 | 0.02 |
| (1,593) | 1:A:66:LEU:HD13 | 1:A:66:LEU:HA | 3 | 0.42 | 0.02 |
| (1,54) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HD3 | 3 | 0.22 | 0.07 |
| (1,54) | 1:A:20:ARG:HG3 | 1:A:10:VAL:HA | 3 | 0.22 | 0.07 |
| (1,54) | 1:A:7:ARG:HG2 | 1:A:10:VAL:HA | 3 | 0.22 | 0.07 |
| (1,54) | 1:A:7:ARG:HG3 | 1:A:10:VAL:HA | 3 | 0.22 | 0.07 |
| (1,468) | 1:A:47:ILE:HA | 1:A:48:LEU:HD11 | 3 | 0.47 | 0.12 |
| (1,468) | 1:A:47:ILE:HA | 1:A:48:LEU:HD12 | 3 | 0.47 | 0.12 |
| (1,468) | 1:A:47:ILE:HA | 1:A:48:LEU:HD13 | 3 | 0.47 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|
| (1,461) | 1:A:47:ILE:HG12 | 1:A:48:LEU:HD11 | 3 | 1.13 | 0.12 |
| (1,461) | 1:A:47:ILE:HG12 | 1:A:48:LEU:HD12 | 3 | 1.13 | 0.12 |
| (1,461) | 1:A:47:ILE:HG12 | 1:A:48:LEU:HD13 | 3 | 1.13 | 0.12 |
| (1,460) | 1:A:47:ILE:HG13 | 1:A:48:LEU:HD11 | 3 | 0.3 | 0.09 |
| (1,460) | 1:A:47:ILE:HG13 | 1:A:48:LEU:HD12 | 3 | 0.3 | 0.09 |
| (1,460) | 1:A:47:ILE:HG13 | 1:A:48:LEU:HD13 | 3 | 0.3 | 0.09 |
| (1,38) | 1:A:58:ILE:HG21 | 1:A:32:ALA:HA | 3 | 0.15 | 0.02 |
| (1,38) | 1:A:58:ILE:HG22 | 1:A:32:ALA:HA | 3 | 0.15 | 0.02 |
| (1,38) | 1:A:58:ILE:HG23 | 1:A:32:ALA:HA | 3 | 0.15 | 0.02 |
| (1,38) | 1:A:47:ILE:HG21 | 1:A:50:ARG:HA | 3 | 0.15 | 0.02 |
| (1,38) | 1:A:47:ILE:HG22 | 1:A:50:ARG:HA | 3 | 0.15 | 0.02 |
| (1,38) | 1:A:47:ILE:HG23 | 1:A:50:ARG:HA | 3 | 0.15 | 0.02 |
| (1,192) | 1:A:29:SER:HB3 | 1:A:34:LEU:HD21 | 3 | 0.15 | 0.03 |
| (1,192) | 1:A:29:SER:HB3 | 1:A:34:LEU:HD22 | 3 | 0.15 | 0.03 |
| (1,192) | 1:A:29:SER:HB3 | 1:A:34:LEU:HD23 | 3 | 0.15 | 0.03 |
| (1,1698) | 1:A:38:SER:H | 1:A:39:LEU:H | 3 | 0.19 | 0.04 |
| (1,1576) | 1:A:66:LEU:HD11 | 1:A:65:THR:HA | 3 | 0.25 | 0.16 |
| (1,1576) | 1:A:66:LEU:HD12 | 1:A:65:THR:HA | 3 | 0.25 | 0.16 |
| (1,1576) | 1:A:66:LEU:HD13 | 1:A:65:THR:HA | 3 | 0.25 | 0.16 |
| (1,1575) | 1:A:66:LEU:HD11 | 1:A:13:VAL:H | 3 | 0.67 | 0.45 |
| (1,1575) | 1:A:66:LEU:HD12 | 1:A:13:VAL:H | 3 | 0.67 | 0.45 |
| (1,1575) | 1:A:66:LEU:HD13 | 1:A:13:VAL:H | 3 | 0.67 | 0.45 |
| (1,1545) | 1:A:44:VAL:HG21 | 1:A:45:ARG:HE | 3 | 0.11 | 0.0 |
| (1,1545) | 1:A:44:VAL:HG22 | 1:A:45:ARG:HE | 3 | 0.11 | 0.0 |
| (1,1545) | 1:A:44:VAL:HG23 | 1:A:45:ARG:HE | 3 | 0.11 | 0.0 |
| (1,1168) | 1:A:54:LEU:HG | 1:A:56:LEU:HD21 | 3 | 0.46 | 0.45 |
| (1,1168) | 1:A:54:LEU:HG | 1:A:56:LEU:HD22 | 3 | 0.46 | 0.45 |
| (1,1168) | 1:A:54:LEU:HG | 1:A:56:LEU:HD23 | 3 | 0.46 | 0.45 |
| (1,1126) | 1:A:48:LEU:HD11 | 1:A:52:HIS:H | 3 | 0.58 | 0.21 |
| (1,1126) | 1:A:48:LEU:HD12 | 1:A:52:HIS:H | 3 | 0.58 | 0.21 |
| (1,1126) | 1:A:48:LEU:HD13 | 1:A:52:HIS:H | 3 | 0.58 | 0.21 |
| (1,1123) | 1:A:48:LEU:HD11 | 1:A:52:HIS:HB2 | 3 | 1.63 | 1.06 |
| (1,1123) | 1:A:48:LEU:HD12 | 1:A:52:HIS:HB2 | 3 | 1.63 | 1.06 |
| (1,1123) | 1:A:48:LEU:HD13 | 1:A:52:HIS:HB2 | 3 | 1.63 | 1.06 |
| (1,1122) | 1:A:48:LEU:HD11 | 1:A:52:HIS:HB3 | 3 | 1.18 | 0.39 |
| (1,1122) | 1:A:48:LEU:HD12 | 1:A:52:HIS:HB3 | 3 | 1.18 | 0.39 |
| (1,1122) | 1:A:48:LEU:HD13 | 1:A:52:HIS:HB3 | 3 | 1.18 | 0.39 |
| (1,1117) | 1:A:48:LEU:HA | 1:A:48:LEU:HD11 | 3 | 0.83 | 0.0 |
| (1,1117) | 1:A:48:LEU:HA | 1:A:48:LEU:HD12 | 3 | 0.83 | 0.0 |
| (1,1117) | 1:A:48:LEU:HA | 1:A:48:LEU:HD13 | 3 | 0.83 | 0.0 |
| (1,1107) | 1:A:48:LEU:HA | 1:A:52:HIS:HB2 | 3 | 0.48 | 0.32 |
| (1,1091) | 1:A:39:LEU:HD11 | 1:A:39:LEU:HA | 3 | 0.18 | 0.06 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|
| (1,1091) | 1:A:39:LEU:HD12 | 1:A:39:LEU:HA | 3 | 0.18 | 0.06 |
| (1,1091) | 1:A:39:LEU:HD13 | 1:A:39:LEU:HA | 3 | 0.18 | 0.06 |
| (1,1012) | 1:A:34:LEU:HD11 | 1:A:31:LEU:H | 3 | 0.54 | 0.31 |
| (1,1012) | 1:A:34:LEU:HD12 | 1:A:31:LEU:H | 3 | 0.54 | 0.31 |
| (1,1012) | 1:A:34:LEU:HD13 | 1:A:31:LEU:H | 3 | 0.54 | 0.31 |
| (1,1008) | 1:A:34:LEU:HD11 | 1:A:31:LEU:HA | 3 | 0.34 | 0.1 |
| (1,1008) | 1:A:34:LEU:HD12 | 1:A:31:LEU:HA | 3 | 0.34 | 0.1 |
| (1,1008) | 1:A:34:LEU:HD13 | 1:A:31:LEU:HA | 3 | 0.34 | 0.1 |
| (1,928) | 1:A:57:PRO:HG2 | 1:A:56:LEU:HD21 | 2 | 0.96 | 0.02 |
| (1,928) | 1:A:57:PRO:HG2 | 1:A:56:LEU:HD22 | 2 | 0.96 | 0.02 |
| (1,928) | 1:A:57:PRO:HG2 | 1:A:56:LEU:HD23 | 2 | 0.96 | 0.02 |
| (1,927) | 1:A:57:PRO:HG3 | 1:A:56:LEU:HD21 | 2 | 0.49 | 0.29 |
| (1,927) | 1:A:57:PRO:HG3 | 1:A:56:LEU:HD22 | 2 | 0.49 | 0.29 |
| (1,927) | 1:A:57:PRO:HG3 | 1:A:56:LEU:HD23 | 2 | 0.49 | 0.29 |
| (1,9) | 1:A:16:ILE:HG21 | 1:A:43:GLU:H | 2 | 0.12 | 0.01 |
| (1,9) | 1:A:16:ILE:HG22 | 1:A:43:GLU:H | 2 | 0.12 | 0.01 |
| (1,9) | 1:A:16:ILE:HG23 | 1:A:43:GLU:H | 2 | 0.12 | 0.01 |
| (1,9) | 1:A:16:ILE:HG21 | 1:A:42:VAL:H | 2 | 0.12 | 0.01 |
| (1,9) | 1:A:16:ILE:HG22 | 1:A:42:VAL:H | 2 | 0.12 | 0.01 |
| (1,9) | 1:A:16:ILE:HG23 | 1:A:42:VAL:H | 2 | 0.12 | 0.01 |
| (1,9) | 1:A:47:ILE:HG21 | 1:A:50:ARG:HE | 2 | 0.12 | 0.01 |
| (1,9) | 1:A:47:ILE:HG22 | 1:A:50:ARG:HE | 2 | 0.12 | 0.01 |
| (1,9) | 1:A:47:ILE:HG23 | 1:A:50:ARG:HE | 2 | 0.12 | 0.01 |
| (1,896) | 1:A:47:ILE:HG21 | 1:A:6:GLN:HE21 | 2 | 0.25 | 0.14 |
| (1,896) | 1:A:47:ILE:HG22 | 1:A:6:GLN:HE21 | 2 | 0.25 | 0.14 |
| (1,896) | 1:A:47:ILE:HG23 | 1:A:6:GLN:HE21 | 2 | 0.25 | 0.14 |
| (1,862) | 1:A:10:VAL:HA | 1:A:9:LEU:HD21 | 2 | 0.14 | 0.03 |
| (1,862) | 1:A:10:VAL:HA | 1:A:9:LEU:HD22 | 2 | 0.14 | 0.03 |
| (1,862) | 1:A:10:VAL:HA | 1:A:9:LEU:HD23 | 2 | 0.14 | 0.03 |
| (1,851) | 1:A:9:LEU:HA | 1:A:9:LEU:HD21 | 2 | 0.16 | 0.01 |
| (1,851) | 1:A:9:LEU:HA | 1:A:9:LEU:HD22 | 2 | 0.16 | 0.01 |
| (1,851) | 1:A:9:LEU:HA | 1:A:9:LEU:HD23 | 2 | 0.16 | 0.01 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD11 | 2 | 0.13 | 0.02 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD12 | 2 | 0.13 | 0.02 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD13 | 2 | 0.13 | 0.02 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD21 | 2 | 0.13 | 0.02 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD22 | 2 | 0.13 | 0.02 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD23 | 2 | 0.13 | 0.02 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:54:LEU:HD21 | 2 | 0.13 | 0.02 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:54:LEU:HD22 | 2 | 0.13 | 0.02 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:54:LEU:HD23 | 2 | 0.13 | 0.02 |
| (1,664) | 1:A:49:GLU:HG2 | 1:A:55:VAL:HG21 | 2 | 0.22 | 0.02 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|
| (1,664) | 1:A:49:GLU:HG2 | 1:A:55:VAL:HG22 | 2 | 0.22 | 0.02 |
| (1,664) | 1:A:49:GLU:HG2 | 1:A:55:VAL:HG23 | 2 | 0.22 | 0.02 |
| (1,469) | 1:A:17:LEU:HD11 | 1:A:16:ILE:H | 2 | 0.21 | 0.08 |
| (1,469) | 1:A:17:LEU:HD12 | 1:A:16:ILE:H | 2 | 0.21 | 0.08 |
| (1,469) | 1:A:17:LEU:HD13 | 1:A:16:ILE:H | 2 | 0.21 | 0.08 |
| (1,391) | 1:A:19:ILE:HG21 | 1:A:21:ASP:HA | 2 | 0.11 | 0.0 |
| (1,391) | 1:A:19:ILE:HG22 | 1:A:21:ASP:HA | 2 | 0.11 | 0.0 |
| (1,391) | 1:A:19:ILE:HG23 | 1:A:21:ASP:HA | 2 | 0.11 | 0.0 |
| (1,296) | 1:A:17:LEU:HD11 | 1:A:19:ILE:HG13 | 2 | 0.5 | 0.08 |
| (1,296) | 1:A:17:LEU:HD12 | 1:A:19:ILE:HG13 | 2 | 0.5 | 0.08 |
| (1,296) | 1:A:17:LEU:HD13 | 1:A:19:ILE:HG13 | 2 | 0.5 | 0.08 |
| (1,291) | 1:A:17:LEU:HG | 1:A:17:LEU:H | 2 | 0.12 | 0.01 |
| (1,236) | 1:A:31:LEU:HD11 | 1:A:66:LEU:H | 2 | 0.64 | 0.33 |
| (1,236) | 1:A:31:LEU:HD12 | 1:A:66:LEU:H | 2 | 0.64 | 0.33 |
| (1,236) | 1:A:31:LEU:HD13 | 1:A:66:LEU:H | 2 | 0.64 | 0.33 |
| (1,213) | 1:A:30:SER:HB3 | 1:A:33:ASP:HA | 2 | 0.12 | 0.01 |
| (1,1727) | 1:A:86:LYS:H | 1:A:85:PRO:HA | 2 | 0.14 | 0.01 |
| (1,171) | 1:A:22:LEU:HG | 1:A:21:ASP:HA | 2 | 0.14 | 0.03 |
| (1,1569) | 1:A:10:VAL:HG21 | 1:A:70:GLN:HB2 | 2 | 0.14 | 0.01 |
| (1,1569) | 1:A:10:VAL:HG21 | 1:A:70:GLN:HB3 | 2 | 0.14 | 0.01 |
| (1,1569) | 1:A:10:VAL:HG22 | 1:A:70:GLN:HB2 | 2 | 0.14 | 0.01 |
| (1,1569) | 1:A:10:VAL:HG22 | 1:A:70:GLN:HB3 | 2 | 0.14 | 0.01 |
| (1,1569) | 1:A:10:VAL:HG23 | 1:A:70:GLN:HB2 | 2 | 0.14 | 0.01 |
| (1,1569) | 1:A:10:VAL:HG23 | 1:A:70:GLN:HB3 | 2 | 0.14 | 0.01 |
| (1,1523) | 1:A:73:SER:HA | 1:A:70:GLN:H | 2 | 0.11 | 0.0 |
| (1,1509) | 1:A:72:MET:HG2 | 1:A:9:LEU:HD11 | 2 | 0.84 | 0.18 |
| (1,1509) | 1:A:72:MET:HG2 | 1:A:9:LEU:HD12 | 2 | 0.84 | 0.18 |
| (1,1509) | 1:A:72:MET:HG2 | 1:A:9:LEU:HD13 | 2 | 0.84 | 0.18 |
| (1,1505) | 1:A:55:VAL:HG11 | 1:A:59:ARG:HD2 | 2 | 0.61 | 0.5 |
| (1,1505) | 1:A:55:VAL:HG11 | 1:A:59:ARG:HD3 | 2 | 0.61 | 0.5 |
| (1,1505) | 1:A:55:VAL:HG12 | 1:A:59:ARG:HD2 | 2 | 0.61 | 0.5 |
| (1,1505) | 1:A:55:VAL:HG12 | 1:A:59:ARG:HD3 | 2 | 0.61 | 0.5 |
| (1,1505) | 1:A:55:VAL:HG13 | 1:A:59:ARG:HD2 | 2 | 0.61 | 0.5 |
| (1,1505) | 1:A:55:VAL:HG13 | 1:A:59:ARG:HD3 | 2 | 0.61 | 0.5 |
| (1,1415) | 1:A:42:VAL:HG11 | 1:A:46:GLN:HE21 | 2 | 0.18 | 0.02 |
| (1,1415) | 1:A:42:VAL:HG12 | 1:A:46:GLN:HE21 | 2 | 0.18 | 0.02 |
| (1,1415) | 1:A:42:VAL:HG13 | 1:A:46:GLN:HE21 | 2 | 0.18 | 0.02 |
| (1,1239) | 1:A:60:GLU:HB3 | 1:A:56:LEU:HB2 | 2 | 0.61 | 0.06 |
| (1,1196) | 1:A:56:LEU:HD21 | 1:A:56:LEU:HA | 2 | 0.72 | 0.22 |
| (1,1196) | 1:A:56:LEU:HD22 | 1:A:56:LEU:HA | 2 | 0.72 | 0.22 |
| (1,1196) | 1:A:56:LEU:HD23 | 1:A:56:LEU:HA | 2 | 0.72 | 0.22 |
| (1,1133) | 1:A:53:ASP:HA | 1:A:53:ASP:H | 2 | 0.2 | 0.03 |

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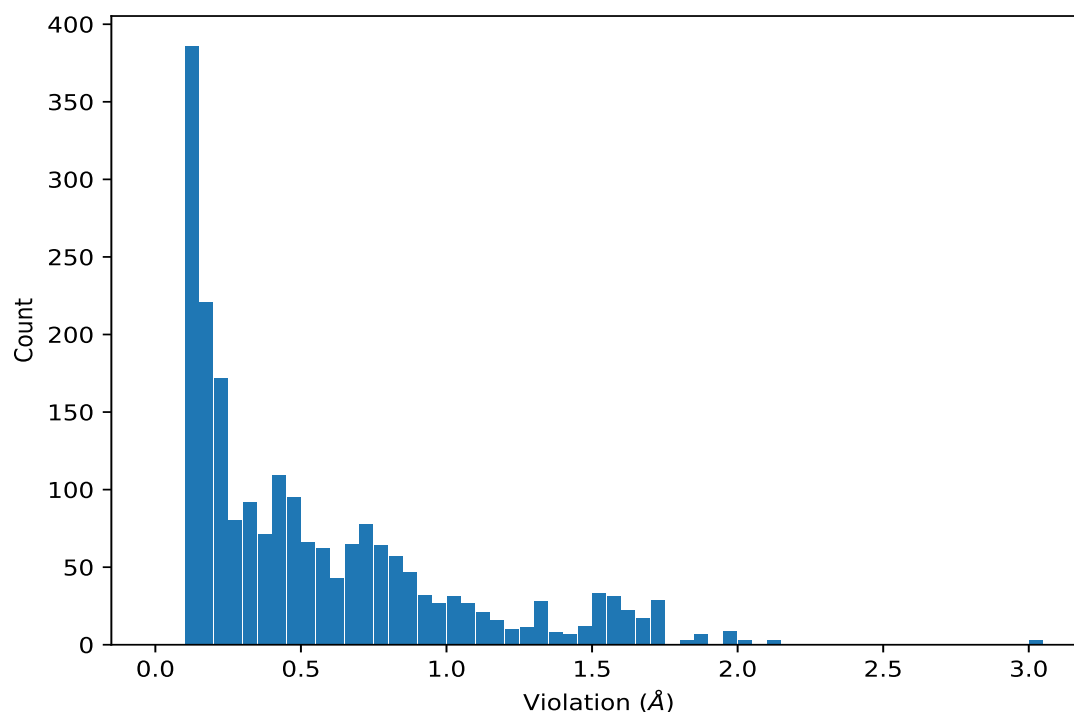
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|
| (1,1100) | 1:A:40:MET:HG2 | 1:A:39:LEU:HD21 | 2 | 0.49 | 0.07 |
| (1,1100) | 1:A:40:MET:HG2 | 1:A:39:LEU:HD22 | 2 | 0.49 | 0.07 |
| (1,1100) | 1:A:40:MET:HG2 | 1:A:39:LEU:HD23 | 2 | 0.49 | 0.07 |
| (1,1061) | 1:A:36:LEU:HD21 | 1:A:38:SER:H | 2 | 0.15 | 0.0 |
| (1,1061) | 1:A:36:LEU:HD22 | 1:A:38:SER:H | 2 | 0.15 | 0.0 |
| (1,1061) | 1:A:36:LEU:HD23 | 1:A:38:SER:H | 2 | 0.15 | 0.0 |

¹Number of violated models, ²Standard deviation

9.5 All distance violations

9.5.1 Histogram : Distribution of distance violations

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1123) | 1:A:48:LEU:HD11 | 1:A:52:HIS:HB2 | 2 | 3.01 |
| (1,1123) | 1:A:48:LEU:HD12 | 1:A:52:HIS:HB2 | 2 | 3.01 |
| (1,1123) | 1:A:48:LEU:HD13 | 1:A:52:HIS:HB2 | 2 | 3.01 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 24 | 2.1 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 24 | 2.1 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 24 | 2.1 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 14 | 2.01 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 14 | 2.01 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 14 | 2.01 |
| (1,1163) | 1:A:54:LEU:HD11 | 1:A:51:GLU:HB2 | 24 | 1.99 |
| (1,1163) | 1:A:54:LEU:HD12 | 1:A:51:GLU:HB2 | 24 | 1.99 |
| (1,1163) | 1:A:54:LEU:HD13 | 1:A:51:GLU:HB2 | 24 | 1.99 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 27 | 1.98 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 27 | 1.98 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 27 | 1.98 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 26 | 1.96 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 26 | 1.96 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 26 | 1.96 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 17 | 1.89 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 17 | 1.89 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 17 | 1.89 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 18 | 1.88 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 13 | 1.87 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 13 | 1.87 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 13 | 1.87 |
| (1,1163) | 1:A:54:LEU:HD11 | 1:A:51:GLU:HB2 | 21 | 1.82 |
| (1,1163) | 1:A:54:LEU:HD12 | 1:A:51:GLU:HB2 | 21 | 1.82 |
| (1,1163) | 1:A:54:LEU:HD13 | 1:A:51:GLU:HB2 | 21 | 1.82 |
| (1,900) | 1:A:47:ILE:HG21 | 1:A:48:LEU:HD11 | 18 | 1.74 |
| (1,900) | 1:A:47:ILE:HG21 | 1:A:48:LEU:HD12 | 18 | 1.74 |
| (1,900) | 1:A:47:ILE:HG21 | 1:A:48:LEU:HD13 | 18 | 1.74 |
| (1,900) | 1:A:47:ILE:HG22 | 1:A:48:LEU:HD11 | 18 | 1.74 |
| (1,900) | 1:A:47:ILE:HG22 | 1:A:48:LEU:HD12 | 18 | 1.74 |
| (1,900) | 1:A:47:ILE:HG22 | 1:A:48:LEU:HD13 | 18 | 1.74 |
| (1,900) | 1:A:47:ILE:HG23 | 1:A:48:LEU:HD11 | 18 | 1.74 |
| (1,900) | 1:A:47:ILE:HG23 | 1:A:48:LEU:HD12 | 18 | 1.74 |
| (1,900) | 1:A:47:ILE:HG23 | 1:A:48:LEU:HD13 | 18 | 1.74 |
| (1,444) | 1:A:47:ILE:HA | 1:A:50:ARG:HB3 | 28 | 1.72 |
| (1,1554) | 1:A:34:LEU:HD21 | 1:A:26:ASN:HB3 | 19 | 1.72 |
| (1,1554) | 1:A:34:LEU:HD22 | 1:A:26:ASN:HB3 | 19 | 1.72 |
| (1,1554) | 1:A:34:LEU:HD23 | 1:A:26:ASN:HB3 | 19 | 1.72 |
| (1,1163) | 1:A:54:LEU:HD11 | 1:A:51:GLU:HB2 | 4 | 1.72 |
| (1,1163) | 1:A:54:LEU:HD12 | 1:A:51:GLU:HB2 | 4 | 1.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1163) | 1:A:54:LEU:HD13 | 1:A:51:GLU:HB2 | 4 | 1.72 |
| (1,1163) | 1:A:54:LEU:HD11 | 1:A:51:GLU:HB2 | 29 | 1.72 |
| (1,1163) | 1:A:54:LEU:HD12 | 1:A:51:GLU:HB2 | 29 | 1.72 |
| (1,1163) | 1:A:54:LEU:HD13 | 1:A:51:GLU:HB2 | 29 | 1.72 |
| (1,444) | 1:A:47:ILE:HA | 1:A:50:ARG:HB3 | 23 | 1.71 |
| (1,900) | 1:A:47:ILE:HG21 | 1:A:48:LEU:HD11 | 2 | 1.7 |
| (1,900) | 1:A:47:ILE:HG21 | 1:A:48:LEU:HD12 | 2 | 1.7 |
| (1,900) | 1:A:47:ILE:HG21 | 1:A:48:LEU:HD13 | 2 | 1.7 |
| (1,900) | 1:A:47:ILE:HG22 | 1:A:48:LEU:HD11 | 2 | 1.7 |
| (1,900) | 1:A:47:ILE:HG22 | 1:A:48:LEU:HD12 | 2 | 1.7 |
| (1,900) | 1:A:47:ILE:HG22 | 1:A:48:LEU:HD13 | 2 | 1.7 |
| (1,900) | 1:A:47:ILE:HG23 | 1:A:48:LEU:HD11 | 2 | 1.7 |
| (1,900) | 1:A:47:ILE:HG23 | 1:A:48:LEU:HD12 | 2 | 1.7 |
| (1,900) | 1:A:47:ILE:HG23 | 1:A:48:LEU:HD13 | 2 | 1.7 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 28 | 1.69 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 28 | 1.69 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 28 | 1.69 |
| (1,1554) | 1:A:34:LEU:HD21 | 1:A:26:ASN:HB3 | 17 | 1.68 |
| (1,1554) | 1:A:34:LEU:HD22 | 1:A:26:ASN:HB3 | 17 | 1.68 |
| (1,1554) | 1:A:34:LEU:HD23 | 1:A:26:ASN:HB3 | 17 | 1.68 |
| (1,1554) | 1:A:34:LEU:HD21 | 1:A:26:ASN:HB3 | 29 | 1.67 |
| (1,1554) | 1:A:34:LEU:HD22 | 1:A:26:ASN:HB3 | 29 | 1.67 |
| (1,1554) | 1:A:34:LEU:HD23 | 1:A:26:ASN:HB3 | 29 | 1.67 |
| (1,1122) | 1:A:48:LEU:HD11 | 1:A:52:HIS:HB3 | 22 | 1.67 |
| (1,1122) | 1:A:48:LEU:HD12 | 1:A:52:HIS:HB3 | 22 | 1.67 |
| (1,1122) | 1:A:48:LEU:HD13 | 1:A:52:HIS:HB3 | 22 | 1.67 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 16 | 1.66 |
| (1,444) | 1:A:47:ILE:HA | 1:A:50:ARG:HB3 | 15 | 1.65 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 16 | 1.65 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 16 | 1.65 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 16 | 1.65 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 9 | 1.64 |
| (1,1555) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB3 | 27 | 1.64 |
| (1,1555) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB3 | 27 | 1.64 |
| (1,1555) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB3 | 27 | 1.64 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 5 | 1.62 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 5 | 1.62 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 5 | 1.62 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 8 | 1.62 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 8 | 1.62 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 8 | 1.62 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 11 | 1.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 11 | 1.62 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 11 | 1.62 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 19 | 1.62 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 19 | 1.62 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 19 | 1.62 |
| (1,1163) | 1:A:54:LEU:HD11 | 1:A:51:GLU:HB2 | 2 | 1.61 |
| (1,1163) | 1:A:54:LEU:HD12 | 1:A:51:GLU:HB2 | 2 | 1.61 |
| (1,1163) | 1:A:54:LEU:HD13 | 1:A:51:GLU:HB2 | 2 | 1.61 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 18 | 1.6 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 18 | 1.6 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 18 | 1.6 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 25 | 1.59 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 25 | 1.59 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 25 | 1.59 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 1 | 1.58 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 1 | 1.58 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 1 | 1.58 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 9 | 1.57 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 9 | 1.57 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 9 | 1.57 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 22 | 1.57 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 22 | 1.57 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 22 | 1.57 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 30 | 1.57 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 30 | 1.57 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 30 | 1.57 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 3 | 1.56 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 6 | 1.56 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 6 | 1.56 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 6 | 1.56 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 27 | 1.56 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 27 | 1.56 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 27 | 1.56 |
| (1,1554) | 1:A:34:LEU:HD21 | 1:A:26:ASN:HB3 | 14 | 1.56 |
| (1,1554) | 1:A:34:LEU:HD22 | 1:A:26:ASN:HB3 | 14 | 1.56 |
| (1,1554) | 1:A:34:LEU:HD23 | 1:A:26:ASN:HB3 | 14 | 1.56 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 23 | 1.55 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 23 | 1.55 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 23 | 1.55 |
| (1,1163) | 1:A:54:LEU:HD11 | 1:A:51:GLU:HB2 | 1 | 1.55 |
| (1,1163) | 1:A:54:LEU:HD12 | 1:A:51:GLU:HB2 | 1 | 1.55 |
| (1,1163) | 1:A:54:LEU:HD13 | 1:A:51:GLU:HB2 | 1 | 1.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 17 | 1.54 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 17 | 1.54 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 17 | 1.54 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD21 | 18 | 1.52 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD22 | 18 | 1.52 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD23 | 18 | 1.52 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD11 | 18 | 1.52 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD12 | 18 | 1.52 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD13 | 18 | 1.52 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 4 | 1.52 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 4 | 1.52 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 4 | 1.52 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 12 | 1.52 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 12 | 1.52 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 12 | 1.52 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 26 | 1.52 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 26 | 1.52 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 26 | 1.52 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 29 | 1.52 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 29 | 1.52 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 29 | 1.52 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 10 | 1.51 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 10 | 1.51 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 10 | 1.51 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 13 | 1.51 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 13 | 1.51 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 13 | 1.51 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 20 | 1.51 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 20 | 1.51 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 20 | 1.51 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 21 | 1.5 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 21 | 1.5 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 21 | 1.5 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 24 | 1.48 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 24 | 1.48 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 24 | 1.48 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 14 | 1.46 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 14 | 1.46 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 14 | 1.46 |
| (1,1554) | 1:A:34:LEU:HD21 | 1:A:26:ASN:HB3 | 26 | 1.46 |
| (1,1554) | 1:A:34:LEU:HD22 | 1:A:26:ASN:HB3 | 26 | 1.46 |
| (1,1554) | 1:A:34:LEU:HD23 | 1:A:26:ASN:HB3 | 26 | 1.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 2 | 1.45 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 2 | 1.45 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 2 | 1.45 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 10 | 1.43 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 15 | 1.43 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 15 | 1.43 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 15 | 1.43 |
| (1,1123) | 1:A:48:LEU:HD11 | 1:A:52:HIS:HB2 | 22 | 1.42 |
| (1,1123) | 1:A:48:LEU:HD12 | 1:A:52:HIS:HB2 | 22 | 1.42 |
| (1,1123) | 1:A:48:LEU:HD13 | 1:A:52:HIS:HB2 | 22 | 1.42 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 7 | 1.39 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 19 | 1.39 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 19 | 1.39 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 19 | 1.39 |
| (1,972) | 1:A:27:LEU:HD21 | 1:A:70:GLN:HE21 | 20 | 1.36 |
| (1,972) | 1:A:27:LEU:HD22 | 1:A:70:GLN:HE21 | 20 | 1.36 |
| (1,972) | 1:A:27:LEU:HD23 | 1:A:70:GLN:HE21 | 20 | 1.36 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 3 | 1.36 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 18 | 1.34 |
| (1,900) | 1:A:47:ILE:HG21 | 1:A:48:LEU:HD11 | 22 | 1.33 |
| (1,900) | 1:A:47:ILE:HG21 | 1:A:48:LEU:HD12 | 22 | 1.33 |
| (1,900) | 1:A:47:ILE:HG21 | 1:A:48:LEU:HD13 | 22 | 1.33 |
| (1,900) | 1:A:47:ILE:HG22 | 1:A:48:LEU:HD11 | 22 | 1.33 |
| (1,900) | 1:A:47:ILE:HG22 | 1:A:48:LEU:HD12 | 22 | 1.33 |
| (1,900) | 1:A:47:ILE:HG22 | 1:A:48:LEU:HD13 | 22 | 1.33 |
| (1,900) | 1:A:47:ILE:HG23 | 1:A:48:LEU:HD11 | 22 | 1.33 |
| (1,900) | 1:A:47:ILE:HG23 | 1:A:48:LEU:HD12 | 22 | 1.33 |
| (1,900) | 1:A:47:ILE:HG23 | 1:A:48:LEU:HD13 | 22 | 1.33 |
| (1,1554) | 1:A:34:LEU:HD21 | 1:A:26:ASN:HB3 | 20 | 1.33 |
| (1,1554) | 1:A:34:LEU:HD22 | 1:A:26:ASN:HB3 | 20 | 1.33 |
| (1,1554) | 1:A:34:LEU:HD23 | 1:A:26:ASN:HB3 | 20 | 1.33 |
| (1,444) | 1:A:47:ILE:HA | 1:A:50:ARG:HB3 | 20 | 1.32 |
| (1,1593) | 1:A:34:LEU:HD21 | 1:A:29:SER:HA | 20 | 1.32 |
| (1,1593) | 1:A:34:LEU:HD22 | 1:A:29:SER:HA | 20 | 1.32 |
| (1,1593) | 1:A:34:LEU:HD23 | 1:A:29:SER:HA | 20 | 1.32 |
| (1,1554) | 1:A:34:LEU:HD21 | 1:A:26:ASN:HB3 | 28 | 1.32 |
| (1,1554) | 1:A:34:LEU:HD22 | 1:A:26:ASN:HB3 | 28 | 1.32 |
| (1,1554) | 1:A:34:LEU:HD23 | 1:A:26:ASN:HB3 | 28 | 1.32 |
| (1,444) | 1:A:47:ILE:HA | 1:A:50:ARG:HB3 | 14 | 1.31 |
| (1,1638) | 1:A:57:PRO:HB3 | 1:A:59:ARG:HB2 | 14 | 1.3 |
| (1,1575) | 1:A:66:LEU:HD11 | 1:A:13:VAL:H | 18 | 1.3 |
| (1,1575) | 1:A:66:LEU:HD12 | 1:A:13:VAL:H | 18 | 1.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1575) | 1:A:66:LEU:HD13 | 1:A:13:VAL:H | 18 | 1.3 |
| (1,1202) | 1:A:56:LEU:HD21 | 1:A:55:VAL:HB | 14 | 1.3 |
| (1,1202) | 1:A:56:LEU:HD22 | 1:A:55:VAL:HB | 14 | 1.3 |
| (1,1202) | 1:A:56:LEU:HD23 | 1:A:55:VAL:HB | 14 | 1.3 |
| (1,444) | 1:A:47:ILE:HA | 1:A:50:ARG:HB3 | 13 | 1.29 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 13 | 1.28 |
| (1,444) | 1:A:47:ILE:HA | 1:A:50:ARG:HB3 | 12 | 1.27 |
| (1,1593) | 1:A:34:LEU:HD21 | 1:A:29:SER:HA | 14 | 1.26 |
| (1,1593) | 1:A:34:LEU:HD22 | 1:A:29:SER:HA | 14 | 1.26 |
| (1,1593) | 1:A:34:LEU:HD23 | 1:A:29:SER:HA | 14 | 1.26 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 25 | 1.26 |
| (1,461) | 1:A:47:ILE:HG12 | 1:A:48:LEU:HD11 | 18 | 1.25 |
| (1,461) | 1:A:47:ILE:HG12 | 1:A:48:LEU:HD12 | 18 | 1.25 |
| (1,461) | 1:A:47:ILE:HG12 | 1:A:48:LEU:HD13 | 18 | 1.25 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 7 | 1.25 |
| (1,1593) | 1:A:34:LEU:HD21 | 1:A:29:SER:HA | 3 | 1.23 |
| (1,1593) | 1:A:34:LEU:HD22 | 1:A:29:SER:HA | 3 | 1.23 |
| (1,1593) | 1:A:34:LEU:HD23 | 1:A:29:SER:HA | 3 | 1.23 |
| (1,972) | 1:A:27:LEU:HD21 | 1:A:70:GLN:HE21 | 23 | 1.22 |
| (1,972) | 1:A:27:LEU:HD22 | 1:A:70:GLN:HE21 | 23 | 1.22 |
| (1,972) | 1:A:27:LEU:HD23 | 1:A:70:GLN:HE21 | 23 | 1.22 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 6 | 1.21 |
| (1,1642) | 1:A:9:LEU:HD11 | 1:A:6:GLN:HE21 | 30 | 1.2 |
| (1,1642) | 1:A:9:LEU:HD12 | 1:A:6:GLN:HE21 | 30 | 1.2 |
| (1,1642) | 1:A:9:LEU:HD13 | 1:A:6:GLN:HE21 | 30 | 1.2 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 20 | 1.19 |
| (1,461) | 1:A:47:ILE:HG12 | 1:A:48:LEU:HD11 | 2 | 1.19 |
| (1,461) | 1:A:47:ILE:HG12 | 1:A:48:LEU:HD12 | 2 | 1.19 |
| (1,461) | 1:A:47:ILE:HG12 | 1:A:48:LEU:HD13 | 2 | 1.19 |
| (1,1593) | 1:A:34:LEU:HD21 | 1:A:29:SER:HA | 24 | 1.19 |
| (1,1593) | 1:A:34:LEU:HD22 | 1:A:29:SER:HA | 24 | 1.19 |
| (1,1593) | 1:A:34:LEU:HD23 | 1:A:29:SER:HA | 24 | 1.19 |
| (1,779) | 1:A:52:HIS:HB2 | 1:A:6:GLN:HE21 | 13 | 1.18 |
| (1,1638) | 1:A:57:PRO:HB3 | 1:A:59:ARG:HB2 | 13 | 1.18 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 5 | 1.18 |
| (1,444) | 1:A:47:ILE:HA | 1:A:50:ARG:HB3 | 1 | 1.17 |
| (1,1302) | 1:A:64:LEU:HB3 | 1:A:31:LEU:HB3 | 28 | 1.17 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 22 | 1.17 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 8 | 1.16 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 29 | 1.15 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 16 | 1.15 |
| (1,1638) | 1:A:57:PRO:HB3 | 1:A:59:ARG:HB2 | 1 | 1.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1200) | 1:A:56:LEU:HD21 | 1:A:55:VAL:H | 14 | 1.14 |
| (1,1200) | 1:A:56:LEU:HD22 | 1:A:55:VAL:H | 14 | 1.14 |
| (1,1200) | 1:A:56:LEU:HD23 | 1:A:55:VAL:H | 14 | 1.14 |
| (1,444) | 1:A:47:ILE:HA | 1:A:50:ARG:HB3 | 25 | 1.13 |
| (1,1593) | 1:A:34:LEU:HD21 | 1:A:29:SER:HA | 13 | 1.13 |
| (1,1593) | 1:A:34:LEU:HD22 | 1:A:29:SER:HA | 13 | 1.13 |
| (1,1593) | 1:A:34:LEU:HD23 | 1:A:29:SER:HA | 13 | 1.13 |
| (1,1122) | 1:A:48:LEU:HD11 | 1:A:52:HIS:HB3 | 2 | 1.13 |
| (1,1122) | 1:A:48:LEU:HD12 | 1:A:52:HIS:HB3 | 2 | 1.13 |
| (1,1122) | 1:A:48:LEU:HD13 | 1:A:52:HIS:HB3 | 2 | 1.13 |
| (1,1505) | 1:A:55:VAL:HG11 | 1:A:59:ARG:HD2 | 1 | 1.11 |
| (1,1505) | 1:A:55:VAL:HG11 | 1:A:59:ARG:HD3 | 1 | 1.11 |
| (1,1505) | 1:A:55:VAL:HG12 | 1:A:59:ARG:HD2 | 1 | 1.11 |
| (1,1505) | 1:A:55:VAL:HG12 | 1:A:59:ARG:HD3 | 1 | 1.11 |
| (1,1505) | 1:A:55:VAL:HG13 | 1:A:59:ARG:HD2 | 1 | 1.11 |
| (1,1505) | 1:A:55:VAL:HG13 | 1:A:59:ARG:HD3 | 1 | 1.11 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 15 | 1.11 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 21 | 1.11 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 1 | 1.1 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 6 | 1.1 |
| (1,1638) | 1:A:57:PRO:HB3 | 1:A:59:ARG:HB2 | 20 | 1.09 |
| (1,1168) | 1:A:54:LEU:HG | 1:A:56:LEU:HD21 | 14 | 1.09 |
| (1,1168) | 1:A:54:LEU:HG | 1:A:56:LEU:HD22 | 14 | 1.09 |
| (1,1168) | 1:A:54:LEU:HG | 1:A:56:LEU:HD23 | 14 | 1.09 |
| (1,197) | 1:A:29:SER:HB3 | 1:A:33:ASP:HB3 | 27 | 1.08 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 20 | 1.08 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 10 | 1.07 |
| (1,1099) | 1:A:40:MET:HG3 | 1:A:39:LEU:HD21 | 28 | 1.07 |
| (1,1099) | 1:A:40:MET:HG3 | 1:A:39:LEU:HD22 | 28 | 1.07 |
| (1,1099) | 1:A:40:MET:HG3 | 1:A:39:LEU:HD23 | 28 | 1.07 |
| (1,1593) | 1:A:34:LEU:HD21 | 1:A:29:SER:HA | 26 | 1.06 |
| (1,1593) | 1:A:34:LEU:HD22 | 1:A:29:SER:HA | 26 | 1.06 |
| (1,1593) | 1:A:34:LEU:HD23 | 1:A:29:SER:HA | 26 | 1.06 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 1 | 1.06 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD11 | 30 | 1.05 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD12 | 30 | 1.05 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD13 | 30 | 1.05 |
| (1,315) | 1:A:40:MET:HB3 | 1:A:39:LEU:HD21 | 28 | 1.05 |
| (1,315) | 1:A:40:MET:HB3 | 1:A:39:LEU:HD22 | 28 | 1.05 |
| (1,315) | 1:A:40:MET:HB3 | 1:A:39:LEU:HD23 | 28 | 1.05 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 14 | 1.05 |
| (1,1555) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB3 | 3 | 1.05 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1555) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB3 | 3 | 1.05 |
| (1,1555) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB3 | 3 | 1.05 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 3 | 1.05 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 13 | 1.05 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 23 | 1.05 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 11 | 1.04 |
| (1,72) | 1:A:48:LEU:HD11 | 1:A:6:GLN:HE21 | 13 | 1.04 |
| (1,72) | 1:A:48:LEU:HD12 | 1:A:6:GLN:HE21 | 13 | 1.04 |
| (1,72) | 1:A:48:LEU:HD13 | 1:A:6:GLN:HE21 | 13 | 1.04 |
| (1,72) | 1:A:9:LEU:HD21 | 1:A:6:GLN:HE21 | 13 | 1.04 |
| (1,72) | 1:A:9:LEU:HD22 | 1:A:6:GLN:HE21 | 13 | 1.04 |
| (1,72) | 1:A:9:LEU:HD23 | 1:A:6:GLN:HE21 | 13 | 1.04 |
| (1,1642) | 1:A:9:LEU:HD11 | 1:A:6:GLN:HE21 | 25 | 1.04 |
| (1,1642) | 1:A:9:LEU:HD12 | 1:A:6:GLN:HE21 | 25 | 1.04 |
| (1,1642) | 1:A:9:LEU:HD13 | 1:A:6:GLN:HE21 | 25 | 1.04 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 28 | 1.03 |
| (1,239) | 1:A:31:LEU:HD11 | 1:A:62:ARG:HG3 | 20 | 1.03 |
| (1,239) | 1:A:31:LEU:HD12 | 1:A:62:ARG:HG3 | 20 | 1.03 |
| (1,239) | 1:A:31:LEU:HD13 | 1:A:62:ARG:HG3 | 20 | 1.03 |
| (1,1544) | 1:A:44:VAL:HG21 | 1:A:44:VAL:H | 18 | 1.03 |
| (1,1544) | 1:A:44:VAL:HG22 | 1:A:44:VAL:H | 18 | 1.03 |
| (1,1544) | 1:A:44:VAL:HG23 | 1:A:44:VAL:H | 18 | 1.03 |
| (1,1509) | 1:A:72:MET:HG2 | 1:A:9:LEU:HD11 | 13 | 1.02 |
| (1,1509) | 1:A:72:MET:HG2 | 1:A:9:LEU:HD12 | 13 | 1.02 |
| (1,1509) | 1:A:72:MET:HG2 | 1:A:9:LEU:HD13 | 13 | 1.02 |
| (1,1302) | 1:A:64:LEU:HB3 | 1:A:31:LEU:HB3 | 7 | 1.02 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 8 | 1.02 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 17 | 1.02 |
| (1,1593) | 1:A:34:LEU:HD21 | 1:A:29:SER:HA | 29 | 1.01 |
| (1,1593) | 1:A:34:LEU:HD22 | 1:A:29:SER:HA | 29 | 1.01 |
| (1,1593) | 1:A:34:LEU:HD23 | 1:A:29:SER:HA | 29 | 1.01 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 30 | 1.0 |
| (1,502) | 1:A:19:ILE:HD11 | 1:A:25:ILE:HG13 | 22 | 1.0 |
| (1,502) | 1:A:19:ILE:HD12 | 1:A:25:ILE:HG13 | 22 | 1.0 |
| (1,502) | 1:A:19:ILE:HD13 | 1:A:25:ILE:HG13 | 22 | 1.0 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 4 | 1.0 |
| (1,928) | 1:A:57:PRO:HG2 | 1:A:56:LEU:HD21 | 14 | 0.98 |
| (1,928) | 1:A:57:PRO:HG2 | 1:A:56:LEU:HD22 | 14 | 0.98 |
| (1,928) | 1:A:57:PRO:HG2 | 1:A:56:LEU:HD23 | 14 | 0.98 |
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB2 | 6 | 0.97 |
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB3 | 6 | 0.97 |
| (1,779) | 1:A:52:HIS:HB2 | 1:A:6:GLN:HE21 | 18 | 0.97 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,236) | 1:A:31:LEU:HD11 | 1:A:66:LEU:H | 19 | 0.97 |
| (1,236) | 1:A:31:LEU:HD12 | 1:A:66:LEU:H | 19 | 0.97 |
| (1,236) | 1:A:31:LEU:HD13 | 1:A:66:LEU:H | 19 | 0.97 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 30 | 0.97 |
| (1,461) | 1:A:47:ILE:HG12 | 1:A:48:LEU:HD11 | 22 | 0.96 |
| (1,461) | 1:A:47:ILE:HG12 | 1:A:48:LEU:HD12 | 22 | 0.96 |
| (1,461) | 1:A:47:ILE:HG12 | 1:A:48:LEU:HD13 | 22 | 0.96 |
| (1,1638) | 1:A:57:PRO:HB3 | 1:A:59:ARG:HB2 | 22 | 0.96 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD11 | 5 | 0.95 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD12 | 5 | 0.95 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD13 | 5 | 0.95 |
| (1,1302) | 1:A:64:LEU:HB3 | 1:A:31:LEU:HB3 | 22 | 0.95 |
| (1,1196) | 1:A:56:LEU:HD21 | 1:A:56:LEU:HA | 14 | 0.95 |
| (1,1196) | 1:A:56:LEU:HD22 | 1:A:56:LEU:HA | 14 | 0.95 |
| (1,1196) | 1:A:56:LEU:HD23 | 1:A:56:LEU:HA | 14 | 0.95 |
| (1,111) | 1:A:55:VAL:HG21 | 1:A:49:GLU:HG3 | 18 | 0.95 |
| (1,111) | 1:A:55:VAL:HG22 | 1:A:49:GLU:HG3 | 18 | 0.95 |
| (1,111) | 1:A:55:VAL:HG23 | 1:A:49:GLU:HG3 | 18 | 0.95 |
| (1,1065) | 1:A:36:LEU:HD11 | 1:A:38:SER:H | 5 | 0.95 |
| (1,1065) | 1:A:36:LEU:HD12 | 1:A:38:SER:H | 5 | 0.95 |
| (1,1065) | 1:A:36:LEU:HD13 | 1:A:38:SER:H | 5 | 0.95 |
| (1,928) | 1:A:57:PRO:HG2 | 1:A:56:LEU:HD21 | 20 | 0.94 |
| (1,928) | 1:A:57:PRO:HG2 | 1:A:56:LEU:HD22 | 20 | 0.94 |
| (1,928) | 1:A:57:PRO:HG2 | 1:A:56:LEU:HD23 | 20 | 0.94 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 15 | 0.94 |
| (1,1648) | 1:A:74:SER:HB3 | 1:A:54:LEU:HD21 | 18 | 0.94 |
| (1,1648) | 1:A:74:SER:HB3 | 1:A:54:LEU:HD22 | 18 | 0.94 |
| (1,1648) | 1:A:74:SER:HB3 | 1:A:54:LEU:HD23 | 18 | 0.94 |
| (1,1638) | 1:A:57:PRO:HB3 | 1:A:59:ARG:HB2 | 15 | 0.94 |
| (1,60) | 1:A:47:ILE:HG21 | 1:A:74:SER:HB2 | 19 | 0.93 |
| (1,60) | 1:A:47:ILE:HG22 | 1:A:74:SER:HB2 | 19 | 0.93 |
| (1,60) | 1:A:47:ILE:HG23 | 1:A:74:SER:HB2 | 19 | 0.93 |
| (1,60) | 1:A:58:ILE:HG21 | 1:A:31:LEU:HA | 19 | 0.93 |
| (1,60) | 1:A:58:ILE:HG22 | 1:A:31:LEU:HA | 19 | 0.93 |
| (1,60) | 1:A:58:ILE:HG23 | 1:A:31:LEU:HA | 19 | 0.93 |
| (1,1638) | 1:A:57:PRO:HB3 | 1:A:59:ARG:HB2 | 23 | 0.93 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 3 | 0.93 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 3 | 0.93 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 3 | 0.93 |
| (1,239) | 1:A:31:LEU:HD11 | 1:A:62:ARG:HG3 | 8 | 0.91 |
| (1,239) | 1:A:31:LEU:HD12 | 1:A:62:ARG:HG3 | 8 | 0.91 |
| (1,239) | 1:A:31:LEU:HD13 | 1:A:62:ARG:HG3 | 8 | 0.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1593) | 1:A:34:LEU:HD21 | 1:A:29:SER:HA | 27 | 0.91 |
| (1,1593) | 1:A:34:LEU:HD22 | 1:A:29:SER:HA | 27 | 0.91 |
| (1,1593) | 1:A:34:LEU:HD23 | 1:A:29:SER:HA | 27 | 0.91 |
| (1,239) | 1:A:31:LEU:HD11 | 1:A:62:ARG:HG3 | 18 | 0.9 |
| (1,239) | 1:A:31:LEU:HD12 | 1:A:62:ARG:HG3 | 18 | 0.9 |
| (1,239) | 1:A:31:LEU:HD13 | 1:A:62:ARG:HG3 | 18 | 0.9 |
| (1,1369) | 1:A:71:GLU:HG2 | 1:A:72:MET:H | 3 | 0.9 |
| (1,1107) | 1:A:48:LEU:HA | 1:A:52:HIS:HB2 | 2 | 0.9 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 28 | 0.9 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 28 | 0.9 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 28 | 0.9 |
| (1,315) | 1:A:40:MET:HB3 | 1:A:39:LEU:HD21 | 24 | 0.89 |
| (1,315) | 1:A:40:MET:HB3 | 1:A:39:LEU:HD22 | 24 | 0.89 |
| (1,315) | 1:A:40:MET:HB3 | 1:A:39:LEU:HD23 | 24 | 0.89 |
| (1,1592) | 1:A:34:LEU:HD21 | 1:A:30:SER:H | 3 | 0.89 |
| (1,1592) | 1:A:34:LEU:HD22 | 1:A:30:SER:H | 3 | 0.89 |
| (1,1592) | 1:A:34:LEU:HD23 | 1:A:30:SER:H | 3 | 0.89 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 11 | 0.89 |
| (1,1302) | 1:A:64:LEU:HB3 | 1:A:31:LEU:HB3 | 19 | 0.89 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 28 | 0.89 |
| (1,1099) | 1:A:40:MET:HG3 | 1:A:39:LEU:HD21 | 24 | 0.89 |
| (1,1099) | 1:A:40:MET:HG3 | 1:A:39:LEU:HD22 | 24 | 0.89 |
| (1,1099) | 1:A:40:MET:HG3 | 1:A:39:LEU:HD23 | 24 | 0.89 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD21 | 24 | 0.88 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD22 | 24 | 0.88 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD23 | 24 | 0.88 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD11 | 24 | 0.88 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD12 | 24 | 0.88 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD13 | 24 | 0.88 |
| (1,1126) | 1:A:48:LEU:HD11 | 1:A:52:HIS:H | 2 | 0.87 |
| (1,1126) | 1:A:48:LEU:HD12 | 1:A:52:HIS:H | 2 | 0.87 |
| (1,1126) | 1:A:48:LEU:HD13 | 1:A:52:HIS:H | 2 | 0.87 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD11 | 16 | 0.86 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD12 | 16 | 0.86 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD13 | 16 | 0.86 |
| (1,700) | 1:A:59:ARG:HA | 1:A:62:ARG:HD2 | 28 | 0.86 |
| (1,244) | 1:A:31:LEU:HD21 | 1:A:64:LEU:HG | 15 | 0.86 |
| (1,244) | 1:A:31:LEU:HD22 | 1:A:64:LEU:HG | 15 | 0.86 |
| (1,244) | 1:A:31:LEU:HD23 | 1:A:64:LEU:HG | 15 | 0.86 |
| (1,244) | 1:A:31:LEU:HD21 | 1:A:64:LEU:HG | 17 | 0.86 |
| (1,244) | 1:A:31:LEU:HD22 | 1:A:64:LEU:HG | 17 | 0.86 |
| (1,244) | 1:A:31:LEU:HD23 | 1:A:64:LEU:HG | 17 | 0.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,244) | 1:A:31:LEU:HD21 | 1:A:64:LEU:HG | 19 | 0.86 |
| (1,244) | 1:A:31:LEU:HD22 | 1:A:64:LEU:HG | 19 | 0.86 |
| (1,244) | 1:A:31:LEU:HD23 | 1:A:64:LEU:HG | 19 | 0.86 |
| (1,229) | 1:A:31:LEU:HA | 1:A:36:LEU:HD21 | 5 | 0.86 |
| (1,229) | 1:A:31:LEU:HA | 1:A:36:LEU:HD22 | 5 | 0.86 |
| (1,229) | 1:A:31:LEU:HA | 1:A:36:LEU:HD23 | 5 | 0.86 |
| (1,972) | 1:A:27:LEU:HD21 | 1:A:70:GLN:HE21 | 14 | 0.85 |
| (1,972) | 1:A:27:LEU:HD22 | 1:A:70:GLN:HE21 | 14 | 0.85 |
| (1,972) | 1:A:27:LEU:HD23 | 1:A:70:GLN:HE21 | 14 | 0.85 |
| (1,719) | 1:A:63:GLN:HB2 | 1:A:63:GLN:HE21 | 29 | 0.85 |
| (1,244) | 1:A:31:LEU:HD21 | 1:A:64:LEU:HG | 13 | 0.85 |
| (1,244) | 1:A:31:LEU:HD22 | 1:A:64:LEU:HG | 13 | 0.85 |
| (1,244) | 1:A:31:LEU:HD23 | 1:A:64:LEU:HG | 13 | 0.85 |
| (1,102) | 1:A:55:VAL:HG21 | 1:A:55:VAL:H | 1 | 0.85 |
| (1,102) | 1:A:55:VAL:HG22 | 1:A:55:VAL:H | 1 | 0.85 |
| (1,102) | 1:A:55:VAL:HG23 | 1:A:55:VAL:H | 1 | 0.85 |
| (1,719) | 1:A:63:GLN:HB2 | 1:A:63:GLN:HE21 | 24 | 0.84 |
| (1,1117) | 1:A:48:LEU:HA | 1:A:48:LEU:HD11 | 22 | 0.84 |
| (1,1117) | 1:A:48:LEU:HA | 1:A:48:LEU:HD12 | 22 | 0.84 |
| (1,1117) | 1:A:48:LEU:HA | 1:A:48:LEU:HD13 | 22 | 0.84 |
| (1,1012) | 1:A:34:LEU:HD11 | 1:A:31:LEU:H | 5 | 0.84 |
| (1,1012) | 1:A:34:LEU:HD12 | 1:A:31:LEU:H | 5 | 0.84 |
| (1,1012) | 1:A:34:LEU:HD13 | 1:A:31:LEU:H | 5 | 0.84 |
| (1,719) | 1:A:63:GLN:HB2 | 1:A:63:GLN:HE21 | 10 | 0.83 |
| (1,244) | 1:A:31:LEU:HD21 | 1:A:64:LEU:HG | 5 | 0.83 |
| (1,244) | 1:A:31:LEU:HD22 | 1:A:64:LEU:HG | 5 | 0.83 |
| (1,244) | 1:A:31:LEU:HD23 | 1:A:64:LEU:HG | 5 | 0.83 |
| (1,244) | 1:A:31:LEU:HD21 | 1:A:64:LEU:HG | 16 | 0.83 |
| (1,244) | 1:A:31:LEU:HD22 | 1:A:64:LEU:HG | 16 | 0.83 |
| (1,244) | 1:A:31:LEU:HD23 | 1:A:64:LEU:HG | 16 | 0.83 |
| (1,239) | 1:A:31:LEU:HD11 | 1:A:62:ARG:HG3 | 6 | 0.83 |
| (1,239) | 1:A:31:LEU:HD12 | 1:A:62:ARG:HG3 | 6 | 0.83 |
| (1,239) | 1:A:31:LEU:HD13 | 1:A:62:ARG:HG3 | 6 | 0.83 |
| (1,1638) | 1:A:57:PRO:HB3 | 1:A:59:ARG:HB2 | 30 | 0.83 |
| (1,1117) | 1:A:48:LEU:HA | 1:A:48:LEU:HD11 | 2 | 0.83 |
| (1,1117) | 1:A:48:LEU:HA | 1:A:48:LEU:HD12 | 2 | 0.83 |
| (1,1117) | 1:A:48:LEU:HA | 1:A:48:LEU:HD13 | 2 | 0.83 |
| (1,1117) | 1:A:48:LEU:HA | 1:A:48:LEU:HD11 | 18 | 0.83 |
| (1,1117) | 1:A:48:LEU:HA | 1:A:48:LEU:HD12 | 18 | 0.83 |
| (1,1117) | 1:A:48:LEU:HA | 1:A:48:LEU:HD13 | 18 | 0.83 |
| (1,499) | 1:A:47:ILE:HD11 | 1:A:43:GLU:HG2 | 21 | 0.82 |
| (1,499) | 1:A:47:ILE:HD12 | 1:A:43:GLU:HG2 | 21 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,499) | 1:A:47:ILE:HD13 | 1:A:43:GLU:HG2 | 21 | 0.82 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 24 | 0.82 |
| (1,719) | 1:A:63:GLN:HB2 | 1:A:63:GLN:HE21 | 5 | 0.81 |
| (1,244) | 1:A:31:LEU:HD21 | 1:A:64:LEU:HG | 30 | 0.81 |
| (1,244) | 1:A:31:LEU:HD22 | 1:A:64:LEU:HG | 30 | 0.81 |
| (1,244) | 1:A:31:LEU:HD23 | 1:A:64:LEU:HG | 30 | 0.81 |
| (1,1302) | 1:A:64:LEU:HB3 | 1:A:31:LEU:HB3 | 18 | 0.81 |
| (1,60) | 1:A:47:ILE:HG21 | 1:A:74:SER:HB2 | 24 | 0.8 |
| (1,60) | 1:A:47:ILE:HG22 | 1:A:74:SER:HB2 | 24 | 0.8 |
| (1,60) | 1:A:47:ILE:HG23 | 1:A:74:SER:HB2 | 24 | 0.8 |
| (1,60) | 1:A:58:ILE:HG21 | 1:A:31:LEU:HA | 24 | 0.8 |
| (1,60) | 1:A:58:ILE:HG22 | 1:A:31:LEU:HA | 24 | 0.8 |
| (1,60) | 1:A:58:ILE:HG23 | 1:A:31:LEU:HA | 24 | 0.8 |
| (1,233) | 1:A:31:LEU:HD11 | 1:A:31:LEU:HA | 30 | 0.8 |
| (1,233) | 1:A:31:LEU:HD12 | 1:A:31:LEU:HA | 30 | 0.8 |
| (1,233) | 1:A:31:LEU:HD13 | 1:A:31:LEU:HA | 30 | 0.8 |
| (1,1593) | 1:A:34:LEU:HD21 | 1:A:29:SER:HA | 17 | 0.8 |
| (1,1593) | 1:A:34:LEU:HD22 | 1:A:29:SER:HA | 17 | 0.8 |
| (1,1593) | 1:A:34:LEU:HD23 | 1:A:29:SER:HA | 17 | 0.8 |
| (1,1592) | 1:A:34:LEU:HD21 | 1:A:30:SER:H | 24 | 0.8 |
| (1,1592) | 1:A:34:LEU:HD22 | 1:A:30:SER:H | 24 | 0.8 |
| (1,1592) | 1:A:34:LEU:HD23 | 1:A:30:SER:H | 24 | 0.8 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 13 | 0.8 |
| (1,1555) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB3 | 20 | 0.8 |
| (1,1555) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB3 | 20 | 0.8 |
| (1,1555) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB3 | 20 | 0.8 |
| (1,1554) | 1:A:34:LEU:HD21 | 1:A:26:ASN:HB3 | 13 | 0.8 |
| (1,1554) | 1:A:34:LEU:HD22 | 1:A:26:ASN:HB3 | 13 | 0.8 |
| (1,1554) | 1:A:34:LEU:HD23 | 1:A:26:ASN:HB3 | 13 | 0.8 |
| (1,1327) | 1:A:68:LYS:HD2 | 1:A:71:GLU:HB2 | 24 | 0.8 |
| (1,1327) | 1:A:68:LYS:HD3 | 1:A:71:GLU:HB2 | 24 | 0.8 |
| (1,927) | 1:A:57:PRO:HG3 | 1:A:56:LEU:HD21 | 14 | 0.79 |
| (1,927) | 1:A:57:PRO:HG3 | 1:A:56:LEU:HD22 | 14 | 0.79 |
| (1,927) | 1:A:57:PRO:HG3 | 1:A:56:LEU:HD23 | 14 | 0.79 |
| (1,719) | 1:A:63:GLN:HB2 | 1:A:63:GLN:HE21 | 30 | 0.79 |
| (1,239) | 1:A:31:LEU:HD11 | 1:A:62:ARG:HG3 | 21 | 0.79 |
| (1,239) | 1:A:31:LEU:HD12 | 1:A:62:ARG:HG3 | 21 | 0.79 |
| (1,239) | 1:A:31:LEU:HD13 | 1:A:62:ARG:HG3 | 21 | 0.79 |
| (1,972) | 1:A:27:LEU:HD21 | 1:A:70:GLN:HE21 | 17 | 0.78 |
| (1,972) | 1:A:27:LEU:HD22 | 1:A:70:GLN:HE21 | 17 | 0.78 |
| (1,972) | 1:A:27:LEU:HD23 | 1:A:70:GLN:HE21 | 17 | 0.78 |
| (1,779) | 1:A:52:HIS:HB2 | 1:A:6:GLN:HE21 | 30 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,700) | 1:A:59:ARG:HA | 1:A:62:ARG:HD2 | 19 | 0.78 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD21 | 13 | 0.78 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD22 | 13 | 0.78 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD23 | 13 | 0.78 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD11 | 13 | 0.78 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD12 | 13 | 0.78 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD13 | 13 | 0.78 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD11 | 15 | 0.77 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD12 | 15 | 0.77 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD13 | 15 | 0.77 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD11 | 19 | 0.77 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD12 | 19 | 0.77 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD13 | 19 | 0.77 |
| (1,60) | 1:A:47:ILE:HG21 | 1:A:74:SER:HB2 | 26 | 0.77 |
| (1,60) | 1:A:47:ILE:HG22 | 1:A:74:SER:HB2 | 26 | 0.77 |
| (1,60) | 1:A:47:ILE:HG23 | 1:A:74:SER:HB2 | 26 | 0.77 |
| (1,60) | 1:A:58:ILE:HG21 | 1:A:31:LEU:HA | 26 | 0.77 |
| (1,60) | 1:A:58:ILE:HG22 | 1:A:31:LEU:HA | 26 | 0.77 |
| (1,60) | 1:A:58:ILE:HG23 | 1:A:31:LEU:HA | 26 | 0.77 |
| (1,233) | 1:A:31:LEU:HD11 | 1:A:31:LEU:HA | 5 | 0.77 |
| (1,233) | 1:A:31:LEU:HD12 | 1:A:31:LEU:HA | 5 | 0.77 |
| (1,233) | 1:A:31:LEU:HD13 | 1:A:31:LEU:HA | 5 | 0.77 |
| (1,233) | 1:A:31:LEU:HD11 | 1:A:31:LEU:HA | 15 | 0.77 |
| (1,233) | 1:A:31:LEU:HD12 | 1:A:31:LEU:HA | 15 | 0.77 |
| (1,233) | 1:A:31:LEU:HD13 | 1:A:31:LEU:HA | 15 | 0.77 |
| (1,1642) | 1:A:9:LEU:HD11 | 1:A:6:GLN:HE21 | 11 | 0.77 |
| (1,1642) | 1:A:9:LEU:HD12 | 1:A:6:GLN:HE21 | 11 | 0.77 |
| (1,1642) | 1:A:9:LEU:HD13 | 1:A:6:GLN:HE21 | 11 | 0.77 |
| (1,1302) | 1:A:64:LEU:HB3 | 1:A:31:LEU:HB3 | 15 | 0.77 |
| (1,572) | 1:A:43:GLU:HB2 | 1:A:44:VAL:HG21 | 18 | 0.76 |
| (1,572) | 1:A:43:GLU:HB2 | 1:A:44:VAL:HG22 | 18 | 0.76 |
| (1,572) | 1:A:43:GLU:HB2 | 1:A:44:VAL:HG23 | 18 | 0.76 |
| (1,412) | 1:A:45:ARG:HD2 | 1:A:58:ILE:HA | 11 | 0.76 |
| (1,412) | 1:A:45:ARG:HD3 | 1:A:58:ILE:HA | 11 | 0.76 |
| (1,412) | 1:A:45:ARG:HD2 | 1:A:58:ILE:HA | 30 | 0.76 |
| (1,412) | 1:A:45:ARG:HD3 | 1:A:58:ILE:HA | 30 | 0.76 |
| (1,233) | 1:A:31:LEU:HD11 | 1:A:31:LEU:HA | 13 | 0.76 |
| (1,233) | 1:A:31:LEU:HD12 | 1:A:31:LEU:HA | 13 | 0.76 |
| (1,233) | 1:A:31:LEU:HD13 | 1:A:31:LEU:HA | 13 | 0.76 |
| (1,233) | 1:A:31:LEU:HD11 | 1:A:31:LEU:HA | 16 | 0.76 |
| (1,233) | 1:A:31:LEU:HD12 | 1:A:31:LEU:HA | 16 | 0.76 |
| (1,233) | 1:A:31:LEU:HD13 | 1:A:31:LEU:HA | 16 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 2 | 0.76 |
| (1,972) | 1:A:27:LEU:HD21 | 1:A:70:GLN:HE21 | 8 | 0.75 |
| (1,972) | 1:A:27:LEU:HD22 | 1:A:70:GLN:HE21 | 8 | 0.75 |
| (1,972) | 1:A:27:LEU:HD23 | 1:A:70:GLN:HE21 | 8 | 0.75 |
| (1,972) | 1:A:27:LEU:HD21 | 1:A:70:GLN:HE21 | 19 | 0.75 |
| (1,972) | 1:A:27:LEU:HD22 | 1:A:70:GLN:HE21 | 19 | 0.75 |
| (1,972) | 1:A:27:LEU:HD23 | 1:A:70:GLN:HE21 | 19 | 0.75 |
| (1,1566) | 1:A:68:LYS:HD2 | 1:A:64:LEU:H | 13 | 0.75 |
| (1,1566) | 1:A:68:LYS:HD3 | 1:A:64:LEU:H | 13 | 0.75 |
| (1,1369) | 1:A:71:GLU:HG2 | 1:A:72:MET:H | 27 | 0.75 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 12 | 0.75 |
| (1,719) | 1:A:63:GLN:HB2 | 1:A:63:GLN:HE21 | 15 | 0.74 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 28 | 0.74 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 28 | 0.74 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 28 | 0.74 |
| (1,394) | 1:A:19:ILE:HG21 | 1:A:25:ILE:HG13 | 2 | 0.73 |
| (1,394) | 1:A:19:ILE:HG22 | 1:A:25:ILE:HG13 | 2 | 0.73 |
| (1,394) | 1:A:19:ILE:HG23 | 1:A:25:ILE:HG13 | 2 | 0.73 |
| (1,239) | 1:A:31:LEU:HD11 | 1:A:62:ARG:HG3 | 23 | 0.73 |
| (1,239) | 1:A:31:LEU:HD12 | 1:A:62:ARG:HG3 | 23 | 0.73 |
| (1,239) | 1:A:31:LEU:HD13 | 1:A:62:ARG:HG3 | 23 | 0.73 |
| (1,233) | 1:A:31:LEU:HD11 | 1:A:31:LEU:HA | 17 | 0.73 |
| (1,233) | 1:A:31:LEU:HD12 | 1:A:31:LEU:HA | 17 | 0.73 |
| (1,233) | 1:A:31:LEU:HD13 | 1:A:31:LEU:HA | 17 | 0.73 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD21 | 6 | 0.73 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD22 | 6 | 0.73 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD23 | 6 | 0.73 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD11 | 6 | 0.73 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD12 | 6 | 0.73 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD13 | 6 | 0.73 |
| (1,1638) | 1:A:57:PRO:HB3 | 1:A:59:ARG:HB2 | 16 | 0.73 |
| (1,1555) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB3 | 29 | 0.73 |
| (1,1555) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB3 | 29 | 0.73 |
| (1,1555) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB3 | 29 | 0.73 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 9 | 0.73 |
| (1,1122) | 1:A:48:LEU:HD11 | 1:A:52:HIS:HB3 | 18 | 0.73 |
| (1,1122) | 1:A:48:LEU:HD12 | 1:A:52:HIS:HB3 | 18 | 0.73 |
| (1,1122) | 1:A:48:LEU:HD13 | 1:A:52:HIS:HB3 | 18 | 0.73 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 9 | 0.73 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 9 | 0.73 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 9 | 0.73 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 25 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 25 | 0.73 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 25 | 0.73 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 5 | 0.72 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 5 | 0.72 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 5 | 0.72 |
| (1,239) | 1:A:31:LEU:HD11 | 1:A:62:ARG:HG3 | 3 | 0.72 |
| (1,239) | 1:A:31:LEU:HD12 | 1:A:62:ARG:HG3 | 3 | 0.72 |
| (1,239) | 1:A:31:LEU:HD13 | 1:A:62:ARG:HG3 | 3 | 0.72 |
| (1,1642) | 1:A:9:LEU:HD11 | 1:A:6:GLN:HE21 | 18 | 0.72 |
| (1,1642) | 1:A:9:LEU:HD12 | 1:A:6:GLN:HE21 | 18 | 0.72 |
| (1,1642) | 1:A:9:LEU:HD13 | 1:A:6:GLN:HE21 | 18 | 0.72 |
| (1,111) | 1:A:55:VAL:HG21 | 1:A:49:GLU:HG3 | 2 | 0.72 |
| (1,111) | 1:A:55:VAL:HG22 | 1:A:49:GLU:HG3 | 2 | 0.72 |
| (1,111) | 1:A:55:VAL:HG23 | 1:A:49:GLU:HG3 | 2 | 0.72 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 12 | 0.72 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 12 | 0.72 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 12 | 0.72 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 11 | 0.71 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 11 | 0.71 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 22 | 0.71 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 22 | 0.71 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 22 | 0.71 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD11 | 17 | 0.7 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD12 | 17 | 0.7 |
| (1,801) | 1:A:65:THR:HA | 1:A:31:LEU:HD13 | 17 | 0.7 |
| (1,668) | 1:A:49:GLU:HG2 | 1:A:46:GLN:HA | 2 | 0.7 |
| (1,239) | 1:A:31:LEU:HD11 | 1:A:62:ARG:HG3 | 1 | 0.7 |
| (1,239) | 1:A:31:LEU:HD12 | 1:A:62:ARG:HG3 | 1 | 0.7 |
| (1,239) | 1:A:31:LEU:HD13 | 1:A:62:ARG:HG3 | 1 | 0.7 |
| (1,177) | 1:A:22:LEU:HD11 | 1:A:24:GLY:HA2 | 8 | 0.7 |
| (1,177) | 1:A:22:LEU:HD12 | 1:A:24:GLY:HA2 | 8 | 0.7 |
| (1,177) | 1:A:22:LEU:HD13 | 1:A:24:GLY:HA2 | 8 | 0.7 |
| (1,177) | 1:A:22:LEU:HD11 | 1:A:24:GLY:HA2 | 17 | 0.7 |
| (1,177) | 1:A:22:LEU:HD12 | 1:A:24:GLY:HA2 | 17 | 0.7 |
| (1,177) | 1:A:22:LEU:HD13 | 1:A:24:GLY:HA2 | 17 | 0.7 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD21 | 1 | 0.7 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD22 | 1 | 0.7 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD23 | 1 | 0.7 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD11 | 1 | 0.7 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD12 | 1 | 0.7 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD13 | 1 | 0.7 |
| (1,1592) | 1:A:34:LEU:HD21 | 1:A:30:SER:H | 13 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1592) | 1:A:34:LEU:HD22 | 1:A:30:SER:H | 13 | 0.7 |
| (1,1592) | 1:A:34:LEU:HD23 | 1:A:30:SER:H | 13 | 0.7 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 1 | 0.7 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 1 | 0.7 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 1 | 0.7 |
| (1,972) | 1:A:27:LEU:HD21 | 1:A:70:GLN:HE21 | 7 | 0.69 |
| (1,972) | 1:A:27:LEU:HD22 | 1:A:70:GLN:HE21 | 7 | 0.69 |
| (1,972) | 1:A:27:LEU:HD23 | 1:A:70:GLN:HE21 | 7 | 0.69 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 18 | 0.69 |
| (1,233) | 1:A:31:LEU:HD11 | 1:A:31:LEU:HA | 19 | 0.69 |
| (1,233) | 1:A:31:LEU:HD12 | 1:A:31:LEU:HA | 19 | 0.69 |
| (1,233) | 1:A:31:LEU:HD13 | 1:A:31:LEU:HA | 19 | 0.69 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 11 | 0.69 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 11 | 0.69 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 11 | 0.69 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 21 | 0.69 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 21 | 0.69 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 21 | 0.69 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 23 | 0.69 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 23 | 0.69 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 23 | 0.69 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD21 | 8 | 0.68 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD22 | 8 | 0.68 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:9:LEU:HD23 | 8 | 0.68 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD11 | 8 | 0.68 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD12 | 8 | 0.68 |
| (1,17) | 1:A:72:MET:HB3 | 1:A:48:LEU:HD13 | 8 | 0.68 |
| (1,1593) | 1:A:34:LEU:HD21 | 1:A:29:SER:HA | 19 | 0.68 |
| (1,1593) | 1:A:34:LEU:HD22 | 1:A:29:SER:HA | 19 | 0.68 |
| (1,1593) | 1:A:34:LEU:HD23 | 1:A:29:SER:HA | 19 | 0.68 |
| (1,566) | 1:A:72:MET:HG2 | 1:A:68:LYS:HB2 | 11 | 0.67 |
| (1,566) | 1:A:72:MET:HG2 | 1:A:68:LYS:HB3 | 11 | 0.67 |
| (1,177) | 1:A:22:LEU:HD11 | 1:A:24:GLY:HA2 | 7 | 0.67 |
| (1,177) | 1:A:22:LEU:HD12 | 1:A:24:GLY:HA2 | 7 | 0.67 |
| (1,177) | 1:A:22:LEU:HD13 | 1:A:24:GLY:HA2 | 7 | 0.67 |
| (1,1592) | 1:A:34:LEU:HD21 | 1:A:30:SER:H | 14 | 0.67 |
| (1,1592) | 1:A:34:LEU:HD22 | 1:A:30:SER:H | 14 | 0.67 |
| (1,1592) | 1:A:34:LEU:HD23 | 1:A:30:SER:H | 14 | 0.67 |
| (1,1239) | 1:A:60:GLU:HB3 | 1:A:56:LEU:HB2 | 10 | 0.67 |
| (1,1012) | 1:A:34:LEU:HD11 | 1:A:31:LEU:H | 28 | 0.67 |
| (1,1012) | 1:A:34:LEU:HD12 | 1:A:31:LEU:H | 28 | 0.67 |
| (1,1012) | 1:A:34:LEU:HD13 | 1:A:31:LEU:H | 28 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB2 | 25 | 0.66 |
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB3 | 25 | 0.66 |
| (1,779) | 1:A:52:HIS:HB2 | 1:A:6:GLN:HE21 | 5 | 0.66 |
| (1,412) | 1:A:45:ARG:HD2 | 1:A:58:ILE:HA | 28 | 0.66 |
| (1,412) | 1:A:45:ARG:HD3 | 1:A:58:ILE:HA | 28 | 0.66 |
| (1,315) | 1:A:40:MET:HB3 | 1:A:39:LEU:HD21 | 27 | 0.66 |
| (1,315) | 1:A:40:MET:HB3 | 1:A:39:LEU:HD22 | 27 | 0.66 |
| (1,315) | 1:A:40:MET:HB3 | 1:A:39:LEU:HD23 | 27 | 0.66 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 26 | 0.66 |
| (1,1509) | 1:A:72:MET:HG2 | 1:A:9:LEU:HD11 | 6 | 0.66 |
| (1,1509) | 1:A:72:MET:HG2 | 1:A:9:LEU:HD12 | 6 | 0.66 |
| (1,1509) | 1:A:72:MET:HG2 | 1:A:9:LEU:HD13 | 6 | 0.66 |
| (1,111) | 1:A:55:VAL:HG21 | 1:A:49:GLU:HG3 | 29 | 0.66 |
| (1,111) | 1:A:55:VAL:HG22 | 1:A:49:GLU:HG3 | 29 | 0.66 |
| (1,111) | 1:A:55:VAL:HG23 | 1:A:49:GLU:HG3 | 29 | 0.66 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 5 | 0.65 |
| (1,412) | 1:A:45:ARG:HD2 | 1:A:58:ILE:HA | 16 | 0.65 |
| (1,412) | 1:A:45:ARG:HD3 | 1:A:58:ILE:HA | 16 | 0.65 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 21 | 0.65 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 21 | 0.65 |
| (1,1445) | 1:A:44:VAL:HG11 | 1:A:47:ILE:HG13 | 18 | 0.65 |
| (1,1445) | 1:A:44:VAL:HG12 | 1:A:47:ILE:HG13 | 18 | 0.65 |
| (1,1445) | 1:A:44:VAL:HG13 | 1:A:47:ILE:HG13 | 18 | 0.65 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 19 | 0.65 |
| (1,1248) | 1:A:61:VAL:HA | 1:A:62:ARG:HB3 | 6 | 0.65 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 7 | 0.65 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 7 | 0.65 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 7 | 0.65 |
| (1,60) | 1:A:47:ILE:HG21 | 1:A:74:SER:HB2 | 11 | 0.64 |
| (1,60) | 1:A:47:ILE:HG22 | 1:A:74:SER:HB2 | 11 | 0.64 |
| (1,60) | 1:A:47:ILE:HG23 | 1:A:74:SER:HB2 | 11 | 0.64 |
| (1,60) | 1:A:58:ILE:HG21 | 1:A:31:LEU:HA | 11 | 0.64 |
| (1,60) | 1:A:58:ILE:HG22 | 1:A:31:LEU:HA | 11 | 0.64 |
| (1,60) | 1:A:58:ILE:HG23 | 1:A:31:LEU:HA | 11 | 0.64 |
| (1,499) | 1:A:47:ILE:HD11 | 1:A:43:GLU:HG2 | 16 | 0.64 |
| (1,499) | 1:A:47:ILE:HD12 | 1:A:43:GLU:HG2 | 16 | 0.64 |
| (1,499) | 1:A:47:ILE:HD13 | 1:A:43:GLU:HG2 | 16 | 0.64 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 15 | 0.64 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 15 | 0.64 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 15 | 0.64 |
| (1,316) | 1:A:40:MET:HB2 | 1:A:39:LEU:HD21 | 28 | 0.63 |
| (1,316) | 1:A:40:MET:HB2 | 1:A:39:LEU:HD22 | 28 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,316) | 1:A:40:MET:HB2 | 1:A:39:LEU:HD23 | 28 | 0.63 |
| (1,240) | 1:A:31:LEU:HD11 | 1:A:34:LEU:HB2 | 15 | 0.63 |
| (1,240) | 1:A:31:LEU:HD12 | 1:A:34:LEU:HB2 | 15 | 0.63 |
| (1,240) | 1:A:31:LEU:HD13 | 1:A:34:LEU:HB2 | 15 | 0.63 |
| (1,240) | 1:A:31:LEU:HD11 | 1:A:34:LEU:HB2 | 19 | 0.63 |
| (1,240) | 1:A:31:LEU:HD12 | 1:A:34:LEU:HB2 | 19 | 0.63 |
| (1,240) | 1:A:31:LEU:HD13 | 1:A:34:LEU:HB2 | 19 | 0.63 |
| (1,1302) | 1:A:64:LEU:HB3 | 1:A:31:LEU:HB3 | 17 | 0.63 |
| (1,240) | 1:A:31:LEU:HD11 | 1:A:34:LEU:HB2 | 30 | 0.62 |
| (1,240) | 1:A:31:LEU:HD12 | 1:A:34:LEU:HB2 | 30 | 0.62 |
| (1,240) | 1:A:31:LEU:HD13 | 1:A:34:LEU:HB2 | 30 | 0.62 |
| (1,1491) | 1:A:42:VAL:HG21 | 1:A:46:GLN:HG2 | 15 | 0.62 |
| (1,1491) | 1:A:42:VAL:HG22 | 1:A:46:GLN:HG2 | 15 | 0.62 |
| (1,1491) | 1:A:42:VAL:HG23 | 1:A:46:GLN:HG2 | 15 | 0.62 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 20 | 0.62 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 20 | 0.62 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 20 | 0.62 |
| (1,468) | 1:A:47:ILE:HA | 1:A:48:LEU:HD11 | 18 | 0.61 |
| (1,468) | 1:A:47:ILE:HA | 1:A:48:LEU:HD12 | 18 | 0.61 |
| (1,468) | 1:A:47:ILE:HA | 1:A:48:LEU:HD13 | 18 | 0.61 |
| (1,239) | 1:A:31:LEU:HD11 | 1:A:62:ARG:HG3 | 7 | 0.61 |
| (1,239) | 1:A:31:LEU:HD12 | 1:A:62:ARG:HG3 | 7 | 0.61 |
| (1,239) | 1:A:31:LEU:HD13 | 1:A:62:ARG:HG3 | 7 | 0.61 |
| (1,1248) | 1:A:61:VAL:HA | 1:A:62:ARG:HB3 | 8 | 0.61 |
| (1,1248) | 1:A:61:VAL:HA | 1:A:62:ARG:HB3 | 20 | 0.61 |
| (1,1592) | 1:A:34:LEU:HD21 | 1:A:30:SER:H | 20 | 0.6 |
| (1,1592) | 1:A:34:LEU:HD22 | 1:A:30:SER:H | 20 | 0.6 |
| (1,1592) | 1:A:34:LEU:HD23 | 1:A:30:SER:H | 20 | 0.6 |
| (1,1248) | 1:A:61:VAL:HA | 1:A:62:ARG:HB3 | 16 | 0.6 |
| (1,502) | 1:A:19:ILE:HD11 | 1:A:25:ILE:HG13 | 2 | 0.59 |
| (1,502) | 1:A:19:ILE:HD12 | 1:A:25:ILE:HG13 | 2 | 0.59 |
| (1,502) | 1:A:19:ILE:HD13 | 1:A:25:ILE:HG13 | 2 | 0.59 |
| (1,239) | 1:A:31:LEU:HD11 | 1:A:62:ARG:HG3 | 22 | 0.59 |
| (1,239) | 1:A:31:LEU:HD12 | 1:A:62:ARG:HG3 | 22 | 0.59 |
| (1,239) | 1:A:31:LEU:HD13 | 1:A:62:ARG:HG3 | 22 | 0.59 |
| (1,1610) | 1:A:13:VAL:HG21 | 1:A:9:LEU:HD11 | 13 | 0.59 |
| (1,1610) | 1:A:13:VAL:HG21 | 1:A:9:LEU:HD12 | 13 | 0.59 |
| (1,1610) | 1:A:13:VAL:HG21 | 1:A:9:LEU:HD13 | 13 | 0.59 |
| (1,1610) | 1:A:13:VAL:HG22 | 1:A:9:LEU:HD11 | 13 | 0.59 |
| (1,1610) | 1:A:13:VAL:HG22 | 1:A:9:LEU:HD12 | 13 | 0.59 |
| (1,1610) | 1:A:13:VAL:HG22 | 1:A:9:LEU:HD13 | 13 | 0.59 |
| (1,1610) | 1:A:13:VAL:HG23 | 1:A:9:LEU:HD11 | 13 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1610) | 1:A:13:VAL:HG23 | 1:A:9:LEU:HD12 | 13 | 0.59 |
| (1,1610) | 1:A:13:VAL:HG23 | 1:A:9:LEU:HD13 | 13 | 0.59 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 12 | 0.59 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 15 | 0.59 |
| (1,1302) | 1:A:64:LEU:HB3 | 1:A:31:LEU:HB3 | 11 | 0.59 |
| (1,1128) | 1:A:36:LEU:HD11 | 1:A:37:ASP:H | 5 | 0.59 |
| (1,1128) | 1:A:36:LEU:HD12 | 1:A:37:ASP:H | 5 | 0.59 |
| (1,1128) | 1:A:36:LEU:HD13 | 1:A:37:ASP:H | 5 | 0.59 |
| (1,296) | 1:A:17:LEU:HD11 | 1:A:19:ILE:HG13 | 16 | 0.58 |
| (1,296) | 1:A:17:LEU:HD12 | 1:A:19:ILE:HG13 | 16 | 0.58 |
| (1,296) | 1:A:17:LEU:HD13 | 1:A:19:ILE:HG13 | 16 | 0.58 |
| (1,177) | 1:A:22:LEU:HD11 | 1:A:24:GLY:HA2 | 10 | 0.58 |
| (1,177) | 1:A:22:LEU:HD12 | 1:A:24:GLY:HA2 | 10 | 0.58 |
| (1,177) | 1:A:22:LEU:HD13 | 1:A:24:GLY:HA2 | 10 | 0.58 |
| (1,177) | 1:A:22:LEU:HD11 | 1:A:24:GLY:HA2 | 20 | 0.58 |
| (1,177) | 1:A:22:LEU:HD12 | 1:A:24:GLY:HA2 | 20 | 0.58 |
| (1,177) | 1:A:22:LEU:HD13 | 1:A:24:GLY:HA2 | 20 | 0.58 |
| (1,1638) | 1:A:57:PRO:HB3 | 1:A:59:ARG:HB2 | 28 | 0.58 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 26 | 0.58 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 26 | 0.58 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 10 | 0.58 |
| (1,1248) | 1:A:61:VAL:HA | 1:A:62:ARG:HB3 | 3 | 0.58 |
| (1,1248) | 1:A:61:VAL:HA | 1:A:62:ARG:HB3 | 15 | 0.58 |
| (1,1248) | 1:A:61:VAL:HA | 1:A:62:ARG:HB3 | 23 | 0.58 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 2 | 0.57 |
| (1,798) | 1:A:51:GLU:HG2 | 1:A:50:ARG:HG2 | 23 | 0.56 |
| (1,798) | 1:A:51:GLU:HG3 | 1:A:50:ARG:HG2 | 23 | 0.56 |
| (1,1303) | 1:A:64:LEU:HB2 | 1:A:31:LEU:HB3 | 28 | 0.56 |
| (1,1100) | 1:A:40:MET:HG2 | 1:A:39:LEU:HD21 | 28 | 0.56 |
| (1,1100) | 1:A:40:MET:HG2 | 1:A:39:LEU:HD22 | 28 | 0.56 |
| (1,1100) | 1:A:40:MET:HG2 | 1:A:39:LEU:HD23 | 28 | 0.56 |
| (1,60) | 1:A:47:ILE:HG21 | 1:A:74:SER:HB2 | 20 | 0.55 |
| (1,60) | 1:A:47:ILE:HG22 | 1:A:74:SER:HB2 | 20 | 0.55 |
| (1,60) | 1:A:47:ILE:HG23 | 1:A:74:SER:HB2 | 20 | 0.55 |
| (1,60) | 1:A:58:ILE:HG21 | 1:A:31:LEU:HA | 20 | 0.55 |
| (1,60) | 1:A:58:ILE:HG22 | 1:A:31:LEU:HA | 20 | 0.55 |
| (1,60) | 1:A:58:ILE:HG23 | 1:A:31:LEU:HA | 20 | 0.55 |
| (1,240) | 1:A:31:LEU:HD11 | 1:A:34:LEU:HB2 | 16 | 0.55 |
| (1,240) | 1:A:31:LEU:HD12 | 1:A:34:LEU:HB2 | 16 | 0.55 |
| (1,240) | 1:A:31:LEU:HD13 | 1:A:34:LEU:HB2 | 16 | 0.55 |
| (1,177) | 1:A:22:LEU:HD11 | 1:A:24:GLY:HA2 | 24 | 0.55 |
| (1,177) | 1:A:22:LEU:HD12 | 1:A:24:GLY:HA2 | 24 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,177) | 1:A:22:LEU:HD13 | 1:A:24:GLY:HA2 | 24 | 0.55 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 18 | 0.55 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 18 | 0.55 |
| (1,1369) | 1:A:71:GLU:HG2 | 1:A:72:MET:H | 22 | 0.55 |
| (1,1248) | 1:A:61:VAL:HA | 1:A:62:ARG:HB3 | 4 | 0.55 |
| (1,1248) | 1:A:61:VAL:HA | 1:A:62:ARG:HB3 | 18 | 0.55 |
| (1,1239) | 1:A:60:GLU:HB3 | 1:A:56:LEU:HB2 | 8 | 0.55 |
| (1,499) | 1:A:47:ILE:HD11 | 1:A:43:GLU:HG2 | 11 | 0.54 |
| (1,499) | 1:A:47:ILE:HD12 | 1:A:43:GLU:HG2 | 11 | 0.54 |
| (1,499) | 1:A:47:ILE:HD13 | 1:A:43:GLU:HG2 | 11 | 0.54 |
| (1,240) | 1:A:31:LEU:HD11 | 1:A:34:LEU:HB2 | 17 | 0.54 |
| (1,240) | 1:A:31:LEU:HD12 | 1:A:34:LEU:HB2 | 17 | 0.54 |
| (1,240) | 1:A:31:LEU:HD13 | 1:A:34:LEU:HB2 | 17 | 0.54 |
| (1,1248) | 1:A:61:VAL:HA | 1:A:62:ARG:HB3 | 5 | 0.54 |
| (1,1248) | 1:A:61:VAL:HA | 1:A:62:ARG:HB3 | 13 | 0.54 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 27 | 0.53 |
| (1,700) | 1:A:59:ARG:HA | 1:A:62:ARG:HD2 | 10 | 0.53 |
| (1,240) | 1:A:31:LEU:HD11 | 1:A:34:LEU:HB2 | 13 | 0.53 |
| (1,240) | 1:A:31:LEU:HD12 | 1:A:34:LEU:HB2 | 13 | 0.53 |
| (1,240) | 1:A:31:LEU:HD13 | 1:A:34:LEU:HB2 | 13 | 0.53 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 8 | 0.53 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 8 | 0.53 |
| (1,1248) | 1:A:61:VAL:HA | 1:A:62:ARG:HB3 | 1 | 0.53 |
| (1,1248) | 1:A:61:VAL:HA | 1:A:62:ARG:HB3 | 17 | 0.53 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 8 | 0.53 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 8 | 0.53 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 8 | 0.53 |
| (1,499) | 1:A:47:ILE:HD11 | 1:A:43:GLU:HG2 | 24 | 0.52 |
| (1,499) | 1:A:47:ILE:HD12 | 1:A:43:GLU:HG2 | 24 | 0.52 |
| (1,499) | 1:A:47:ILE:HD13 | 1:A:43:GLU:HG2 | 24 | 0.52 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 5 | 0.52 |
| (1,972) | 1:A:27:LEU:HD21 | 1:A:70:GLN:HE21 | 29 | 0.51 |
| (1,972) | 1:A:27:LEU:HD22 | 1:A:70:GLN:HE21 | 29 | 0.51 |
| (1,972) | 1:A:27:LEU:HD23 | 1:A:70:GLN:HE21 | 29 | 0.51 |
| (1,394) | 1:A:19:ILE:HG21 | 1:A:25:ILE:HG13 | 10 | 0.51 |
| (1,394) | 1:A:19:ILE:HG22 | 1:A:25:ILE:HG13 | 10 | 0.51 |
| (1,394) | 1:A:19:ILE:HG23 | 1:A:25:ILE:HG13 | 10 | 0.51 |
| (1,177) | 1:A:22:LEU:HD11 | 1:A:24:GLY:HA2 | 29 | 0.51 |
| (1,177) | 1:A:22:LEU:HD12 | 1:A:24:GLY:HA2 | 29 | 0.51 |
| (1,177) | 1:A:22:LEU:HD13 | 1:A:24:GLY:HA2 | 29 | 0.51 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD2 | 13 | 0.51 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD3 | 13 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 28 | 0.51 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 28 | 0.51 |
| (1,1248) | 1:A:61:VAL:HA | 1:A:62:ARG:HB3 | 21 | 0.51 |
| (1,60) | 1:A:47:ILE:HG21 | 1:A:74:SER:HB2 | 13 | 0.5 |
| (1,60) | 1:A:47:ILE:HG22 | 1:A:74:SER:HB2 | 13 | 0.5 |
| (1,60) | 1:A:47:ILE:HG23 | 1:A:74:SER:HB2 | 13 | 0.5 |
| (1,60) | 1:A:58:ILE:HG21 | 1:A:31:LEU:HA | 13 | 0.5 |
| (1,60) | 1:A:58:ILE:HG22 | 1:A:31:LEU:HA | 13 | 0.5 |
| (1,60) | 1:A:58:ILE:HG23 | 1:A:31:LEU:HA | 13 | 0.5 |
| (1,499) | 1:A:47:ILE:HD11 | 1:A:43:GLU:HG2 | 27 | 0.5 |
| (1,499) | 1:A:47:ILE:HD12 | 1:A:43:GLU:HG2 | 27 | 0.5 |
| (1,499) | 1:A:47:ILE:HD13 | 1:A:43:GLU:HG2 | 27 | 0.5 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 12 | 0.5 |
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 12 | 0.5 |
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 12 | 0.5 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD2 | 15 | 0.5 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD3 | 15 | 0.5 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 14 | 0.5 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 14 | 0.5 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 19 | 0.5 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 19 | 0.5 |
| (1,1248) | 1:A:61:VAL:HA | 1:A:62:ARG:HB3 | 22 | 0.5 |
| (1,1196) | 1:A:56:LEU:HD21 | 1:A:56:LEU:HA | 20 | 0.5 |
| (1,1196) | 1:A:56:LEU:HD22 | 1:A:56:LEU:HA | 20 | 0.5 |
| (1,1196) | 1:A:56:LEU:HD23 | 1:A:56:LEU:HA | 20 | 0.5 |
| (1,1019) | 1:A:34:LEU:HD21 | 1:A:34:LEU:HA | 13 | 0.5 |
| (1,1019) | 1:A:34:LEU:HD22 | 1:A:34:LEU:HA | 13 | 0.5 |
| (1,1019) | 1:A:34:LEU:HD23 | 1:A:34:LEU:HA | 13 | 0.5 |
| (1,1019) | 1:A:34:LEU:HD21 | 1:A:34:LEU:HA | 24 | 0.5 |
| (1,1019) | 1:A:34:LEU:HD22 | 1:A:34:LEU:HA | 24 | 0.5 |
| (1,1019) | 1:A:34:LEU:HD23 | 1:A:34:LEU:HA | 24 | 0.5 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 19 | 0.49 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 19 | 0.49 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 19 | 0.49 |
| (1,239) | 1:A:31:LEU:HD11 | 1:A:62:ARG:HG3 | 4 | 0.49 |
| (1,239) | 1:A:31:LEU:HD12 | 1:A:62:ARG:HG3 | 4 | 0.49 |
| (1,239) | 1:A:31:LEU:HD13 | 1:A:62:ARG:HG3 | 4 | 0.49 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 17 | 0.49 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 17 | 0.49 |
| (1,1327) | 1:A:68:LYS:HD2 | 1:A:71:GLU:HB2 | 3 | 0.49 |
| (1,1327) | 1:A:68:LYS:HD3 | 1:A:71:GLU:HB2 | 3 | 0.49 |
| (1,1019) | 1:A:34:LEU:HD21 | 1:A:34:LEU:HA | 14 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1019) | 1:A:34:LEU:HD22 | 1:A:34:LEU:HA | 14 | 0.49 |
| (1,1019) | 1:A:34:LEU:HD23 | 1:A:34:LEU:HA | 14 | 0.49 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 12 | 0.48 |
| (1,394) | 1:A:19:ILE:HG21 | 1:A:25:ILE:HG13 | 1 | 0.48 |
| (1,394) | 1:A:19:ILE:HG22 | 1:A:25:ILE:HG13 | 1 | 0.48 |
| (1,394) | 1:A:19:ILE:HG23 | 1:A:25:ILE:HG13 | 1 | 0.48 |
| (1,177) | 1:A:22:LEU:HD11 | 1:A:24:GLY:HA2 | 27 | 0.48 |
| (1,177) | 1:A:22:LEU:HD12 | 1:A:24:GLY:HA2 | 27 | 0.48 |
| (1,177) | 1:A:22:LEU:HD13 | 1:A:24:GLY:HA2 | 27 | 0.48 |
| (1,1642) | 1:A:9:LEU:HD11 | 1:A:6:GLN:HE21 | 10 | 0.48 |
| (1,1642) | 1:A:9:LEU:HD12 | 1:A:6:GLN:HE21 | 10 | 0.48 |
| (1,1642) | 1:A:9:LEU:HD13 | 1:A:6:GLN:HE21 | 10 | 0.48 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD2 | 23 | 0.48 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD3 | 23 | 0.48 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 9 | 0.48 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 9 | 0.48 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 24 | 0.48 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 24 | 0.48 |
| (1,1019) | 1:A:34:LEU:HD21 | 1:A:34:LEU:HA | 27 | 0.48 |
| (1,1019) | 1:A:34:LEU:HD22 | 1:A:34:LEU:HA | 27 | 0.48 |
| (1,1019) | 1:A:34:LEU:HD23 | 1:A:34:LEU:HA | 27 | 0.48 |
| (1,468) | 1:A:47:ILE:HA | 1:A:48:LEU:HD11 | 2 | 0.47 |
| (1,468) | 1:A:47:ILE:HA | 1:A:48:LEU:HD12 | 2 | 0.47 |
| (1,468) | 1:A:47:ILE:HA | 1:A:48:LEU:HD13 | 2 | 0.47 |
| (1,294) | 1:A:17:LEU:HD11 | 1:A:36:LEU:HB2 | 26 | 0.47 |
| (1,294) | 1:A:17:LEU:HD12 | 1:A:36:LEU:HB2 | 26 | 0.47 |
| (1,294) | 1:A:17:LEU:HD13 | 1:A:36:LEU:HB2 | 26 | 0.47 |
| (1,294) | 1:A:17:LEU:HD21 | 1:A:36:LEU:HB2 | 26 | 0.47 |
| (1,294) | 1:A:17:LEU:HD22 | 1:A:36:LEU:HB2 | 26 | 0.47 |
| (1,294) | 1:A:17:LEU:HD23 | 1:A:36:LEU:HB2 | 26 | 0.47 |
| (1,1576) | 1:A:66:LEU:HD11 | 1:A:65:THR:HA | 11 | 0.47 |
| (1,1576) | 1:A:66:LEU:HD12 | 1:A:65:THR:HA | 11 | 0.47 |
| (1,1576) | 1:A:66:LEU:HD13 | 1:A:65:THR:HA | 11 | 0.47 |
| (1,1369) | 1:A:71:GLU:HG2 | 1:A:72:MET:H | 24 | 0.47 |
| (1,1302) | 1:A:64:LEU:HB3 | 1:A:31:LEU:HB3 | 13 | 0.47 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 11 | 0.47 |
| (1,1248) | 1:A:61:VAL:HA | 1:A:62:ARG:HB3 | 7 | 0.47 |
| (1,1019) | 1:A:34:LEU:HD21 | 1:A:34:LEU:HA | 17 | 0.47 |
| (1,1019) | 1:A:34:LEU:HD22 | 1:A:34:LEU:HA | 17 | 0.47 |
| (1,1019) | 1:A:34:LEU:HD23 | 1:A:34:LEU:HA | 17 | 0.47 |
| (1,1019) | 1:A:34:LEU:HD21 | 1:A:34:LEU:HA | 20 | 0.47 |
| (1,1019) | 1:A:34:LEU:HD22 | 1:A:34:LEU:HA | 20 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1019) | 1:A:34:LEU:HD23 | 1:A:34:LEU:HA | 20 | 0.47 |
| (1,1019) | 1:A:34:LEU:HD21 | 1:A:34:LEU:HA | 29 | 0.47 |
| (1,1019) | 1:A:34:LEU:HD22 | 1:A:34:LEU:HA | 29 | 0.47 |
| (1,1019) | 1:A:34:LEU:HD23 | 1:A:34:LEU:HA | 29 | 0.47 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 1 | 0.46 |
| (1,1638) | 1:A:57:PRO:HB3 | 1:A:59:ARG:HB2 | 12 | 0.46 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD2 | 1 | 0.46 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD3 | 1 | 0.46 |
| (1,1575) | 1:A:66:LEU:HD11 | 1:A:13:VAL:H | 30 | 0.46 |
| (1,1575) | 1:A:66:LEU:HD12 | 1:A:13:VAL:H | 30 | 0.46 |
| (1,1575) | 1:A:66:LEU:HD13 | 1:A:13:VAL:H | 30 | 0.46 |
| (1,1508) | 1:A:72:MET:HG3 | 1:A:9:LEU:HD11 | 13 | 0.46 |
| (1,1508) | 1:A:72:MET:HG3 | 1:A:9:LEU:HD12 | 13 | 0.46 |
| (1,1508) | 1:A:72:MET:HG3 | 1:A:9:LEU:HD13 | 13 | 0.46 |
| (1,972) | 1:A:27:LEU:HD21 | 1:A:70:GLN:HE21 | 12 | 0.45 |
| (1,972) | 1:A:27:LEU:HD22 | 1:A:70:GLN:HE21 | 12 | 0.45 |
| (1,972) | 1:A:27:LEU:HD23 | 1:A:70:GLN:HE21 | 12 | 0.45 |
| (1,798) | 1:A:51:GLU:HG2 | 1:A:50:ARG:HG2 | 12 | 0.45 |
| (1,798) | 1:A:51:GLU:HG3 | 1:A:50:ARG:HG2 | 12 | 0.45 |
| (1,60) | 1:A:47:ILE:HG21 | 1:A:74:SER:HB2 | 16 | 0.45 |
| (1,60) | 1:A:47:ILE:HG22 | 1:A:74:SER:HB2 | 16 | 0.45 |
| (1,60) | 1:A:47:ILE:HG23 | 1:A:74:SER:HB2 | 16 | 0.45 |
| (1,60) | 1:A:58:ILE:HG21 | 1:A:31:LEU:HA | 16 | 0.45 |
| (1,60) | 1:A:58:ILE:HG22 | 1:A:31:LEU:HA | 16 | 0.45 |
| (1,60) | 1:A:58:ILE:HG23 | 1:A:31:LEU:HA | 16 | 0.45 |
| (1,394) | 1:A:19:ILE:HG21 | 1:A:25:ILE:HG13 | 22 | 0.45 |
| (1,394) | 1:A:19:ILE:HG22 | 1:A:25:ILE:HG13 | 22 | 0.45 |
| (1,394) | 1:A:19:ILE:HG23 | 1:A:25:ILE:HG13 | 22 | 0.45 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 22 | 0.45 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 22 | 0.45 |
| (1,1592) | 1:A:34:LEU:HD21 | 1:A:30:SER:H | 26 | 0.45 |
| (1,1592) | 1:A:34:LEU:HD22 | 1:A:30:SER:H | 26 | 0.45 |
| (1,1592) | 1:A:34:LEU:HD23 | 1:A:30:SER:H | 26 | 0.45 |
| (1,1126) | 1:A:48:LEU:HD11 | 1:A:52:HIS:H | 22 | 0.45 |
| (1,1126) | 1:A:48:LEU:HD12 | 1:A:52:HIS:H | 22 | 0.45 |
| (1,1126) | 1:A:48:LEU:HD13 | 1:A:52:HIS:H | 22 | 0.45 |
| (1,1123) | 1:A:48:LEU:HD11 | 1:A:52:HIS:HB2 | 18 | 0.45 |
| (1,1123) | 1:A:48:LEU:HD12 | 1:A:52:HIS:HB2 | 18 | 0.45 |
| (1,1123) | 1:A:48:LEU:HD13 | 1:A:52:HIS:HB2 | 18 | 0.45 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 18 | 0.45 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 18 | 0.45 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 18 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,72) | 1:A:48:LEU:HD11 | 1:A:6:GLN:HE21 | 18 | 0.44 |
| (1,72) | 1:A:48:LEU:HD12 | 1:A:6:GLN:HE21 | 18 | 0.44 |
| (1,72) | 1:A:48:LEU:HD13 | 1:A:6:GLN:HE21 | 18 | 0.44 |
| (1,72) | 1:A:9:LEU:HD21 | 1:A:6:GLN:HE21 | 18 | 0.44 |
| (1,72) | 1:A:9:LEU:HD22 | 1:A:6:GLN:HE21 | 18 | 0.44 |
| (1,72) | 1:A:9:LEU:HD23 | 1:A:6:GLN:HE21 | 18 | 0.44 |
| (1,593) | 1:A:66:LEU:HD11 | 1:A:66:LEU:HA | 30 | 0.44 |
| (1,593) | 1:A:66:LEU:HD12 | 1:A:66:LEU:HA | 30 | 0.44 |
| (1,593) | 1:A:66:LEU:HD13 | 1:A:66:LEU:HA | 30 | 0.44 |
| (1,394) | 1:A:19:ILE:HG21 | 1:A:25:ILE:HG13 | 24 | 0.44 |
| (1,394) | 1:A:19:ILE:HG22 | 1:A:25:ILE:HG13 | 24 | 0.44 |
| (1,394) | 1:A:19:ILE:HG23 | 1:A:25:ILE:HG13 | 24 | 0.44 |
| (1,316) | 1:A:40:MET:HB2 | 1:A:39:LEU:HD21 | 24 | 0.44 |
| (1,316) | 1:A:40:MET:HB2 | 1:A:39:LEU:HD22 | 24 | 0.44 |
| (1,316) | 1:A:40:MET:HB2 | 1:A:39:LEU:HD23 | 24 | 0.44 |
| (1,316) | 1:A:40:MET:HB2 | 1:A:39:LEU:HD21 | 27 | 0.44 |
| (1,316) | 1:A:40:MET:HB2 | 1:A:39:LEU:HD22 | 27 | 0.44 |
| (1,316) | 1:A:40:MET:HB2 | 1:A:39:LEU:HD23 | 27 | 0.44 |
| (1,1554) | 1:A:34:LEU:HD21 | 1:A:26:ASN:HB3 | 5 | 0.44 |
| (1,1554) | 1:A:34:LEU:HD22 | 1:A:26:ASN:HB3 | 5 | 0.44 |
| (1,1554) | 1:A:34:LEU:HD23 | 1:A:26:ASN:HB3 | 5 | 0.44 |
| (1,1221) | 1:A:58:ILE:HG21 | 1:A:57:PRO:HB3 | 14 | 0.44 |
| (1,1221) | 1:A:58:ILE:HG22 | 1:A:57:PRO:HB3 | 14 | 0.44 |
| (1,1221) | 1:A:58:ILE:HG23 | 1:A:57:PRO:HB3 | 14 | 0.44 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 16 | 0.44 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 16 | 0.44 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 16 | 0.44 |
| (1,1019) | 1:A:34:LEU:HD21 | 1:A:34:LEU:HA | 3 | 0.44 |
| (1,1019) | 1:A:34:LEU:HD22 | 1:A:34:LEU:HA | 3 | 0.44 |
| (1,1019) | 1:A:34:LEU:HD23 | 1:A:34:LEU:HA | 3 | 0.44 |
| (1,1008) | 1:A:34:LEU:HD11 | 1:A:31:LEU:HA | 5 | 0.44 |
| (1,1008) | 1:A:34:LEU:HD12 | 1:A:31:LEU:HA | 5 | 0.44 |
| (1,1008) | 1:A:34:LEU:HD13 | 1:A:31:LEU:HA | 5 | 0.44 |
| (1,1006) | 1:A:33:ASP:HB2 | 1:A:30:SER:H | 27 | 0.44 |
| (1,972) | 1:A:27:LEU:HD21 | 1:A:70:GLN:HE21 | 30 | 0.43 |
| (1,972) | 1:A:27:LEU:HD22 | 1:A:70:GLN:HE21 | 30 | 0.43 |
| (1,972) | 1:A:27:LEU:HD23 | 1:A:70:GLN:HE21 | 30 | 0.43 |
| (1,847) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HD2 | 25 | 0.43 |
| (1,847) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HD3 | 25 | 0.43 |
| (1,1554) | 1:A:34:LEU:HD21 | 1:A:26:ASN:HB3 | 3 | 0.43 |
| (1,1554) | 1:A:34:LEU:HD22 | 1:A:26:ASN:HB3 | 3 | 0.43 |
| (1,1554) | 1:A:34:LEU:HD23 | 1:A:26:ASN:HB3 | 3 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1099) | 1:A:40:MET:HG3 | 1:A:39:LEU:HD21 | 27 | 0.43 |
| (1,1099) | 1:A:40:MET:HG3 | 1:A:39:LEU:HD22 | 27 | 0.43 |
| (1,1099) | 1:A:40:MET:HG3 | 1:A:39:LEU:HD23 | 27 | 0.43 |
| (1,1019) | 1:A:34:LEU:HD21 | 1:A:34:LEU:HA | 19 | 0.43 |
| (1,1019) | 1:A:34:LEU:HD22 | 1:A:34:LEU:HA | 19 | 0.43 |
| (1,1019) | 1:A:34:LEU:HD23 | 1:A:34:LEU:HA | 19 | 0.43 |
| (1,1019) | 1:A:34:LEU:HD21 | 1:A:34:LEU:HA | 26 | 0.43 |
| (1,1019) | 1:A:34:LEU:HD22 | 1:A:34:LEU:HA | 26 | 0.43 |
| (1,1019) | 1:A:34:LEU:HD23 | 1:A:34:LEU:HA | 26 | 0.43 |
| (1,739) | 1:A:70:GLN:HA | 1:A:71:GLU:HB2 | 15 | 0.42 |
| (1,593) | 1:A:66:LEU:HD11 | 1:A:66:LEU:HA | 18 | 0.42 |
| (1,593) | 1:A:66:LEU:HD12 | 1:A:66:LEU:HA | 18 | 0.42 |
| (1,593) | 1:A:66:LEU:HD13 | 1:A:66:LEU:HA | 18 | 0.42 |
| (1,296) | 1:A:17:LEU:HD11 | 1:A:19:ILE:HG13 | 7 | 0.42 |
| (1,296) | 1:A:17:LEU:HD12 | 1:A:19:ILE:HG13 | 7 | 0.42 |
| (1,296) | 1:A:17:LEU:HD13 | 1:A:19:ILE:HG13 | 7 | 0.42 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD2 | 22 | 0.42 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD3 | 22 | 0.42 |
| (1,1369) | 1:A:71:GLU:HG2 | 1:A:72:MET:H | 25 | 0.42 |
| (1,1100) | 1:A:40:MET:HG2 | 1:A:39:LEU:HD21 | 24 | 0.42 |
| (1,1100) | 1:A:40:MET:HG2 | 1:A:39:LEU:HD22 | 24 | 0.42 |
| (1,1100) | 1:A:40:MET:HG2 | 1:A:39:LEU:HD23 | 24 | 0.42 |
| (1,972) | 1:A:27:LEU:HD21 | 1:A:70:GLN:HE21 | 24 | 0.41 |
| (1,972) | 1:A:27:LEU:HD22 | 1:A:70:GLN:HE21 | 24 | 0.41 |
| (1,972) | 1:A:27:LEU:HD23 | 1:A:70:GLN:HE21 | 24 | 0.41 |
| (1,798) | 1:A:51:GLU:HG2 | 1:A:50:ARG:HG2 | 25 | 0.41 |
| (1,798) | 1:A:51:GLU:HG3 | 1:A:50:ARG:HG2 | 25 | 0.41 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 7 | 0.41 |
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 7 | 0.41 |
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 7 | 0.41 |
| (1,222) | 1:A:31:LEU:HB3 | 1:A:36:LEU:HD21 | 5 | 0.41 |
| (1,222) | 1:A:31:LEU:HB3 | 1:A:36:LEU:HD22 | 5 | 0.41 |
| (1,222) | 1:A:31:LEU:HB3 | 1:A:36:LEU:HD23 | 5 | 0.41 |
| (1,1592) | 1:A:34:LEU:HD21 | 1:A:30:SER:H | 29 | 0.41 |
| (1,1592) | 1:A:34:LEU:HD22 | 1:A:30:SER:H | 29 | 0.41 |
| (1,1592) | 1:A:34:LEU:HD23 | 1:A:30:SER:H | 29 | 0.41 |
| (1,1491) | 1:A:42:VAL:HG21 | 1:A:46:GLN:HG2 | 12 | 0.41 |
| (1,1491) | 1:A:42:VAL:HG22 | 1:A:46:GLN:HG2 | 12 | 0.41 |
| (1,1491) | 1:A:42:VAL:HG23 | 1:A:46:GLN:HG2 | 12 | 0.41 |
| (1,1491) | 1:A:42:VAL:HG21 | 1:A:46:GLN:HG2 | 22 | 0.41 |
| (1,1491) | 1:A:42:VAL:HG22 | 1:A:46:GLN:HG2 | 22 | 0.41 |
| (1,1491) | 1:A:42:VAL:HG23 | 1:A:46:GLN:HG2 | 22 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 26 | 0.41 |
| (1,1241) | 1:A:60:GLU:HB2 | 1:A:61:VAL:HG21 | 2 | 0.41 |
| (1,1241) | 1:A:60:GLU:HB2 | 1:A:61:VAL:HG22 | 2 | 0.41 |
| (1,1241) | 1:A:60:GLU:HB2 | 1:A:61:VAL:HG23 | 2 | 0.41 |
| (1,1126) | 1:A:48:LEU:HD11 | 1:A:52:HIS:H | 18 | 0.41 |
| (1,1126) | 1:A:48:LEU:HD12 | 1:A:52:HIS:H | 18 | 0.41 |
| (1,1126) | 1:A:48:LEU:HD13 | 1:A:52:HIS:H | 18 | 0.41 |
| (1,1107) | 1:A:48:LEU:HA | 1:A:52:HIS:HB2 | 1 | 0.41 |
| (1,1028) | 1:A:34:LEU:HD21 | 1:A:33:ASP:H | 27 | 0.41 |
| (1,1028) | 1:A:34:LEU:HD22 | 1:A:33:ASP:H | 27 | 0.41 |
| (1,1028) | 1:A:34:LEU:HD23 | 1:A:33:ASP:H | 27 | 0.41 |
| (1,787) | 1:A:51:GLU:HB3 | 1:A:6:GLN:HE21 | 5 | 0.4 |
| (1,460) | 1:A:47:ILE:HG13 | 1:A:48:LEU:HD11 | 18 | 0.4 |
| (1,460) | 1:A:47:ILE:HG13 | 1:A:48:LEU:HD12 | 18 | 0.4 |
| (1,460) | 1:A:47:ILE:HG13 | 1:A:48:LEU:HD13 | 18 | 0.4 |
| (1,1584) | 1:A:59:ARG:HG3 | 1:A:58:ILE:H | 20 | 0.4 |
| (1,1491) | 1:A:42:VAL:HG21 | 1:A:46:GLN:HG2 | 2 | 0.4 |
| (1,1491) | 1:A:42:VAL:HG22 | 1:A:46:GLN:HG2 | 2 | 0.4 |
| (1,1491) | 1:A:42:VAL:HG23 | 1:A:46:GLN:HG2 | 2 | 0.4 |
| (1,1028) | 1:A:34:LEU:HD21 | 1:A:33:ASP:H | 3 | 0.4 |
| (1,1028) | 1:A:34:LEU:HD22 | 1:A:33:ASP:H | 3 | 0.4 |
| (1,1028) | 1:A:34:LEU:HD23 | 1:A:33:ASP:H | 3 | 0.4 |
| (1,1019) | 1:A:34:LEU:HD21 | 1:A:34:LEU:HA | 28 | 0.4 |
| (1,1019) | 1:A:34:LEU:HD22 | 1:A:34:LEU:HA | 28 | 0.4 |
| (1,1019) | 1:A:34:LEU:HD23 | 1:A:34:LEU:HA | 28 | 0.4 |
| (1,972) | 1:A:27:LEU:HD21 | 1:A:70:GLN:HE21 | 27 | 0.39 |
| (1,972) | 1:A:27:LEU:HD22 | 1:A:70:GLN:HE21 | 27 | 0.39 |
| (1,972) | 1:A:27:LEU:HD23 | 1:A:70:GLN:HE21 | 27 | 0.39 |
| (1,896) | 1:A:47:ILE:HG21 | 1:A:6:GLN:HE21 | 12 | 0.39 |
| (1,896) | 1:A:47:ILE:HG22 | 1:A:6:GLN:HE21 | 12 | 0.39 |
| (1,896) | 1:A:47:ILE:HG23 | 1:A:6:GLN:HE21 | 12 | 0.39 |
| (1,593) | 1:A:66:LEU:HD11 | 1:A:66:LEU:HA | 11 | 0.39 |
| (1,593) | 1:A:66:LEU:HD12 | 1:A:66:LEU:HA | 11 | 0.39 |
| (1,593) | 1:A:66:LEU:HD13 | 1:A:66:LEU:HA | 11 | 0.39 |
| (1,1592) | 1:A:34:LEU:HD21 | 1:A:30:SER:H | 17 | 0.39 |
| (1,1592) | 1:A:34:LEU:HD22 | 1:A:30:SER:H | 17 | 0.39 |
| (1,1592) | 1:A:34:LEU:HD23 | 1:A:30:SER:H | 17 | 0.39 |
| (1,1548) | 1:A:19:ILE:HG21 | 1:A:21:ASP:HB2 | 22 | 0.39 |
| (1,1548) | 1:A:19:ILE:HG22 | 1:A:21:ASP:HB2 | 22 | 0.39 |
| (1,1548) | 1:A:19:ILE:HG23 | 1:A:21:ASP:HB2 | 22 | 0.39 |
| (1,1491) | 1:A:42:VAL:HG21 | 1:A:46:GLN:HG2 | 6 | 0.39 |
| (1,1491) | 1:A:42:VAL:HG22 | 1:A:46:GLN:HG2 | 6 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1491) | 1:A:42:VAL:HG23 | 1:A:46:GLN:HG2 | 6 | 0.39 |
| (1,1303) | 1:A:64:LEU:HB2 | 1:A:31:LEU:HB3 | 7 | 0.39 |
| (1,1302) | 1:A:64:LEU:HB3 | 1:A:31:LEU:HB3 | 30 | 0.39 |
| (1,1179) | 1:A:55:VAL:HG11 | 1:A:56:LEU:HB3 | 1 | 0.39 |
| (1,1179) | 1:A:55:VAL:HG12 | 1:A:56:LEU:HB3 | 1 | 0.39 |
| (1,1179) | 1:A:55:VAL:HG13 | 1:A:56:LEU:HB3 | 1 | 0.39 |
| (1,116) | 1:A:55:VAL:HG21 | 1:A:54:LEU:HB3 | 1 | 0.39 |
| (1,116) | 1:A:55:VAL:HG22 | 1:A:54:LEU:HB3 | 1 | 0.39 |
| (1,116) | 1:A:55:VAL:HG23 | 1:A:54:LEU:HB3 | 1 | 0.39 |
| (1,32) | 1:A:27:LEU:HD11 | 1:A:70:GLN:HE21 | 12 | 0.38 |
| (1,32) | 1:A:27:LEU:HD12 | 1:A:70:GLN:HE21 | 12 | 0.38 |
| (1,32) | 1:A:27:LEU:HD13 | 1:A:70:GLN:HE21 | 12 | 0.38 |
| (1,32) | 1:A:66:LEU:HD11 | 1:A:70:GLN:HE21 | 12 | 0.38 |
| (1,32) | 1:A:66:LEU:HD12 | 1:A:70:GLN:HE21 | 12 | 0.38 |
| (1,32) | 1:A:66:LEU:HD13 | 1:A:70:GLN:HE21 | 12 | 0.38 |
| (1,1589) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HE | 21 | 0.38 |
| (1,1642) | 1:A:9:LEU:HD11 | 1:A:6:GLN:HE21 | 28 | 0.37 |
| (1,1642) | 1:A:9:LEU:HD12 | 1:A:6:GLN:HE21 | 28 | 0.37 |
| (1,1642) | 1:A:9:LEU:HD13 | 1:A:6:GLN:HE21 | 28 | 0.37 |
| (1,114) | 1:A:55:VAL:HG11 | 1:A:57:PRO:HG3 | 1 | 0.37 |
| (1,114) | 1:A:55:VAL:HG12 | 1:A:57:PRO:HG3 | 1 | 0.37 |
| (1,114) | 1:A:55:VAL:HG13 | 1:A:57:PRO:HG3 | 1 | 0.37 |
| (1,1638) | 1:A:57:PRO:HB3 | 1:A:59:ARG:HB2 | 7 | 0.36 |
| (1,1638) | 1:A:57:PRO:HB3 | 1:A:59:ARG:HB2 | 24 | 0.36 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 7 | 0.36 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 7 | 0.36 |
| (1,1008) | 1:A:34:LEU:HD11 | 1:A:31:LEU:HA | 28 | 0.36 |
| (1,1008) | 1:A:34:LEU:HD12 | 1:A:31:LEU:HA | 28 | 0.36 |
| (1,1008) | 1:A:34:LEU:HD13 | 1:A:31:LEU:HA | 28 | 0.36 |
| (1,315) | 1:A:40:MET:HB3 | 1:A:39:LEU:HD21 | 8 | 0.35 |
| (1,315) | 1:A:40:MET:HB3 | 1:A:39:LEU:HD22 | 8 | 0.35 |
| (1,315) | 1:A:40:MET:HB3 | 1:A:39:LEU:HD23 | 8 | 0.35 |
| (1,294) | 1:A:17:LEU:HD11 | 1:A:36:LEU:HB2 | 11 | 0.35 |
| (1,294) | 1:A:17:LEU:HD12 | 1:A:36:LEU:HB2 | 11 | 0.35 |
| (1,294) | 1:A:17:LEU:HD13 | 1:A:36:LEU:HB2 | 11 | 0.35 |
| (1,294) | 1:A:17:LEU:HD21 | 1:A:36:LEU:HB2 | 11 | 0.35 |
| (1,294) | 1:A:17:LEU:HD22 | 1:A:36:LEU:HB2 | 11 | 0.35 |
| (1,294) | 1:A:17:LEU:HD23 | 1:A:36:LEU:HB2 | 11 | 0.35 |
| (1,177) | 1:A:22:LEU:HD11 | 1:A:24:GLY:HA2 | 3 | 0.35 |
| (1,177) | 1:A:22:LEU:HD12 | 1:A:24:GLY:HA2 | 3 | 0.35 |
| (1,177) | 1:A:22:LEU:HD13 | 1:A:24:GLY:HA2 | 3 | 0.35 |
| (1,1642) | 1:A:9:LEU:HD11 | 1:A:6:GLN:HE21 | 1 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1642) | 1:A:9:LEU:HD12 | 1:A:6:GLN:HE21 | 1 | 0.35 |
| (1,1642) | 1:A:9:LEU:HD13 | 1:A:6:GLN:HE21 | 1 | 0.35 |
| (1,1638) | 1:A:57:PRO:HB3 | 1:A:59:ARG:HB2 | 19 | 0.35 |
| (1,1491) | 1:A:42:VAL:HG21 | 1:A:46:GLN:HG2 | 16 | 0.35 |
| (1,1491) | 1:A:42:VAL:HG22 | 1:A:46:GLN:HG2 | 16 | 0.35 |
| (1,1491) | 1:A:42:VAL:HG23 | 1:A:46:GLN:HG2 | 16 | 0.35 |
| (1,1369) | 1:A:71:GLU:HG2 | 1:A:72:MET:H | 19 | 0.35 |
| (1,1303) | 1:A:64:LEU:HB2 | 1:A:31:LEU:HB3 | 19 | 0.35 |
| (1,1303) | 1:A:64:LEU:HB2 | 1:A:31:LEU:HB3 | 22 | 0.35 |
| (1,1302) | 1:A:64:LEU:HB3 | 1:A:31:LEU:HB3 | 16 | 0.35 |
| (1,1183) | 1:A:56:LEU:HB2 | 1:A:57:PRO:HB2 | 14 | 0.35 |
| (1,1183) | 1:A:56:LEU:HB2 | 1:A:57:PRO:HG2 | 14 | 0.35 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD21 | 27 | 0.34 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD22 | 27 | 0.34 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD23 | 27 | 0.34 |
| (1,787) | 1:A:51:GLU:HB3 | 1:A:6:GLN:HE21 | 3 | 0.34 |
| (1,394) | 1:A:19:ILE:HG21 | 1:A:25:ILE:HG13 | 7 | 0.34 |
| (1,394) | 1:A:19:ILE:HG22 | 1:A:25:ILE:HG13 | 7 | 0.34 |
| (1,394) | 1:A:19:ILE:HG23 | 1:A:25:ILE:HG13 | 7 | 0.34 |
| (1,1369) | 1:A:71:GLU:HG2 | 1:A:72:MET:H | 10 | 0.34 |
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB2 | 20 | 0.33 |
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB3 | 20 | 0.33 |
| (1,502) | 1:A:19:ILE:HD11 | 1:A:25:ILE:HG13 | 1 | 0.33 |
| (1,502) | 1:A:19:ILE:HD12 | 1:A:25:ILE:HG13 | 1 | 0.33 |
| (1,502) | 1:A:19:ILE:HD13 | 1:A:25:ILE:HG13 | 1 | 0.33 |
| (1,1389) | 1:A:12:ALA:HB1 | 1:A:9:LEU:HD21 | 13 | 0.33 |
| (1,1389) | 1:A:12:ALA:HB1 | 1:A:9:LEU:HD22 | 13 | 0.33 |
| (1,1389) | 1:A:12:ALA:HB1 | 1:A:9:LEU:HD23 | 13 | 0.33 |
| (1,1389) | 1:A:12:ALA:HB2 | 1:A:9:LEU:HD21 | 13 | 0.33 |
| (1,1389) | 1:A:12:ALA:HB2 | 1:A:9:LEU:HD22 | 13 | 0.33 |
| (1,1389) | 1:A:12:ALA:HB2 | 1:A:9:LEU:HD23 | 13 | 0.33 |
| (1,1389) | 1:A:12:ALA:HB3 | 1:A:9:LEU:HD21 | 13 | 0.33 |
| (1,1389) | 1:A:12:ALA:HB3 | 1:A:9:LEU:HD22 | 13 | 0.33 |
| (1,1389) | 1:A:12:ALA:HB3 | 1:A:9:LEU:HD23 | 13 | 0.33 |
| (1,1369) | 1:A:71:GLU:HG2 | 1:A:72:MET:H | 28 | 0.33 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD21 | 3 | 0.32 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD22 | 3 | 0.32 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD23 | 3 | 0.32 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 14 | 0.32 |
| (1,668) | 1:A:49:GLU:HG2 | 1:A:46:GLN:HA | 18 | 0.32 |
| (1,468) | 1:A:47:ILE:HA | 1:A:48:LEU:HD11 | 22 | 0.32 |
| (1,468) | 1:A:47:ILE:HA | 1:A:48:LEU:HD12 | 22 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,468) | 1:A:47:ILE:HA | 1:A:48:LEU:HD13 | 22 | 0.32 |
| (1,460) | 1:A:47:ILE:HG13 | 1:A:48:LEU:HD11 | 2 | 0.32 |
| (1,460) | 1:A:47:ILE:HG13 | 1:A:48:LEU:HD12 | 2 | 0.32 |
| (1,460) | 1:A:47:ILE:HG13 | 1:A:48:LEU:HD13 | 2 | 0.32 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 27 | 0.32 |
| (1,1018) | 1:A:34:LEU:HD21 | 1:A:29:SER:HB2 | 13 | 0.32 |
| (1,1018) | 1:A:34:LEU:HD22 | 1:A:29:SER:HB2 | 13 | 0.32 |
| (1,1018) | 1:A:34:LEU:HD23 | 1:A:29:SER:HB2 | 13 | 0.32 |
| (1,1018) | 1:A:34:LEU:HD21 | 1:A:29:SER:HB2 | 20 | 0.32 |
| (1,1018) | 1:A:34:LEU:HD22 | 1:A:29:SER:HB2 | 20 | 0.32 |
| (1,1018) | 1:A:34:LEU:HD23 | 1:A:29:SER:HB2 | 20 | 0.32 |
| (1,54) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HD3 | 16 | 0.31 |
| (1,54) | 1:A:20:ARG:HG3 | 1:A:10:VAL:HA | 16 | 0.31 |
| (1,54) | 1:A:7:ARG:HG2 | 1:A:10:VAL:HA | 16 | 0.31 |
| (1,54) | 1:A:7:ARG:HG3 | 1:A:10:VAL:HA | 16 | 0.31 |
| (1,236) | 1:A:31:LEU:HD11 | 1:A:66:LEU:H | 13 | 0.31 |
| (1,236) | 1:A:31:LEU:HD12 | 1:A:66:LEU:H | 13 | 0.31 |
| (1,236) | 1:A:31:LEU:HD13 | 1:A:66:LEU:H | 13 | 0.31 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD2 | 14 | 0.31 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD3 | 14 | 0.31 |
| (1,1369) | 1:A:71:GLU:HG2 | 1:A:72:MET:H | 21 | 0.31 |
| (1,1220) | 1:A:58:ILE:HG21 | 1:A:62:ARG:HD2 | 26 | 0.31 |
| (1,1220) | 1:A:58:ILE:HG22 | 1:A:62:ARG:HD2 | 26 | 0.31 |
| (1,1220) | 1:A:58:ILE:HG23 | 1:A:62:ARG:HD2 | 26 | 0.31 |
| (1,1018) | 1:A:34:LEU:HD21 | 1:A:29:SER:HB2 | 14 | 0.31 |
| (1,1018) | 1:A:34:LEU:HD22 | 1:A:29:SER:HB2 | 14 | 0.31 |
| (1,1018) | 1:A:34:LEU:HD23 | 1:A:29:SER:HB2 | 14 | 0.31 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD21 | 17 | 0.3 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD22 | 17 | 0.3 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD23 | 17 | 0.3 |
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB2 | 3 | 0.3 |
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB3 | 3 | 0.3 |
| (1,60) | 1:A:47:ILE:HG21 | 1:A:74:SER:HB2 | 14 | 0.3 |
| (1,60) | 1:A:47:ILE:HG22 | 1:A:74:SER:HB2 | 14 | 0.3 |
| (1,60) | 1:A:47:ILE:HG23 | 1:A:74:SER:HB2 | 14 | 0.3 |
| (1,60) | 1:A:58:ILE:HG21 | 1:A:31:LEU:HA | 14 | 0.3 |
| (1,60) | 1:A:58:ILE:HG22 | 1:A:31:LEU:HA | 14 | 0.3 |
| (1,60) | 1:A:58:ILE:HG23 | 1:A:31:LEU:HA | 14 | 0.3 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 19 | 0.3 |
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 19 | 0.3 |
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 19 | 0.3 |
| (1,469) | 1:A:17:LEU:HD11 | 1:A:16:ILE:H | 16 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,469) | 1:A:17:LEU:HD12 | 1:A:16:ILE:H | 16 | 0.3 |
| (1,469) | 1:A:17:LEU:HD13 | 1:A:16:ILE:H | 16 | 0.3 |
| (1,294) | 1:A:17:LEU:HD11 | 1:A:36:LEU:HB2 | 3 | 0.3 |
| (1,294) | 1:A:17:LEU:HD12 | 1:A:36:LEU:HB2 | 3 | 0.3 |
| (1,294) | 1:A:17:LEU:HD13 | 1:A:36:LEU:HB2 | 3 | 0.3 |
| (1,294) | 1:A:17:LEU:HD21 | 1:A:36:LEU:HB2 | 3 | 0.3 |
| (1,294) | 1:A:17:LEU:HD22 | 1:A:36:LEU:HB2 | 3 | 0.3 |
| (1,294) | 1:A:17:LEU:HD23 | 1:A:36:LEU:HB2 | 3 | 0.3 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD2 | 9 | 0.3 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD3 | 9 | 0.3 |
| (1,1542) | 1:A:44:VAL:HG21 | 1:A:40:MET:HB2 | 18 | 0.3 |
| (1,1542) | 1:A:44:VAL:HG22 | 1:A:40:MET:HB2 | 18 | 0.3 |
| (1,1542) | 1:A:44:VAL:HG23 | 1:A:40:MET:HB2 | 18 | 0.3 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 25 | 0.3 |
| (1,1263) | 1:A:61:VAL:HG11 | 1:A:62:ARG:HB3 | 22 | 0.3 |
| (1,1263) | 1:A:61:VAL:HG12 | 1:A:62:ARG:HB3 | 22 | 0.3 |
| (1,1263) | 1:A:61:VAL:HG13 | 1:A:62:ARG:HB3 | 22 | 0.3 |
| (1,1018) | 1:A:34:LEU:HD21 | 1:A:29:SER:HB2 | 26 | 0.3 |
| (1,1018) | 1:A:34:LEU:HD22 | 1:A:29:SER:HB2 | 26 | 0.3 |
| (1,1018) | 1:A:34:LEU:HD23 | 1:A:29:SER:HB2 | 26 | 0.3 |
| (1,668) | 1:A:49:GLU:HG2 | 1:A:46:GLN:HA | 29 | 0.29 |
| (1,1263) | 1:A:61:VAL:HG11 | 1:A:62:ARG:HB3 | 7 | 0.29 |
| (1,1263) | 1:A:61:VAL:HG12 | 1:A:62:ARG:HB3 | 7 | 0.29 |
| (1,1263) | 1:A:61:VAL:HG13 | 1:A:62:ARG:HB3 | 7 | 0.29 |
| (1,1099) | 1:A:40:MET:HG3 | 1:A:39:LEU:HD21 | 8 | 0.29 |
| (1,1099) | 1:A:40:MET:HG3 | 1:A:39:LEU:HD22 | 8 | 0.29 |
| (1,1099) | 1:A:40:MET:HG3 | 1:A:39:LEU:HD23 | 8 | 0.29 |
| (1,1019) | 1:A:34:LEU:HD21 | 1:A:34:LEU:HA | 5 | 0.29 |
| (1,1019) | 1:A:34:LEU:HD22 | 1:A:34:LEU:HA | 5 | 0.29 |
| (1,1019) | 1:A:34:LEU:HD23 | 1:A:34:LEU:HA | 5 | 0.29 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD21 | 13 | 0.28 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD22 | 13 | 0.28 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD23 | 13 | 0.28 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD21 | 14 | 0.28 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD22 | 14 | 0.28 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD23 | 14 | 0.28 |
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB2 | 30 | 0.28 |
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB3 | 30 | 0.28 |
| (1,1491) | 1:A:42:VAL:HG21 | 1:A:46:GLN:HG2 | 4 | 0.28 |
| (1,1491) | 1:A:42:VAL:HG22 | 1:A:46:GLN:HG2 | 4 | 0.28 |
| (1,1491) | 1:A:42:VAL:HG23 | 1:A:46:GLN:HG2 | 4 | 0.28 |
| (1,1018) | 1:A:34:LEU:HD21 | 1:A:29:SER:HB2 | 24 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1018) | 1:A:34:LEU:HD22 | 1:A:29:SER:HB2 | 24 | 0.28 |
| (1,1018) | 1:A:34:LEU:HD23 | 1:A:29:SER:HB2 | 24 | 0.28 |
| (1,787) | 1:A:51:GLU:HB3 | 1:A:6:GLN:HE21 | 26 | 0.27 |
| (1,549) | 1:A:72:MET:HB2 | 1:A:72:MET:H | 18 | 0.27 |
| (1,502) | 1:A:19:ILE:HD11 | 1:A:25:ILE:HG13 | 24 | 0.27 |
| (1,502) | 1:A:19:ILE:HD12 | 1:A:25:ILE:HG13 | 24 | 0.27 |
| (1,502) | 1:A:19:ILE:HD13 | 1:A:25:ILE:HG13 | 24 | 0.27 |
| (1,1584) | 1:A:59:ARG:HG3 | 1:A:58:ILE:H | 22 | 0.27 |
| (1,1548) | 1:A:19:ILE:HG21 | 1:A:21:ASP:HB2 | 25 | 0.27 |
| (1,1548) | 1:A:19:ILE:HG22 | 1:A:21:ASP:HB2 | 25 | 0.27 |
| (1,1548) | 1:A:19:ILE:HG23 | 1:A:21:ASP:HB2 | 25 | 0.27 |
| (1,1540) | 1:A:44:VAL:HG21 | 1:A:40:MET:HA | 18 | 0.27 |
| (1,1540) | 1:A:44:VAL:HG22 | 1:A:40:MET:HA | 18 | 0.27 |
| (1,1540) | 1:A:44:VAL:HG23 | 1:A:40:MET:HA | 18 | 0.27 |
| (1,1180) | 1:A:55:VAL:HG21 | 1:A:53:ASP:HA | 1 | 0.27 |
| (1,1180) | 1:A:55:VAL:HG22 | 1:A:53:ASP:HA | 1 | 0.27 |
| (1,1180) | 1:A:55:VAL:HG23 | 1:A:53:ASP:HA | 1 | 0.27 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD21 | 24 | 0.26 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD22 | 24 | 0.26 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD23 | 24 | 0.26 |
| (1,549) | 1:A:72:MET:HB2 | 1:A:72:MET:H | 6 | 0.26 |
| (1,1643) | 1:A:9:LEU:HD11 | 1:A:72:MET:H | 13 | 0.26 |
| (1,1643) | 1:A:9:LEU:HD12 | 1:A:72:MET:H | 13 | 0.26 |
| (1,1643) | 1:A:9:LEU:HD13 | 1:A:72:MET:H | 13 | 0.26 |
| (1,1584) | 1:A:59:ARG:HG3 | 1:A:58:ILE:H | 1 | 0.26 |
| (1,1575) | 1:A:66:LEU:HD11 | 1:A:13:VAL:H | 11 | 0.26 |
| (1,1575) | 1:A:66:LEU:HD12 | 1:A:13:VAL:H | 11 | 0.26 |
| (1,1575) | 1:A:66:LEU:HD13 | 1:A:13:VAL:H | 11 | 0.26 |
| (1,1554) | 1:A:34:LEU:HD21 | 1:A:26:ASN:HB3 | 24 | 0.26 |
| (1,1554) | 1:A:34:LEU:HD22 | 1:A:26:ASN:HB3 | 24 | 0.26 |
| (1,1554) | 1:A:34:LEU:HD23 | 1:A:26:ASN:HB3 | 24 | 0.26 |
| (1,111) | 1:A:55:VAL:HG21 | 1:A:49:GLU:HG3 | 25 | 0.26 |
| (1,111) | 1:A:55:VAL:HG22 | 1:A:49:GLU:HG3 | 25 | 0.26 |
| (1,111) | 1:A:55:VAL:HG23 | 1:A:49:GLU:HG3 | 25 | 0.26 |
| (1,1091) | 1:A:39:LEU:HD11 | 1:A:39:LEU:HA | 8 | 0.26 |
| (1,1091) | 1:A:39:LEU:HD12 | 1:A:39:LEU:HA | 8 | 0.26 |
| (1,1091) | 1:A:39:LEU:HD13 | 1:A:39:LEU:HA | 8 | 0.26 |
| (1,1020) | 1:A:34:LEU:HD21 | 1:A:33:ASP:HB2 | 29 | 0.26 |
| (1,1020) | 1:A:34:LEU:HD22 | 1:A:33:ASP:HB2 | 29 | 0.26 |
| (1,1020) | 1:A:34:LEU:HD23 | 1:A:33:ASP:HB2 | 29 | 0.26 |
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB2 | 24 | 0.25 |
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB3 | 24 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB2 | 28 | 0.25 |
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB3 | 28 | 0.25 |
| (1,798) | 1:A:51:GLU:HG2 | 1:A:50:ARG:HG2 | 15 | 0.25 |
| (1,798) | 1:A:51:GLU:HG3 | 1:A:50:ARG:HG2 | 15 | 0.25 |
| (1,60) | 1:A:47:ILE:HG21 | 1:A:74:SER:HB2 | 23 | 0.25 |
| (1,60) | 1:A:47:ILE:HG22 | 1:A:74:SER:HB2 | 23 | 0.25 |
| (1,60) | 1:A:47:ILE:HG23 | 1:A:74:SER:HB2 | 23 | 0.25 |
| (1,60) | 1:A:58:ILE:HG21 | 1:A:31:LEU:HA | 23 | 0.25 |
| (1,60) | 1:A:58:ILE:HG22 | 1:A:31:LEU:HA | 23 | 0.25 |
| (1,60) | 1:A:58:ILE:HG23 | 1:A:31:LEU:HA | 23 | 0.25 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 1 | 0.25 |
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 1 | 0.25 |
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 1 | 0.25 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 15 | 0.25 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 15 | 0.25 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 29 | 0.25 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD21 | 26 | 0.24 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD22 | 26 | 0.24 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD23 | 26 | 0.24 |
| (1,787) | 1:A:51:GLU:HB3 | 1:A:6:GLN:HE21 | 15 | 0.24 |
| (1,779) | 1:A:52:HIS:HB2 | 1:A:6:GLN:HE21 | 11 | 0.24 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 17 | 0.24 |
| (1,664) | 1:A:49:GLU:HG2 | 1:A:55:VAL:HG21 | 15 | 0.24 |
| (1,664) | 1:A:49:GLU:HG2 | 1:A:55:VAL:HG22 | 15 | 0.24 |
| (1,664) | 1:A:49:GLU:HG2 | 1:A:55:VAL:HG23 | 15 | 0.24 |
| (1,1698) | 1:A:38:SER:H | 1:A:39:LEU:H | 22 | 0.24 |
| (1,1642) | 1:A:9:LEU:HD11 | 1:A:6:GLN:HE21 | 7 | 0.24 |
| (1,1642) | 1:A:9:LEU:HD12 | 1:A:6:GLN:HE21 | 7 | 0.24 |
| (1,1642) | 1:A:9:LEU:HD13 | 1:A:6:GLN:HE21 | 7 | 0.24 |
| (1,54) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HD3 | 18 | 0.23 |
| (1,54) | 1:A:20:ARG:HG3 | 1:A:10:VAL:HA | 18 | 0.23 |
| (1,54) | 1:A:7:ARG:HG2 | 1:A:10:VAL:HA | 18 | 0.23 |
| (1,54) | 1:A:7:ARG:HG3 | 1:A:10:VAL:HA | 18 | 0.23 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 3 | 0.23 |
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 3 | 0.23 |
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 3 | 0.23 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 15 | 0.23 |
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 15 | 0.23 |
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 15 | 0.23 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 26 | 0.23 |
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 26 | 0.23 |
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 26 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,177) | 1:A:22:LEU:HD11 | 1:A:24:GLY:HA2 | 2 | 0.23 |
| (1,177) | 1:A:22:LEU:HD12 | 1:A:24:GLY:HA2 | 2 | 0.23 |
| (1,177) | 1:A:22:LEU:HD13 | 1:A:24:GLY:HA2 | 2 | 0.23 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 5 | 0.23 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 5 | 0.23 |
| (1,1303) | 1:A:64:LEU:HB2 | 1:A:31:LEU:HB3 | 15 | 0.23 |
| (1,1263) | 1:A:61:VAL:HG11 | 1:A:62:ARG:HB3 | 21 | 0.23 |
| (1,1263) | 1:A:61:VAL:HG12 | 1:A:62:ARG:HB3 | 21 | 0.23 |
| (1,1263) | 1:A:61:VAL:HG13 | 1:A:62:ARG:HB3 | 21 | 0.23 |
| (1,1133) | 1:A:53:ASP:HA | 1:A:53:ASP:H | 12 | 0.23 |
| (1,1082) | 1:A:39:LEU:HB3 | 1:A:39:LEU:H | 17 | 0.23 |
| (1,1028) | 1:A:34:LEU:HD21 | 1:A:33:ASP:H | 26 | 0.23 |
| (1,1028) | 1:A:34:LEU:HD22 | 1:A:33:ASP:H | 26 | 0.23 |
| (1,1028) | 1:A:34:LEU:HD23 | 1:A:33:ASP:H | 26 | 0.23 |
| (1,774) | 1:A:6:GLN:HA | 1:A:6:GLN:HG3 | 16 | 0.22 |
| (1,700) | 1:A:59:ARG:HA | 1:A:62:ARG:HD2 | 30 | 0.22 |
| (1,502) | 1:A:19:ILE:HD11 | 1:A:25:ILE:HG13 | 7 | 0.22 |
| (1,502) | 1:A:19:ILE:HD12 | 1:A:25:ILE:HG13 | 7 | 0.22 |
| (1,502) | 1:A:19:ILE:HD13 | 1:A:25:ILE:HG13 | 7 | 0.22 |
| (1,394) | 1:A:19:ILE:HG21 | 1:A:25:ILE:HG13 | 9 | 0.22 |
| (1,394) | 1:A:19:ILE:HG22 | 1:A:25:ILE:HG13 | 9 | 0.22 |
| (1,394) | 1:A:19:ILE:HG23 | 1:A:25:ILE:HG13 | 9 | 0.22 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD2 | 12 | 0.22 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD3 | 12 | 0.22 |
| (1,1303) | 1:A:64:LEU:HB2 | 1:A:31:LEU:HB3 | 18 | 0.22 |
| (1,1271) | 1:A:62:ARG:HA | 1:A:58:ILE:HG12 | 14 | 0.22 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD21 | 20 | 0.21 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD22 | 20 | 0.21 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD23 | 20 | 0.21 |
| (1,952) | 1:A:11:LYS:HG2 | 1:A:11:LYS:H | 8 | 0.21 |
| (1,844) | 1:A:8:ASP:HB3 | 1:A:11:LYS:HB2 | 18 | 0.21 |
| (1,844) | 1:A:8:ASP:HB3 | 1:A:11:LYS:HB3 | 18 | 0.21 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 13 | 0.21 |
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 13 | 0.21 |
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 13 | 0.21 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 14 | 0.21 |
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 14 | 0.21 |
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 14 | 0.21 |
| (1,394) | 1:A:19:ILE:HG21 | 1:A:25:ILE:HG13 | 4 | 0.21 |
| (1,394) | 1:A:19:ILE:HG22 | 1:A:25:ILE:HG13 | 4 | 0.21 |
| (1,394) | 1:A:19:ILE:HG23 | 1:A:25:ILE:HG13 | 4 | 0.21 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 1 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 3 | 0.21 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 8 | 0.21 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 13 | 0.21 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 16 | 0.21 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 24 | 0.21 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 17 | 0.21 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 17 | 0.21 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 17 | 0.21 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 26 | 0.21 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 26 | 0.21 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 26 | 0.21 |
| (1,1593) | 1:A:34:LEU:HD21 | 1:A:29:SER:HA | 28 | 0.21 |
| (1,1593) | 1:A:34:LEU:HD22 | 1:A:29:SER:HA | 28 | 0.21 |
| (1,1593) | 1:A:34:LEU:HD23 | 1:A:29:SER:HA | 28 | 0.21 |
| (1,1327) | 1:A:68:LYS:HD2 | 1:A:71:GLU:HB2 | 11 | 0.21 |
| (1,1327) | 1:A:68:LYS:HD3 | 1:A:71:GLU:HB2 | 11 | 0.21 |
| (1,1302) | 1:A:64:LEU:HB3 | 1:A:31:LEU:HB3 | 5 | 0.21 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB1 | 16 | 0.21 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB2 | 16 | 0.21 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB3 | 16 | 0.21 |
| (1,1049) | 1:A:36:LEU:HD21 | 1:A:40:MET:HB3 | 9 | 0.21 |
| (1,1049) | 1:A:36:LEU:HD22 | 1:A:40:MET:HB3 | 9 | 0.21 |
| (1,1049) | 1:A:36:LEU:HD23 | 1:A:40:MET:HB3 | 9 | 0.21 |
| (1,1018) | 1:A:34:LEU:HD21 | 1:A:29:SER:HB2 | 17 | 0.21 |
| (1,1018) | 1:A:34:LEU:HD22 | 1:A:29:SER:HB2 | 17 | 0.21 |
| (1,1018) | 1:A:34:LEU:HD23 | 1:A:29:SER:HB2 | 17 | 0.21 |
| (1,1018) | 1:A:34:LEU:HD21 | 1:A:29:SER:HB2 | 19 | 0.21 |
| (1,1018) | 1:A:34:LEU:HD22 | 1:A:29:SER:HB2 | 19 | 0.21 |
| (1,1018) | 1:A:34:LEU:HD23 | 1:A:29:SER:HB2 | 19 | 0.21 |
| (1,1018) | 1:A:34:LEU:HD21 | 1:A:29:SER:HB2 | 28 | 0.21 |
| (1,1018) | 1:A:34:LEU:HD22 | 1:A:29:SER:HB2 | 28 | 0.21 |
| (1,1018) | 1:A:34:LEU:HD23 | 1:A:29:SER:HB2 | 28 | 0.21 |
| (1,1008) | 1:A:34:LEU:HD11 | 1:A:31:LEU:HA | 19 | 0.21 |
| (1,1008) | 1:A:34:LEU:HD12 | 1:A:31:LEU:HA | 19 | 0.21 |
| (1,1008) | 1:A:34:LEU:HD13 | 1:A:31:LEU:HA | 19 | 0.21 |
| (1,927) | 1:A:57:PRO:HG3 | 1:A:56:LEU:HD21 | 20 | 0.2 |
| (1,927) | 1:A:57:PRO:HG3 | 1:A:56:LEU:HD22 | 20 | 0.2 |
| (1,927) | 1:A:57:PRO:HG3 | 1:A:56:LEU:HD23 | 20 | 0.2 |
| (1,85) | 1:A:24:GLY:H | 1:A:23:ALA:HA | 1 | 0.2 |
| (1,85) | 1:A:24:GLY:H | 1:A:25:ILE:HA | 1 | 0.2 |
| (1,664) | 1:A:49:GLU:HG2 | 1:A:55:VAL:HG21 | 25 | 0.2 |
| (1,664) | 1:A:49:GLU:HG2 | 1:A:55:VAL:HG22 | 25 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,664) | 1:A:49:GLU:HG2 | 1:A:55:VAL:HG23 | 25 | 0.2 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 2 | 0.2 |
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 2 | 0.2 |
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 2 | 0.2 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 8 | 0.2 |
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 8 | 0.2 |
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 8 | 0.2 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 22 | 0.2 |
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 22 | 0.2 |
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 22 | 0.2 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 4 | 0.2 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 5 | 0.2 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 6 | 0.2 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 7 | 0.2 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 9 | 0.2 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 11 | 0.2 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 12 | 0.2 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 20 | 0.2 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 21 | 0.2 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 23 | 0.2 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 26 | 0.2 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 27 | 0.2 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 29 | 0.2 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 30 | 0.2 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 11 | 0.2 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 11 | 0.2 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 11 | 0.2 |
| (1,192) | 1:A:29:SER:HB3 | 1:A:34:LEU:HD21 | 24 | 0.2 |
| (1,192) | 1:A:29:SER:HB3 | 1:A:34:LEU:HD22 | 24 | 0.2 |
| (1,192) | 1:A:29:SER:HB3 | 1:A:34:LEU:HD23 | 24 | 0.2 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD2 | 19 | 0.2 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD3 | 19 | 0.2 |
| (1,1584) | 1:A:59:ARG:HG3 | 1:A:58:ILE:H | 15 | 0.2 |
| (1,1554) | 1:A:34:LEU:HD21 | 1:A:26:ASN:HB3 | 27 | 0.2 |
| (1,1554) | 1:A:34:LEU:HD22 | 1:A:26:ASN:HB3 | 27 | 0.2 |
| (1,1554) | 1:A:34:LEU:HD23 | 1:A:26:ASN:HB3 | 27 | 0.2 |
| (1,1548) | 1:A:19:ILE:HG21 | 1:A:21:ASP:HB2 | 1 | 0.2 |
| (1,1548) | 1:A:19:ILE:HG22 | 1:A:21:ASP:HB2 | 1 | 0.2 |
| (1,1548) | 1:A:19:ILE:HG23 | 1:A:21:ASP:HB2 | 1 | 0.2 |
| (1,1491) | 1:A:42:VAL:HG21 | 1:A:46:GLN:HG2 | 20 | 0.2 |
| (1,1491) | 1:A:42:VAL:HG22 | 1:A:46:GLN:HG2 | 20 | 0.2 |
| (1,1491) | 1:A:42:VAL:HG23 | 1:A:46:GLN:HG2 | 20 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1415) | 1:A:42:VAL:HG11 | 1:A:46:GLN:HE21 | 6 | 0.2 |
| (1,1415) | 1:A:42:VAL:HG12 | 1:A:46:GLN:HE21 | 6 | 0.2 |
| (1,1415) | 1:A:42:VAL:HG13 | 1:A:46:GLN:HE21 | 6 | 0.2 |
| (1,1369) | 1:A:71:GLU:HG2 | 1:A:72:MET:H | 12 | 0.2 |
| (1,1354) | 1:A:69:LEU:HD21 | 1:A:67:ARG:HD3 | 9 | 0.2 |
| (1,1354) | 1:A:69:LEU:HD22 | 1:A:67:ARG:HD3 | 9 | 0.2 |
| (1,1354) | 1:A:69:LEU:HD23 | 1:A:67:ARG:HD3 | 9 | 0.2 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB1 | 13 | 0.2 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB2 | 13 | 0.2 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB3 | 13 | 0.2 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB1 | 17 | 0.2 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB2 | 17 | 0.2 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB3 | 17 | 0.2 |
| (1,1037) | 1:A:36:LEU:HB3 | 1:A:40:MET:HA | 5 | 0.2 |
| (1,1028) | 1:A:34:LEU:HD21 | 1:A:33:ASP:H | 17 | 0.2 |
| (1,1028) | 1:A:34:LEU:HD22 | 1:A:33:ASP:H | 17 | 0.2 |
| (1,1028) | 1:A:34:LEU:HD23 | 1:A:33:ASP:H | 17 | 0.2 |
| (1,1018) | 1:A:34:LEU:HD21 | 1:A:29:SER:HB2 | 29 | 0.2 |
| (1,1018) | 1:A:34:LEU:HD22 | 1:A:29:SER:HB2 | 29 | 0.2 |
| (1,1018) | 1:A:34:LEU:HD23 | 1:A:29:SER:HB2 | 29 | 0.2 |
| (1,700) | 1:A:59:ARG:HA | 1:A:62:ARG:HD2 | 27 | 0.19 |
| (1,571) | 1:A:43:GLU:HB3 | 1:A:44:VAL:HG21 | 18 | 0.19 |
| (1,571) | 1:A:43:GLU:HB3 | 1:A:44:VAL:HG22 | 18 | 0.19 |
| (1,571) | 1:A:43:GLU:HB3 | 1:A:44:VAL:HG23 | 18 | 0.19 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 2 | 0.19 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 10 | 0.19 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 15 | 0.19 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 18 | 0.19 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 19 | 0.19 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 22 | 0.19 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 25 | 0.19 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 28 | 0.19 |
| (1,294) | 1:A:17:LEU:HD11 | 1:A:36:LEU:HB2 | 4 | 0.19 |
| (1,294) | 1:A:17:LEU:HD12 | 1:A:36:LEU:HB2 | 4 | 0.19 |
| (1,294) | 1:A:17:LEU:HD13 | 1:A:36:LEU:HB2 | 4 | 0.19 |
| (1,294) | 1:A:17:LEU:HD21 | 1:A:36:LEU:HB2 | 4 | 0.19 |
| (1,294) | 1:A:17:LEU:HD22 | 1:A:36:LEU:HB2 | 4 | 0.19 |
| (1,294) | 1:A:17:LEU:HD23 | 1:A:36:LEU:HB2 | 4 | 0.19 |
| (1,18) | 1:A:71:GLU:HA | 1:A:74:SER:H | 6 | 0.19 |
| (1,18) | 1:A:71:GLU:HA | 1:A:69:LEU:H | 6 | 0.19 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD2 | 16 | 0.19 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD3 | 16 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1491) | 1:A:42:VAL:HG21 | 1:A:46:GLN:HG2 | 21 | 0.19 |
| (1,1491) | 1:A:42:VAL:HG22 | 1:A:46:GLN:HG2 | 21 | 0.19 |
| (1,1491) | 1:A:42:VAL:HG23 | 1:A:46:GLN:HG2 | 21 | 0.19 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB1 | 15 | 0.19 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB2 | 15 | 0.19 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB3 | 15 | 0.19 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB1 | 20 | 0.19 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB2 | 20 | 0.19 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB3 | 20 | 0.19 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD21 | 29 | 0.18 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD22 | 29 | 0.18 |
| (1,994) | 1:A:33:ASP:HA | 1:A:34:LEU:HD23 | 29 | 0.18 |
| (1,972) | 1:A:27:LEU:HD21 | 1:A:70:GLN:HE21 | 2 | 0.18 |
| (1,972) | 1:A:27:LEU:HD22 | 1:A:70:GLN:HE21 | 2 | 0.18 |
| (1,972) | 1:A:27:LEU:HD23 | 1:A:70:GLN:HE21 | 2 | 0.18 |
| (1,85) | 1:A:24:GLY:H | 1:A:23:ALA:HA | 14 | 0.18 |
| (1,85) | 1:A:24:GLY:H | 1:A:25:ILE:HA | 14 | 0.18 |
| (1,779) | 1:A:52:HIS:HB2 | 1:A:6:GLN:HE21 | 7 | 0.18 |
| (1,668) | 1:A:49:GLU:HG2 | 1:A:46:GLN:HA | 19 | 0.18 |
| (1,460) | 1:A:47:ILE:HG13 | 1:A:48:LEU:HD11 | 22 | 0.18 |
| (1,460) | 1:A:47:ILE:HG13 | 1:A:48:LEU:HD12 | 22 | 0.18 |
| (1,460) | 1:A:47:ILE:HG13 | 1:A:48:LEU:HD13 | 22 | 0.18 |
| (1,394) | 1:A:19:ILE:HG21 | 1:A:25:ILE:HG13 | 29 | 0.18 |
| (1,394) | 1:A:19:ILE:HG22 | 1:A:25:ILE:HG13 | 29 | 0.18 |
| (1,394) | 1:A:19:ILE:HG23 | 1:A:25:ILE:HG13 | 29 | 0.18 |
| (1,38) | 1:A:58:ILE:HG21 | 1:A:32:ALA:HA | 24 | 0.18 |
| (1,38) | 1:A:58:ILE:HG22 | 1:A:32:ALA:HA | 24 | 0.18 |
| (1,38) | 1:A:58:ILE:HG23 | 1:A:32:ALA:HA | 24 | 0.18 |
| (1,38) | 1:A:47:ILE:HG21 | 1:A:50:ARG:HA | 24 | 0.18 |
| (1,38) | 1:A:47:ILE:HG22 | 1:A:50:ARG:HA | 24 | 0.18 |
| (1,38) | 1:A:47:ILE:HG23 | 1:A:50:ARG:HA | 24 | 0.18 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 14 | 0.18 |
| (1,323) | 1:A:45:ARG:HB2 | 1:A:45:ARG:HG2 | 17 | 0.18 |
| (1,316) | 1:A:40:MET:HB2 | 1:A:39:LEU:HD21 | 8 | 0.18 |
| (1,316) | 1:A:40:MET:HB2 | 1:A:39:LEU:HD22 | 8 | 0.18 |
| (1,316) | 1:A:40:MET:HB2 | 1:A:39:LEU:HD23 | 8 | 0.18 |
| (1,294) | 1:A:17:LEU:HD11 | 1:A:36:LEU:HB2 | 16 | 0.18 |
| (1,294) | 1:A:17:LEU:HD12 | 1:A:36:LEU:HB2 | 16 | 0.18 |
| (1,294) | 1:A:17:LEU:HD13 | 1:A:36:LEU:HB2 | 16 | 0.18 |
| (1,294) | 1:A:17:LEU:HD21 | 1:A:36:LEU:HB2 | 16 | 0.18 |
| (1,294) | 1:A:17:LEU:HD22 | 1:A:36:LEU:HB2 | 16 | 0.18 |
| (1,294) | 1:A:17:LEU:HD23 | 1:A:36:LEU:HB2 | 16 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,294) | 1:A:17:LEU:HD11 | 1:A:36:LEU:HB2 | 22 | 0.18 |
| (1,294) | 1:A:17:LEU:HD12 | 1:A:36:LEU:HB2 | 22 | 0.18 |
| (1,294) | 1:A:17:LEU:HD13 | 1:A:36:LEU:HB2 | 22 | 0.18 |
| (1,294) | 1:A:17:LEU:HD21 | 1:A:36:LEU:HB2 | 22 | 0.18 |
| (1,294) | 1:A:17:LEU:HD22 | 1:A:36:LEU:HB2 | 22 | 0.18 |
| (1,294) | 1:A:17:LEU:HD23 | 1:A:36:LEU:HB2 | 22 | 0.18 |
| (1,1698) | 1:A:38:SER:H | 1:A:39:LEU:H | 17 | 0.18 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 6 | 0.18 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 6 | 0.18 |
| (1,1584) | 1:A:59:ARG:HG3 | 1:A:58:ILE:H | 13 | 0.18 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 3 | 0.18 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 3 | 0.18 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 3 | 0.18 |
| (1,1491) | 1:A:42:VAL:HG21 | 1:A:46:GLN:HG2 | 24 | 0.18 |
| (1,1491) | 1:A:42:VAL:HG22 | 1:A:46:GLN:HG2 | 24 | 0.18 |
| (1,1491) | 1:A:42:VAL:HG23 | 1:A:46:GLN:HG2 | 24 | 0.18 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB1 | 18 | 0.18 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB2 | 18 | 0.18 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB3 | 18 | 0.18 |
| (1,1071) | 1:A:36:LEU:HG | 1:A:38:SER:H | 18 | 0.18 |
| (1,851) | 1:A:9:LEU:HA | 1:A:9:LEU:HD21 | 13 | 0.17 |
| (1,851) | 1:A:9:LEU:HA | 1:A:9:LEU:HD22 | 13 | 0.17 |
| (1,851) | 1:A:9:LEU:HA | 1:A:9:LEU:HD23 | 13 | 0.17 |
| (1,813) | 1:A:65:THR:HG21 | 1:A:69:LEU:H | 20 | 0.17 |
| (1,813) | 1:A:65:THR:HG22 | 1:A:69:LEU:H | 20 | 0.17 |
| (1,813) | 1:A:65:THR:HG23 | 1:A:69:LEU:H | 20 | 0.17 |
| (1,813) | 1:A:65:THR:HG21 | 1:A:69:LEU:H | 22 | 0.17 |
| (1,813) | 1:A:65:THR:HG22 | 1:A:69:LEU:H | 22 | 0.17 |
| (1,813) | 1:A:65:THR:HG23 | 1:A:69:LEU:H | 22 | 0.17 |
| (1,813) | 1:A:65:THR:HG21 | 1:A:69:LEU:H | 29 | 0.17 |
| (1,813) | 1:A:65:THR:HG22 | 1:A:69:LEU:H | 29 | 0.17 |
| (1,813) | 1:A:65:THR:HG23 | 1:A:69:LEU:H | 29 | 0.17 |
| (1,662) | 1:A:49:GLU:HA | 1:A:46:GLN:HA | 5 | 0.17 |
| (1,662) | 1:A:49:GLU:HA | 1:A:46:GLN:HA | 8 | 0.17 |
| (1,549) | 1:A:72:MET:HB2 | 1:A:72:MET:H | 13 | 0.17 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 5 | 0.17 |
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 5 | 0.17 |
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 5 | 0.17 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 17 | 0.17 |
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 17 | 0.17 |
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 17 | 0.17 |
| (1,240) | 1:A:31:LEU:HD11 | 1:A:34:LEU:HB2 | 5 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,240) | 1:A:31:LEU:HD12 | 1:A:34:LEU:HB2 | 5 | 0.17 |
| (1,240) | 1:A:31:LEU:HD13 | 1:A:34:LEU:HB2 | 5 | 0.17 |
| (1,18) | 1:A:71:GLU:HA | 1:A:74:SER:H | 13 | 0.17 |
| (1,18) | 1:A:71:GLU:HA | 1:A:69:LEU:H | 13 | 0.17 |
| (1,177) | 1:A:22:LEU:HD11 | 1:A:24:GLY:HA2 | 6 | 0.17 |
| (1,177) | 1:A:22:LEU:HD12 | 1:A:24:GLY:HA2 | 6 | 0.17 |
| (1,177) | 1:A:22:LEU:HD13 | 1:A:24:GLY:HA2 | 6 | 0.17 |
| (1,171) | 1:A:22:LEU:HG | 1:A:21:ASP:HA | 23 | 0.17 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD2 | 17 | 0.17 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD3 | 17 | 0.17 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 27 | 0.17 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 27 | 0.17 |
| (1,1548) | 1:A:19:ILE:HG21 | 1:A:21:ASP:HB2 | 10 | 0.17 |
| (1,1548) | 1:A:19:ILE:HG22 | 1:A:21:ASP:HB2 | 10 | 0.17 |
| (1,1548) | 1:A:19:ILE:HG23 | 1:A:21:ASP:HB2 | 10 | 0.17 |
| (1,1491) | 1:A:42:VAL:HG21 | 1:A:46:GLN:HG2 | 27 | 0.17 |
| (1,1491) | 1:A:42:VAL:HG22 | 1:A:46:GLN:HG2 | 27 | 0.17 |
| (1,1491) | 1:A:42:VAL:HG23 | 1:A:46:GLN:HG2 | 27 | 0.17 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB1 | 7 | 0.17 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB2 | 7 | 0.17 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB3 | 7 | 0.17 |
| (1,1133) | 1:A:53:ASP:HA | 1:A:53:ASP:H | 19 | 0.17 |
| (1,1028) | 1:A:34:LEU:HD21 | 1:A:33:ASP:H | 24 | 0.17 |
| (1,1028) | 1:A:34:LEU:HD22 | 1:A:33:ASP:H | 24 | 0.17 |
| (1,1028) | 1:A:34:LEU:HD23 | 1:A:33:ASP:H | 24 | 0.17 |
| (1,862) | 1:A:10:VAL:HA | 1:A:9:LEU:HD21 | 13 | 0.16 |
| (1,862) | 1:A:10:VAL:HA | 1:A:9:LEU:HD22 | 13 | 0.16 |
| (1,862) | 1:A:10:VAL:HA | 1:A:9:LEU:HD23 | 13 | 0.16 |
| (1,85) | 1:A:24:GLY:H | 1:A:23:ALA:HA | 9 | 0.16 |
| (1,85) | 1:A:24:GLY:H | 1:A:25:ILE:HA | 9 | 0.16 |
| (1,813) | 1:A:65:THR:HG21 | 1:A:69:LEU:H | 2 | 0.16 |
| (1,813) | 1:A:65:THR:HG22 | 1:A:69:LEU:H | 2 | 0.16 |
| (1,813) | 1:A:65:THR:HG23 | 1:A:69:LEU:H | 2 | 0.16 |
| (1,813) | 1:A:65:THR:HG21 | 1:A:69:LEU:H | 4 | 0.16 |
| (1,813) | 1:A:65:THR:HG22 | 1:A:69:LEU:H | 4 | 0.16 |
| (1,813) | 1:A:65:THR:HG23 | 1:A:69:LEU:H | 4 | 0.16 |
| (1,813) | 1:A:65:THR:HG21 | 1:A:69:LEU:H | 8 | 0.16 |
| (1,813) | 1:A:65:THR:HG22 | 1:A:69:LEU:H | 8 | 0.16 |
| (1,813) | 1:A:65:THR:HG23 | 1:A:69:LEU:H | 8 | 0.16 |
| (1,549) | 1:A:72:MET:HB2 | 1:A:72:MET:H | 24 | 0.16 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 6 | 0.16 |
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 6 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 6 | 0.16 |
| (1,20) | 1:A:66:LEU:HB3 | 1:A:19:ILE:HD11 | 14 | 0.16 |
| (1,20) | 1:A:66:LEU:HB3 | 1:A:19:ILE:HD12 | 14 | 0.16 |
| (1,20) | 1:A:66:LEU:HB3 | 1:A:19:ILE:HD13 | 14 | 0.16 |
| (1,20) | 1:A:66:LEU:HB3 | 1:A:69:LEU:HD21 | 14 | 0.16 |
| (1,20) | 1:A:66:LEU:HB3 | 1:A:69:LEU:HD22 | 14 | 0.16 |
| (1,20) | 1:A:66:LEU:HB3 | 1:A:69:LEU:HD23 | 14 | 0.16 |
| (1,20) | 1:A:66:LEU:HB3 | 1:A:27:LEU:HD21 | 14 | 0.16 |
| (1,20) | 1:A:66:LEU:HB3 | 1:A:27:LEU:HD22 | 14 | 0.16 |
| (1,20) | 1:A:66:LEU:HB3 | 1:A:27:LEU:HD23 | 14 | 0.16 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 3 | 0.16 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 3 | 0.16 |
| (1,1415) | 1:A:42:VAL:HG11 | 1:A:46:GLN:HE21 | 15 | 0.16 |
| (1,1415) | 1:A:42:VAL:HG12 | 1:A:46:GLN:HE21 | 15 | 0.16 |
| (1,1415) | 1:A:42:VAL:HG13 | 1:A:46:GLN:HE21 | 15 | 0.16 |
| (1,1394) | 1:A:44:VAL:HA | 1:A:44:VAL:HG11 | 18 | 0.16 |
| (1,1394) | 1:A:44:VAL:HA | 1:A:44:VAL:HG12 | 18 | 0.16 |
| (1,1394) | 1:A:44:VAL:HA | 1:A:44:VAL:HG13 | 18 | 0.16 |
| (1,1327) | 1:A:68:LYS:HD2 | 1:A:71:GLU:HB2 | 6 | 0.16 |
| (1,1327) | 1:A:68:LYS:HD3 | 1:A:71:GLU:HB2 | 6 | 0.16 |
| (1,1314) | 1:A:64:LEU:HD21 | 1:A:68:LYS:HD2 | 12 | 0.16 |
| (1,1314) | 1:A:64:LEU:HD21 | 1:A:68:LYS:HD3 | 12 | 0.16 |
| (1,1314) | 1:A:64:LEU:HD22 | 1:A:68:LYS:HD2 | 12 | 0.16 |
| (1,1314) | 1:A:64:LEU:HD22 | 1:A:68:LYS:HD3 | 12 | 0.16 |
| (1,1314) | 1:A:64:LEU:HD23 | 1:A:68:LYS:HD2 | 12 | 0.16 |
| (1,1314) | 1:A:64:LEU:HD23 | 1:A:68:LYS:HD3 | 12 | 0.16 |
| (1,851) | 1:A:9:LEU:HA | 1:A:9:LEU:HD21 | 6 | 0.15 |
| (1,851) | 1:A:9:LEU:HA | 1:A:9:LEU:HD22 | 6 | 0.15 |
| (1,851) | 1:A:9:LEU:HA | 1:A:9:LEU:HD23 | 6 | 0.15 |
| (1,85) | 1:A:24:GLY:H | 1:A:23:ALA:HA | 30 | 0.15 |
| (1,85) | 1:A:24:GLY:H | 1:A:25:ILE:HA | 30 | 0.15 |
| (1,704) | 1:A:59:ARG:HB2 | 1:A:59:ARG:H | 9 | 0.15 |
| (1,704) | 1:A:59:ARG:HB2 | 1:A:59:ARG:H | 12 | 0.15 |
| (1,704) | 1:A:59:ARG:HB2 | 1:A:59:ARG:H | 14 | 0.15 |
| (1,502) | 1:A:19:ILE:HD11 | 1:A:25:ILE:HG13 | 9 | 0.15 |
| (1,502) | 1:A:19:ILE:HD12 | 1:A:25:ILE:HG13 | 9 | 0.15 |
| (1,502) | 1:A:19:ILE:HD13 | 1:A:25:ILE:HG13 | 9 | 0.15 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 16 | 0.15 |
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 16 | 0.15 |
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 16 | 0.15 |
| (1,394) | 1:A:19:ILE:HG21 | 1:A:25:ILE:HG13 | 6 | 0.15 |
| (1,394) | 1:A:19:ILE:HG22 | 1:A:25:ILE:HG13 | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,394) | 1:A:19:ILE:HG23 | 1:A:25:ILE:HG13 | 6 | 0.15 |
| (1,38) | 1:A:58:ILE:HG21 | 1:A:32:ALA:HA | 20 | 0.15 |
| (1,38) | 1:A:58:ILE:HG22 | 1:A:32:ALA:HA | 20 | 0.15 |
| (1,38) | 1:A:58:ILE:HG23 | 1:A:32:ALA:HA | 20 | 0.15 |
| (1,38) | 1:A:47:ILE:HG21 | 1:A:50:ARG:HA | 20 | 0.15 |
| (1,38) | 1:A:47:ILE:HG22 | 1:A:50:ARG:HA | 20 | 0.15 |
| (1,38) | 1:A:47:ILE:HG23 | 1:A:50:ARG:HA | 20 | 0.15 |
| (1,1727) | 1:A:86:LYS:H | 1:A:85:PRO:HA | 5 | 0.15 |
| (1,1698) | 1:A:38:SER:H | 1:A:39:LEU:H | 30 | 0.15 |
| (1,1584) | 1:A:59:ARG:HG3 | 1:A:58:ILE:H | 16 | 0.15 |
| (1,1569) | 1:A:10:VAL:HG21 | 1:A:70:GLN:HB2 | 7 | 0.15 |
| (1,1569) | 1:A:10:VAL:HG21 | 1:A:70:GLN:HB3 | 7 | 0.15 |
| (1,1569) | 1:A:10:VAL:HG22 | 1:A:70:GLN:HB2 | 7 | 0.15 |
| (1,1569) | 1:A:10:VAL:HG22 | 1:A:70:GLN:HB3 | 7 | 0.15 |
| (1,1569) | 1:A:10:VAL:HG23 | 1:A:70:GLN:HB2 | 7 | 0.15 |
| (1,1569) | 1:A:10:VAL:HG23 | 1:A:70:GLN:HB3 | 7 | 0.15 |
| (1,1327) | 1:A:68:LYS:HD2 | 1:A:71:GLU:HB2 | 19 | 0.15 |
| (1,1327) | 1:A:68:LYS:HD3 | 1:A:71:GLU:HB2 | 19 | 0.15 |
| (1,1163) | 1:A:54:LEU:HD11 | 1:A:51:GLU:HB2 | 18 | 0.15 |
| (1,1163) | 1:A:54:LEU:HD12 | 1:A:51:GLU:HB2 | 18 | 0.15 |
| (1,1163) | 1:A:54:LEU:HD13 | 1:A:51:GLU:HB2 | 18 | 0.15 |
| (1,1091) | 1:A:39:LEU:HD11 | 1:A:39:LEU:HA | 12 | 0.15 |
| (1,1091) | 1:A:39:LEU:HD12 | 1:A:39:LEU:HA | 12 | 0.15 |
| (1,1091) | 1:A:39:LEU:HD13 | 1:A:39:LEU:HA | 12 | 0.15 |
| (1,1061) | 1:A:36:LEU:HD21 | 1:A:38:SER:H | 7 | 0.15 |
| (1,1061) | 1:A:36:LEU:HD22 | 1:A:38:SER:H | 7 | 0.15 |
| (1,1061) | 1:A:36:LEU:HD23 | 1:A:38:SER:H | 7 | 0.15 |
| (1,1037) | 1:A:36:LEU:HB3 | 1:A:40:MET:HA | 29 | 0.15 |
| (1,1028) | 1:A:34:LEU:HD21 | 1:A:33:ASP:H | 14 | 0.15 |
| (1,1028) | 1:A:34:LEU:HD22 | 1:A:33:ASP:H | 14 | 0.15 |
| (1,1028) | 1:A:34:LEU:HD23 | 1:A:33:ASP:H | 14 | 0.15 |
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB2 | 14 | 0.14 |
| (1,845) | 1:A:8:ASP:HB2 | 1:A:11:LYS:HB3 | 14 | 0.14 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD11 | 9 | 0.14 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD12 | 9 | 0.14 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD13 | 9 | 0.14 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD21 | 9 | 0.14 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD22 | 9 | 0.14 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD23 | 9 | 0.14 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:54:LEU:HD21 | 9 | 0.14 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:54:LEU:HD22 | 9 | 0.14 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:54:LEU:HD23 | 9 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,813) | 1:A:65:THR:HG21 | 1:A:69:LEU:H | 6 | 0.14 |
| (1,813) | 1:A:65:THR:HG22 | 1:A:69:LEU:H | 6 | 0.14 |
| (1,813) | 1:A:65:THR:HG23 | 1:A:69:LEU:H | 6 | 0.14 |
| (1,704) | 1:A:59:ARG:HB2 | 1:A:59:ARG:H | 19 | 0.14 |
| (1,475) | 1:A:22:LEU:HD21 | 1:A:20:ARG:HB2 | 18 | 0.14 |
| (1,475) | 1:A:22:LEU:HD22 | 1:A:20:ARG:HB2 | 18 | 0.14 |
| (1,475) | 1:A:22:LEU:HD23 | 1:A:20:ARG:HB2 | 18 | 0.14 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 6 | 0.14 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 6 | 0.14 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 6 | 0.14 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 7 | 0.14 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 7 | 0.14 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 7 | 0.14 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 21 | 0.14 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 21 | 0.14 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 21 | 0.14 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 30 | 0.14 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 30 | 0.14 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 30 | 0.14 |
| (1,192) | 1:A:29:SER:HB3 | 1:A:34:LEU:HD21 | 20 | 0.14 |
| (1,192) | 1:A:29:SER:HB3 | 1:A:34:LEU:HD22 | 20 | 0.14 |
| (1,192) | 1:A:29:SER:HB3 | 1:A:34:LEU:HD23 | 20 | 0.14 |
| (1,1584) | 1:A:59:ARG:HG3 | 1:A:58:ILE:H | 12 | 0.14 |
| (1,1584) | 1:A:59:ARG:HG3 | 1:A:58:ILE:H | 23 | 0.14 |
| (1,1576) | 1:A:66:LEU:HD11 | 1:A:65:THR:HA | 14 | 0.14 |
| (1,1576) | 1:A:66:LEU:HD12 | 1:A:65:THR:HA | 14 | 0.14 |
| (1,1576) | 1:A:66:LEU:HD13 | 1:A:65:THR:HA | 14 | 0.14 |
| (1,1576) | 1:A:66:LEU:HD11 | 1:A:65:THR:HA | 18 | 0.14 |
| (1,1576) | 1:A:66:LEU:HD12 | 1:A:65:THR:HA | 18 | 0.14 |
| (1,1576) | 1:A:66:LEU:HD13 | 1:A:65:THR:HA | 18 | 0.14 |
| (1,1497) | 1:A:65:THR:HG21 | 1:A:63:GLN:HB2 | 13 | 0.14 |
| (1,1497) | 1:A:65:THR:HG22 | 1:A:63:GLN:HB2 | 13 | 0.14 |
| (1,1497) | 1:A:65:THR:HG23 | 1:A:63:GLN:HB2 | 13 | 0.14 |
| (1,1484) | 1:A:14:ALA:HB1 | 1:A:19:ILE:HB | 9 | 0.14 |
| (1,1484) | 1:A:14:ALA:HB2 | 1:A:19:ILE:HB | 9 | 0.14 |
| (1,1484) | 1:A:14:ALA:HB3 | 1:A:19:ILE:HB | 9 | 0.14 |
| (1,1376) | 1:A:12:ALA:HB1 | 1:A:7:ARG:HD2 | 5 | 0.14 |
| (1,1376) | 1:A:12:ALA:HB1 | 1:A:7:ARG:HD3 | 5 | 0.14 |
| (1,1376) | 1:A:12:ALA:HB2 | 1:A:7:ARG:HD2 | 5 | 0.14 |
| (1,1376) | 1:A:12:ALA:HB2 | 1:A:7:ARG:HD3 | 5 | 0.14 |
| (1,1376) | 1:A:12:ALA:HB3 | 1:A:7:ARG:HD2 | 5 | 0.14 |
| (1,1376) | 1:A:12:ALA:HB3 | 1:A:7:ARG:HD3 | 5 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1369) | 1:A:71:GLU:HG2 | 1:A:72:MET:H | 7 | 0.14 |
| (1,1327) | 1:A:68:LYS:HD2 | 1:A:71:GLU:HB2 | 18 | 0.14 |
| (1,1327) | 1:A:68:LYS:HD3 | 1:A:71:GLU:HB2 | 18 | 0.14 |
| (1,1308) | 1:A:64:LEU:HA | 1:A:63:GLN:HE21 | 16 | 0.14 |
| (1,1263) | 1:A:61:VAL:HG11 | 1:A:62:ARG:HB3 | 4 | 0.14 |
| (1,1263) | 1:A:61:VAL:HG12 | 1:A:62:ARG:HB3 | 4 | 0.14 |
| (1,1263) | 1:A:61:VAL:HG13 | 1:A:62:ARG:HB3 | 4 | 0.14 |
| (1,1168) | 1:A:54:LEU:HG | 1:A:56:LEU:HD21 | 17 | 0.14 |
| (1,1168) | 1:A:54:LEU:HG | 1:A:56:LEU:HD22 | 17 | 0.14 |
| (1,1168) | 1:A:54:LEU:HG | 1:A:56:LEU:HD23 | 17 | 0.14 |
| (1,1168) | 1:A:54:LEU:HG | 1:A:56:LEU:HD21 | 26 | 0.14 |
| (1,1168) | 1:A:54:LEU:HG | 1:A:56:LEU:HD22 | 26 | 0.14 |
| (1,1168) | 1:A:54:LEU:HG | 1:A:56:LEU:HD23 | 26 | 0.14 |
| (1,1061) | 1:A:36:LEU:HD21 | 1:A:38:SER:H | 11 | 0.14 |
| (1,1061) | 1:A:36:LEU:HD22 | 1:A:38:SER:H | 11 | 0.14 |
| (1,1061) | 1:A:36:LEU:HD23 | 1:A:38:SER:H | 11 | 0.14 |
| (1,1037) | 1:A:36:LEU:HB3 | 1:A:40:MET:HA | 21 | 0.14 |
| (1,1028) | 1:A:34:LEU:HD21 | 1:A:33:ASP:H | 20 | 0.14 |
| (1,1028) | 1:A:34:LEU:HD22 | 1:A:33:ASP:H | 20 | 0.14 |
| (1,1028) | 1:A:34:LEU:HD23 | 1:A:33:ASP:H | 20 | 0.14 |
| (1,9) | 1:A:16:ILE:HG21 | 1:A:43:GLU:H | 23 | 0.13 |
| (1,9) | 1:A:16:ILE:HG22 | 1:A:43:GLU:H | 23 | 0.13 |
| (1,9) | 1:A:16:ILE:HG23 | 1:A:43:GLU:H | 23 | 0.13 |
| (1,9) | 1:A:16:ILE:HG21 | 1:A:42:VAL:H | 23 | 0.13 |
| (1,9) | 1:A:16:ILE:HG22 | 1:A:42:VAL:H | 23 | 0.13 |
| (1,9) | 1:A:16:ILE:HG23 | 1:A:42:VAL:H | 23 | 0.13 |
| (1,9) | 1:A:47:ILE:HG21 | 1:A:50:ARG:HE | 23 | 0.13 |
| (1,9) | 1:A:47:ILE:HG22 | 1:A:50:ARG:HE | 23 | 0.13 |
| (1,9) | 1:A:47:ILE:HG23 | 1:A:50:ARG:HE | 23 | 0.13 |
| (1,85) | 1:A:24:GLY:H | 1:A:23:ALA:HA | 12 | 0.13 |
| (1,85) | 1:A:24:GLY:H | 1:A:25:ILE:HA | 12 | 0.13 |
| (1,85) | 1:A:24:GLY:H | 1:A:23:ALA:HA | 18 | 0.13 |
| (1,85) | 1:A:24:GLY:H | 1:A:25:ILE:HA | 18 | 0.13 |
| (1,813) | 1:A:65:THR:HG21 | 1:A:69:LEU:H | 1 | 0.13 |
| (1,813) | 1:A:65:THR:HG22 | 1:A:69:LEU:H | 1 | 0.13 |
| (1,813) | 1:A:65:THR:HG23 | 1:A:69:LEU:H | 1 | 0.13 |
| (1,813) | 1:A:65:THR:HG21 | 1:A:69:LEU:H | 3 | 0.13 |
| (1,813) | 1:A:65:THR:HG22 | 1:A:69:LEU:H | 3 | 0.13 |
| (1,813) | 1:A:65:THR:HG23 | 1:A:69:LEU:H | 3 | 0.13 |
| (1,813) | 1:A:65:THR:HG21 | 1:A:69:LEU:H | 5 | 0.13 |
| (1,813) | 1:A:65:THR:HG22 | 1:A:69:LEU:H | 5 | 0.13 |
| (1,813) | 1:A:65:THR:HG23 | 1:A:69:LEU:H | 5 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,813) | 1:A:65:THR:HG21 | 1:A:69:LEU:H | 7 | 0.13 |
| (1,813) | 1:A:65:THR:HG22 | 1:A:69:LEU:H | 7 | 0.13 |
| (1,813) | 1:A:65:THR:HG23 | 1:A:69:LEU:H | 7 | 0.13 |
| (1,813) | 1:A:65:THR:HG21 | 1:A:69:LEU:H | 28 | 0.13 |
| (1,813) | 1:A:65:THR:HG22 | 1:A:69:LEU:H | 28 | 0.13 |
| (1,813) | 1:A:65:THR:HG23 | 1:A:69:LEU:H | 28 | 0.13 |
| (1,72) | 1:A:48:LEU:HD11 | 1:A:6:GLN:HE21 | 30 | 0.13 |
| (1,72) | 1:A:48:LEU:HD12 | 1:A:6:GLN:HE21 | 30 | 0.13 |
| (1,72) | 1:A:48:LEU:HD13 | 1:A:6:GLN:HE21 | 30 | 0.13 |
| (1,72) | 1:A:9:LEU:HD21 | 1:A:6:GLN:HE21 | 30 | 0.13 |
| (1,72) | 1:A:9:LEU:HD22 | 1:A:6:GLN:HE21 | 30 | 0.13 |
| (1,72) | 1:A:9:LEU:HD23 | 1:A:6:GLN:HE21 | 30 | 0.13 |
| (1,549) | 1:A:72:MET:HB2 | 1:A:72:MET:H | 8 | 0.13 |
| (1,54) | 1:A:20:ARG:HG3 | 1:A:67:ARG:HD3 | 25 | 0.13 |
| (1,54) | 1:A:20:ARG:HG3 | 1:A:10:VAL:HA | 25 | 0.13 |
| (1,54) | 1:A:7:ARG:HG2 | 1:A:10:VAL:HA | 25 | 0.13 |
| (1,54) | 1:A:7:ARG:HG3 | 1:A:10:VAL:HA | 25 | 0.13 |
| (1,479) | 1:A:23:ALA:HA | 1:A:21:ASP:HA | 19 | 0.13 |
| (1,469) | 1:A:17:LEU:HD11 | 1:A:16:ILE:H | 7 | 0.13 |
| (1,469) | 1:A:17:LEU:HD12 | 1:A:16:ILE:H | 7 | 0.13 |
| (1,469) | 1:A:17:LEU:HD13 | 1:A:16:ILE:H | 7 | 0.13 |
| (1,291) | 1:A:17:LEU:HG | 1:A:17:LEU:H | 7 | 0.13 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 12 | 0.13 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 12 | 0.13 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 12 | 0.13 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 29 | 0.13 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 29 | 0.13 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 29 | 0.13 |
| (1,213) | 1:A:30:SER:HB3 | 1:A:33:ASP:HA | 27 | 0.13 |
| (1,1727) | 1:A:86:LYS:H | 1:A:85:PRO:HA | 22 | 0.13 |
| (1,1638) | 1:A:57:PRO:HB3 | 1:A:59:ARG:HB2 | 9 | 0.13 |
| (1,1595) | 1:A:68:LYS:HB2 | 1:A:64:LEU:H | 10 | 0.13 |
| (1,1595) | 1:A:68:LYS:HB3 | 1:A:64:LEU:H | 10 | 0.13 |
| (1,1484) | 1:A:14:ALA:HB1 | 1:A:19:ILE:HB | 1 | 0.13 |
| (1,1484) | 1:A:14:ALA:HB2 | 1:A:19:ILE:HB | 1 | 0.13 |
| (1,1484) | 1:A:14:ALA:HB3 | 1:A:19:ILE:HB | 1 | 0.13 |
| (1,1484) | 1:A:14:ALA:HB1 | 1:A:19:ILE:HB | 4 | 0.13 |
| (1,1484) | 1:A:14:ALA:HB2 | 1:A:19:ILE:HB | 4 | 0.13 |
| (1,1484) | 1:A:14:ALA:HB3 | 1:A:19:ILE:HB | 4 | 0.13 |
| (1,1484) | 1:A:14:ALA:HB1 | 1:A:19:ILE:HB | 12 | 0.13 |
| (1,1484) | 1:A:14:ALA:HB2 | 1:A:19:ILE:HB | 12 | 0.13 |
| (1,1484) | 1:A:14:ALA:HB3 | 1:A:19:ILE:HB | 12 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1484) | 1:A:14:ALA:HB1 | 1:A:19:ILE:HB | 18 | 0.13 |
| (1,1484) | 1:A:14:ALA:HB2 | 1:A:19:ILE:HB | 18 | 0.13 |
| (1,1484) | 1:A:14:ALA:HB3 | 1:A:19:ILE:HB | 18 | 0.13 |
| (1,1484) | 1:A:14:ALA:HB1 | 1:A:19:ILE:HB | 25 | 0.13 |
| (1,1484) | 1:A:14:ALA:HB2 | 1:A:19:ILE:HB | 25 | 0.13 |
| (1,1484) | 1:A:14:ALA:HB3 | 1:A:19:ILE:HB | 25 | 0.13 |
| (1,1263) | 1:A:61:VAL:HG11 | 1:A:62:ARG:HB3 | 18 | 0.13 |
| (1,1263) | 1:A:61:VAL:HG12 | 1:A:62:ARG:HB3 | 18 | 0.13 |
| (1,1263) | 1:A:61:VAL:HG13 | 1:A:62:ARG:HB3 | 18 | 0.13 |
| (1,1107) | 1:A:48:LEU:HA | 1:A:52:HIS:HB2 | 17 | 0.13 |
| (1,1050) | 1:A:36:LEU:HD11 | 1:A:44:VAL:HG21 | 18 | 0.13 |
| (1,1050) | 1:A:36:LEU:HD11 | 1:A:44:VAL:HG22 | 18 | 0.13 |
| (1,1050) | 1:A:36:LEU:HD11 | 1:A:44:VAL:HG23 | 18 | 0.13 |
| (1,1050) | 1:A:36:LEU:HD12 | 1:A:44:VAL:HG21 | 18 | 0.13 |
| (1,1050) | 1:A:36:LEU:HD12 | 1:A:44:VAL:HG22 | 18 | 0.13 |
| (1,1050) | 1:A:36:LEU:HD12 | 1:A:44:VAL:HG23 | 18 | 0.13 |
| (1,1050) | 1:A:36:LEU:HD13 | 1:A:44:VAL:HG21 | 18 | 0.13 |
| (1,1050) | 1:A:36:LEU:HD13 | 1:A:44:VAL:HG22 | 18 | 0.13 |
| (1,1050) | 1:A:36:LEU:HD13 | 1:A:44:VAL:HG23 | 18 | 0.13 |
| (1,1037) | 1:A:36:LEU:HB3 | 1:A:40:MET:HA | 6 | 0.13 |
| (1,1037) | 1:A:36:LEU:HB3 | 1:A:40:MET:HA | 26 | 0.13 |
| (1,1037) | 1:A:36:LEU:HB3 | 1:A:40:MET:HA | 27 | 0.13 |
| (1,1017) | 1:A:34:LEU:HD21 | 1:A:31:LEU:HA | 28 | 0.13 |
| (1,1017) | 1:A:34:LEU:HD22 | 1:A:31:LEU:HA | 28 | 0.13 |
| (1,1017) | 1:A:34:LEU:HD23 | 1:A:31:LEU:HA | 28 | 0.13 |
| (1,972) | 1:A:27:LEU:HD21 | 1:A:70:GLN:HE21 | 21 | 0.12 |
| (1,972) | 1:A:27:LEU:HD22 | 1:A:70:GLN:HE21 | 21 | 0.12 |
| (1,972) | 1:A:27:LEU:HD23 | 1:A:70:GLN:HE21 | 21 | 0.12 |
| (1,85) | 1:A:24:GLY:H | 1:A:23:ALA:HA | 25 | 0.12 |
| (1,85) | 1:A:24:GLY:H | 1:A:25:ILE:HA | 25 | 0.12 |
| (1,85) | 1:A:24:GLY:H | 1:A:23:ALA:HA | 26 | 0.12 |
| (1,85) | 1:A:24:GLY:H | 1:A:25:ILE:HA | 26 | 0.12 |
| (1,85) | 1:A:24:GLY:H | 1:A:23:ALA:HA | 28 | 0.12 |
| (1,85) | 1:A:24:GLY:H | 1:A:25:ILE:HA | 28 | 0.12 |
| (1,813) | 1:A:65:THR:HG21 | 1:A:69:LEU:H | 10 | 0.12 |
| (1,813) | 1:A:65:THR:HG22 | 1:A:69:LEU:H | 10 | 0.12 |
| (1,813) | 1:A:65:THR:HG23 | 1:A:69:LEU:H | 10 | 0.12 |
| (1,813) | 1:A:65:THR:HG21 | 1:A:69:LEU:H | 12 | 0.12 |
| (1,813) | 1:A:65:THR:HG22 | 1:A:69:LEU:H | 12 | 0.12 |
| (1,813) | 1:A:65:THR:HG23 | 1:A:69:LEU:H | 12 | 0.12 |
| (1,778) | 1:A:52:HIS:HB3 | 1:A:6:GLN:HE21 | 22 | 0.12 |
| (1,662) | 1:A:49:GLU:HA | 1:A:46:GLN:HA | 10 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,662) | 1:A:49:GLU:HA | 1:A:46:GLN:HA | 18 | 0.12 |
| (1,662) | 1:A:49:GLU:HA | 1:A:46:GLN:HA | 21 | 0.12 |
| (1,391) | 1:A:19:ILE:HG21 | 1:A:21:ASP:HA | 25 | 0.12 |
| (1,391) | 1:A:19:ILE:HG22 | 1:A:21:ASP:HA | 25 | 0.12 |
| (1,391) | 1:A:19:ILE:HG23 | 1:A:21:ASP:HA | 25 | 0.12 |
| (1,38) | 1:A:58:ILE:HG21 | 1:A:32:ALA:HA | 14 | 0.12 |
| (1,38) | 1:A:58:ILE:HG22 | 1:A:32:ALA:HA | 14 | 0.12 |
| (1,38) | 1:A:58:ILE:HG23 | 1:A:32:ALA:HA | 14 | 0.12 |
| (1,38) | 1:A:47:ILE:HG21 | 1:A:50:ARG:HA | 14 | 0.12 |
| (1,38) | 1:A:47:ILE:HG22 | 1:A:50:ARG:HA | 14 | 0.12 |
| (1,38) | 1:A:47:ILE:HG23 | 1:A:50:ARG:HA | 14 | 0.12 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 2 | 0.12 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 2 | 0.12 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 2 | 0.12 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 18 | 0.12 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 18 | 0.12 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 18 | 0.12 |
| (1,239) | 1:A:31:LEU:HD11 | 1:A:62:ARG:HG3 | 9 | 0.12 |
| (1,239) | 1:A:31:LEU:HD12 | 1:A:62:ARG:HG3 | 9 | 0.12 |
| (1,239) | 1:A:31:LEU:HD13 | 1:A:62:ARG:HG3 | 9 | 0.12 |
| (1,239) | 1:A:31:LEU:HD11 | 1:A:62:ARG:HG3 | 29 | 0.12 |
| (1,239) | 1:A:31:LEU:HD12 | 1:A:62:ARG:HG3 | 29 | 0.12 |
| (1,239) | 1:A:31:LEU:HD13 | 1:A:62:ARG:HG3 | 29 | 0.12 |
| (1,192) | 1:A:29:SER:HB3 | 1:A:34:LEU:HD21 | 3 | 0.12 |
| (1,192) | 1:A:29:SER:HB3 | 1:A:34:LEU:HD22 | 3 | 0.12 |
| (1,192) | 1:A:29:SER:HB3 | 1:A:34:LEU:HD23 | 3 | 0.12 |
| (1,18) | 1:A:71:GLU:HA | 1:A:74:SER:H | 18 | 0.12 |
| (1,18) | 1:A:71:GLU:HA | 1:A:69:LEU:H | 18 | 0.12 |
| (1,1581) | 1:A:14:ALA:HB1 | 1:A:70:GLN:HG3 | 7 | 0.12 |
| (1,1581) | 1:A:14:ALA:HB2 | 1:A:70:GLN:HG3 | 7 | 0.12 |
| (1,1581) | 1:A:14:ALA:HB3 | 1:A:70:GLN:HG3 | 7 | 0.12 |
| (1,1569) | 1:A:10:VAL:HG21 | 1:A:70:GLN:HB2 | 3 | 0.12 |
| (1,1569) | 1:A:10:VAL:HG21 | 1:A:70:GLN:HB3 | 3 | 0.12 |
| (1,1569) | 1:A:10:VAL:HG22 | 1:A:70:GLN:HB2 | 3 | 0.12 |
| (1,1569) | 1:A:10:VAL:HG22 | 1:A:70:GLN:HB3 | 3 | 0.12 |
| (1,1569) | 1:A:10:VAL:HG23 | 1:A:70:GLN:HB2 | 3 | 0.12 |
| (1,1569) | 1:A:10:VAL:HG23 | 1:A:70:GLN:HB3 | 3 | 0.12 |
| (1,1545) | 1:A:44:VAL:HG21 | 1:A:45:ARG:HE | 9 | 0.12 |
| (1,1545) | 1:A:44:VAL:HG22 | 1:A:45:ARG:HE | 9 | 0.12 |
| (1,1545) | 1:A:44:VAL:HG23 | 1:A:45:ARG:HE | 9 | 0.12 |
| (1,1484) | 1:A:14:ALA:HB1 | 1:A:19:ILE:HB | 21 | 0.12 |
| (1,1484) | 1:A:14:ALA:HB2 | 1:A:19:ILE:HB | 21 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1484) | 1:A:14:ALA:HB3 | 1:A:19:ILE:HB | 21 | 0.12 |
| (1,1484) | 1:A:14:ALA:HB1 | 1:A:19:ILE:HB | 28 | 0.12 |
| (1,1484) | 1:A:14:ALA:HB2 | 1:A:19:ILE:HB | 28 | 0.12 |
| (1,1484) | 1:A:14:ALA:HB3 | 1:A:19:ILE:HB | 28 | 0.12 |
| (1,1400) | 1:A:44:VAL:HB | 1:A:45:ARG:HE | 18 | 0.12 |
| (1,1369) | 1:A:71:GLU:HG2 | 1:A:72:MET:H | 5 | 0.12 |
| (1,1327) | 1:A:68:LYS:HD2 | 1:A:71:GLU:HB2 | 8 | 0.12 |
| (1,1327) | 1:A:68:LYS:HD3 | 1:A:71:GLU:HB2 | 8 | 0.12 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB1 | 5 | 0.12 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB2 | 5 | 0.12 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB3 | 5 | 0.12 |
| (1,1263) | 1:A:61:VAL:HG11 | 1:A:62:ARG:HB3 | 20 | 0.12 |
| (1,1263) | 1:A:61:VAL:HG12 | 1:A:62:ARG:HB3 | 20 | 0.12 |
| (1,1263) | 1:A:61:VAL:HG13 | 1:A:62:ARG:HB3 | 20 | 0.12 |
| (1,1091) | 1:A:39:LEU:HD11 | 1:A:39:LEU:HA | 27 | 0.12 |
| (1,1091) | 1:A:39:LEU:HD12 | 1:A:39:LEU:HA | 27 | 0.12 |
| (1,1091) | 1:A:39:LEU:HD13 | 1:A:39:LEU:HA | 27 | 0.12 |
| (1,1037) | 1:A:36:LEU:HB3 | 1:A:40:MET:HA | 22 | 0.12 |
| (1,1018) | 1:A:34:LEU:HD21 | 1:A:29:SER:HB2 | 3 | 0.12 |
| (1,1018) | 1:A:34:LEU:HD22 | 1:A:29:SER:HB2 | 3 | 0.12 |
| (1,1018) | 1:A:34:LEU:HD23 | 1:A:29:SER:HB2 | 3 | 0.12 |
| (1,1017) | 1:A:34:LEU:HD21 | 1:A:31:LEU:HA | 19 | 0.12 |
| (1,1017) | 1:A:34:LEU:HD22 | 1:A:31:LEU:HA | 19 | 0.12 |
| (1,1017) | 1:A:34:LEU:HD23 | 1:A:31:LEU:HA | 19 | 0.12 |
| (1,1017) | 1:A:34:LEU:HD21 | 1:A:31:LEU:HA | 21 | 0.12 |
| (1,1017) | 1:A:34:LEU:HD22 | 1:A:31:LEU:HA | 21 | 0.12 |
| (1,1017) | 1:A:34:LEU:HD23 | 1:A:31:LEU:HA | 21 | 0.12 |
| (1,1017) | 1:A:34:LEU:HD21 | 1:A:31:LEU:HA | 30 | 0.12 |
| (1,1017) | 1:A:34:LEU:HD22 | 1:A:31:LEU:HA | 30 | 0.12 |
| (1,1017) | 1:A:34:LEU:HD23 | 1:A:31:LEU:HA | 30 | 0.12 |
| (1,1012) | 1:A:34:LEU:HD11 | 1:A:31:LEU:H | 19 | 0.12 |
| (1,1012) | 1:A:34:LEU:HD12 | 1:A:31:LEU:H | 19 | 0.12 |
| (1,1012) | 1:A:34:LEU:HD13 | 1:A:31:LEU:H | 19 | 0.12 |
| (1,9) | 1:A:16:ILE:HG21 | 1:A:43:GLU:H | 4 | 0.11 |
| (1,9) | 1:A:16:ILE:HG22 | 1:A:43:GLU:H | 4 | 0.11 |
| (1,9) | 1:A:16:ILE:HG23 | 1:A:43:GLU:H | 4 | 0.11 |
| (1,9) | 1:A:16:ILE:HG21 | 1:A:42:VAL:H | 4 | 0.11 |
| (1,9) | 1:A:16:ILE:HG22 | 1:A:42:VAL:H | 4 | 0.11 |
| (1,9) | 1:A:16:ILE:HG23 | 1:A:42:VAL:H | 4 | 0.11 |
| (1,9) | 1:A:47:ILE:HG21 | 1:A:50:ARG:HE | 4 | 0.11 |
| (1,9) | 1:A:47:ILE:HG22 | 1:A:50:ARG:HE | 4 | 0.11 |
| (1,9) | 1:A:47:ILE:HG23 | 1:A:50:ARG:HE | 4 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,896) | 1:A:47:ILE:HG21 | 1:A:6:GLN:HE21 | 6 | 0.11 |
| (1,896) | 1:A:47:ILE:HG22 | 1:A:6:GLN:HE21 | 6 | 0.11 |
| (1,896) | 1:A:47:ILE:HG23 | 1:A:6:GLN:HE21 | 6 | 0.11 |
| (1,862) | 1:A:10:VAL:HA | 1:A:9:LEU:HD21 | 8 | 0.11 |
| (1,862) | 1:A:10:VAL:HA | 1:A:9:LEU:HD22 | 8 | 0.11 |
| (1,862) | 1:A:10:VAL:HA | 1:A:9:LEU:HD23 | 8 | 0.11 |
| (1,85) | 1:A:24:GLY:H | 1:A:23:ALA:HA | 11 | 0.11 |
| (1,85) | 1:A:24:GLY:H | 1:A:25:ILE:HA | 11 | 0.11 |
| (1,85) | 1:A:24:GLY:H | 1:A:23:ALA:HA | 23 | 0.11 |
| (1,85) | 1:A:24:GLY:H | 1:A:25:ILE:HA | 23 | 0.11 |
| (1,841) | 1:A:8:ASP:HB2 | 1:A:11:LYS:H | 25 | 0.11 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD11 | 19 | 0.11 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD12 | 19 | 0.11 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD13 | 19 | 0.11 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD21 | 19 | 0.11 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD22 | 19 | 0.11 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:69:LEU:HD23 | 19 | 0.11 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:54:LEU:HD21 | 19 | 0.11 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:54:LEU:HD22 | 19 | 0.11 |
| (1,83) | 1:A:73:SER:HB3 | 1:A:54:LEU:HD23 | 19 | 0.11 |
| (1,813) | 1:A:65:THR:HG21 | 1:A:69:LEU:H | 27 | 0.11 |
| (1,813) | 1:A:65:THR:HG22 | 1:A:69:LEU:H | 27 | 0.11 |
| (1,813) | 1:A:65:THR:HG23 | 1:A:69:LEU:H | 27 | 0.11 |
| (1,806) | 1:A:65:THR:HG21 | 1:A:67:ARG:HB2 | 2 | 0.11 |
| (1,806) | 1:A:65:THR:HG21 | 1:A:67:ARG:HB3 | 2 | 0.11 |
| (1,806) | 1:A:65:THR:HG22 | 1:A:67:ARG:HB2 | 2 | 0.11 |
| (1,806) | 1:A:65:THR:HG22 | 1:A:67:ARG:HB3 | 2 | 0.11 |
| (1,806) | 1:A:65:THR:HG23 | 1:A:67:ARG:HB2 | 2 | 0.11 |
| (1,806) | 1:A:65:THR:HG23 | 1:A:67:ARG:HB3 | 2 | 0.11 |
| (1,704) | 1:A:59:ARG:HB2 | 1:A:59:ARG:H | 7 | 0.11 |
| (1,704) | 1:A:59:ARG:HB2 | 1:A:59:ARG:H | 15 | 0.11 |
| (1,394) | 1:A:19:ILE:HG21 | 1:A:25:ILE:HG13 | 3 | 0.11 |
| (1,394) | 1:A:19:ILE:HG22 | 1:A:25:ILE:HG13 | 3 | 0.11 |
| (1,394) | 1:A:19:ILE:HG23 | 1:A:25:ILE:HG13 | 3 | 0.11 |
| (1,391) | 1:A:19:ILE:HG21 | 1:A:21:ASP:HA | 17 | 0.11 |
| (1,391) | 1:A:19:ILE:HG22 | 1:A:21:ASP:HA | 17 | 0.11 |
| (1,391) | 1:A:19:ILE:HG23 | 1:A:21:ASP:HA | 17 | 0.11 |
| (1,291) | 1:A:17:LEU:HG | 1:A:17:LEU:H | 16 | 0.11 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 8 | 0.11 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 8 | 0.11 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 8 | 0.11 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 20 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 20 | 0.11 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 20 | 0.11 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 22 | 0.11 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 22 | 0.11 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 22 | 0.11 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD11 | 25 | 0.11 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD12 | 25 | 0.11 |
| (1,264) | 1:A:32:ALA:HA | 1:A:34:LEU:HD13 | 25 | 0.11 |
| (1,213) | 1:A:30:SER:HB3 | 1:A:33:ASP:HA | 26 | 0.11 |
| (1,18) | 1:A:71:GLU:HA | 1:A:74:SER:H | 12 | 0.11 |
| (1,18) | 1:A:71:GLU:HA | 1:A:69:LEU:H | 12 | 0.11 |
| (1,18) | 1:A:71:GLU:HA | 1:A:74:SER:H | 29 | 0.11 |
| (1,18) | 1:A:71:GLU:HA | 1:A:69:LEU:H | 29 | 0.11 |
| (1,177) | 1:A:22:LEU:HD11 | 1:A:24:GLY:HA2 | 14 | 0.11 |
| (1,177) | 1:A:22:LEU:HD12 | 1:A:24:GLY:HA2 | 14 | 0.11 |
| (1,177) | 1:A:22:LEU:HD13 | 1:A:24:GLY:HA2 | 14 | 0.11 |
| (1,1732) | 1:A:32:ALA:H | 1:A:65:THR:HG21 | 17 | 0.11 |
| (1,1732) | 1:A:32:ALA:H | 1:A:65:THR:HG22 | 17 | 0.11 |
| (1,1732) | 1:A:32:ALA:H | 1:A:65:THR:HG23 | 17 | 0.11 |
| (1,171) | 1:A:22:LEU:HG | 1:A:21:ASP:HA | 27 | 0.11 |
| (1,1646) | 1:A:9:LEU:HG | 1:A:9:LEU:H | 3 | 0.11 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD2 | 20 | 0.11 |
| (1,1618) | 1:A:58:ILE:HG12 | 1:A:59:ARG:HD3 | 20 | 0.11 |
| (1,1553) | 1:A:19:ILE:HG21 | 1:A:26:ASN:H | 6 | 0.11 |
| (1,1553) | 1:A:19:ILE:HG22 | 1:A:26:ASN:H | 6 | 0.11 |
| (1,1553) | 1:A:19:ILE:HG23 | 1:A:26:ASN:H | 6 | 0.11 |
| (1,1546) | 1:A:44:VAL:HG11 | 1:A:42:VAL:HA | 11 | 0.11 |
| (1,1546) | 1:A:44:VAL:HG12 | 1:A:42:VAL:HA | 11 | 0.11 |
| (1,1546) | 1:A:44:VAL:HG13 | 1:A:42:VAL:HA | 11 | 0.11 |
| (1,1545) | 1:A:44:VAL:HG21 | 1:A:45:ARG:HE | 8 | 0.11 |
| (1,1545) | 1:A:44:VAL:HG22 | 1:A:45:ARG:HE | 8 | 0.11 |
| (1,1545) | 1:A:44:VAL:HG23 | 1:A:45:ARG:HE | 8 | 0.11 |
| (1,1545) | 1:A:44:VAL:HG21 | 1:A:45:ARG:HE | 15 | 0.11 |
| (1,1545) | 1:A:44:VAL:HG22 | 1:A:45:ARG:HE | 15 | 0.11 |
| (1,1545) | 1:A:44:VAL:HG23 | 1:A:45:ARG:HE | 15 | 0.11 |
| (1,1525) | 1:A:73:SER:HA | 1:A:9:LEU:HD21 | 13 | 0.11 |
| (1,1525) | 1:A:73:SER:HA | 1:A:9:LEU:HD22 | 13 | 0.11 |
| (1,1525) | 1:A:73:SER:HA | 1:A:9:LEU:HD23 | 13 | 0.11 |
| (1,1523) | 1:A:73:SER:HA | 1:A:70:GLN:H | 3 | 0.11 |
| (1,1523) | 1:A:73:SER:HA | 1:A:70:GLN:H | 22 | 0.11 |
| (1,1505) | 1:A:55:VAL:HG11 | 1:A:59:ARG:HD2 | 25 | 0.11 |
| (1,1505) | 1:A:55:VAL:HG11 | 1:A:59:ARG:HD3 | 25 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1505) | 1:A:55:VAL:HG12 | 1:A:59:ARG:HD2 | 25 | 0.11 |
| (1,1505) | 1:A:55:VAL:HG12 | 1:A:59:ARG:HD3 | 25 | 0.11 |
| (1,1505) | 1:A:55:VAL:HG13 | 1:A:59:ARG:HD2 | 25 | 0.11 |
| (1,1505) | 1:A:55:VAL:HG13 | 1:A:59:ARG:HD3 | 25 | 0.11 |
| (1,1402) | 1:A:42:VAL:HA | 1:A:45:ARG:HB3 | 15 | 0.11 |
| (1,1332) | 1:A:68:LYS:HE2 | 1:A:69:LEU:H | 20 | 0.11 |
| (1,1332) | 1:A:68:LYS:HE3 | 1:A:69:LEU:H | 20 | 0.11 |
| (1,1327) | 1:A:68:LYS:HD2 | 1:A:71:GLU:HB2 | 15 | 0.11 |
| (1,1327) | 1:A:68:LYS:HD3 | 1:A:71:GLU:HB2 | 15 | 0.11 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB1 | 4 | 0.11 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB2 | 4 | 0.11 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB3 | 4 | 0.11 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB1 | 6 | 0.11 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB2 | 6 | 0.11 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB3 | 6 | 0.11 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB1 | 22 | 0.11 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB2 | 22 | 0.11 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB3 | 22 | 0.11 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB1 | 23 | 0.11 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB2 | 23 | 0.11 |
| (1,1276) | 1:A:62:ARG:HB3 | 1:A:32:ALA:HB3 | 23 | 0.11 |
| (1,1037) | 1:A:36:LEU:HB3 | 1:A:40:MET:HA | 2 | 0.11 |
| (1,1037) | 1:A:36:LEU:HB3 | 1:A:40:MET:HA | 3 | 0.11 |
| (1,1037) | 1:A:36:LEU:HB3 | 1:A:40:MET:HA | 28 | 0.11 |
| (1,1017) | 1:A:34:LEU:HD21 | 1:A:31:LEU:HA | 2 | 0.11 |
| (1,1017) | 1:A:34:LEU:HD22 | 1:A:31:LEU:HA | 2 | 0.11 |
| (1,1017) | 1:A:34:LEU:HD23 | 1:A:31:LEU:HA | 2 | 0.11 |
| (1,1017) | 1:A:34:LEU:HD21 | 1:A:31:LEU:HA | 15 | 0.11 |
| (1,1017) | 1:A:34:LEU:HD22 | 1:A:31:LEU:HA | 15 | 0.11 |
| (1,1017) | 1:A:34:LEU:HD23 | 1:A:31:LEU:HA | 15 | 0.11 |
| (1,1017) | 1:A:34:LEU:HD21 | 1:A:31:LEU:HA | 16 | 0.11 |
| (1,1017) | 1:A:34:LEU:HD22 | 1:A:31:LEU:HA | 16 | 0.11 |
| (1,1017) | 1:A:34:LEU:HD23 | 1:A:31:LEU:HA | 16 | 0.11 |
| (1,1017) | 1:A:34:LEU:HD21 | 1:A:31:LEU:HA | 17 | 0.11 |
| (1,1017) | 1:A:34:LEU:HD22 | 1:A:31:LEU:HA | 17 | 0.11 |
| (1,1017) | 1:A:34:LEU:HD23 | 1:A:31:LEU:HA | 17 | 0.11 |
| (1,1017) | 1:A:34:LEU:HD21 | 1:A:31:LEU:HA | 26 | 0.11 |
| (1,1017) | 1:A:34:LEU:HD22 | 1:A:31:LEU:HA | 26 | 0.11 |
| (1,1017) | 1:A:34:LEU:HD23 | 1:A:31:LEU:HA | 26 | 0.11 |

10 Dihedral-angle violation analysis

No dihedral-angle restraints found