



# wwPDB NMR Structure Validation Summary Report ⓘ

Feb 25, 2020 – 04:43 PM CST

PDB ID : 2KKO  
Title : Solution NMR structure of the homodimeric winged helix-turn-helix DNA-binding domain (fragment 1-100) Mb0332 from Mycobacterium bovis, a possible ArsR-family transcriptional regulator. Northeast Structural Genomics Consortium Target MbR242E.  
Authors : Ramelot, T.A.; Cort, J.R.; Wang, D.; Ciccocanti, C.; Jiang, M.; Nair, R.; Rost, B.; Swapna, G.; Acton, T.B.; Xiao, R.; Everett, J.K.; Montelione, G.T.; Kennedy, M.A.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2009-06-26

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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

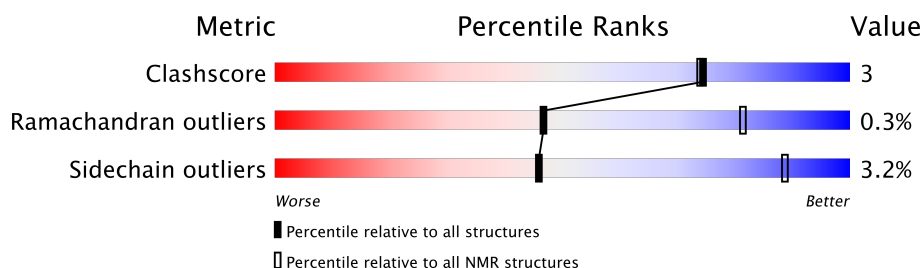
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*



The overall completeness of chemical shifts assignment is 63%.

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  $\geq 3$ , 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	108	 84% • 14%
1	B	108	 83% • 14%

## 2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:7-A:99, B:8-B:100 (186)	0.55	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 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3328 atoms, of which 1678 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called POSSIBLE TRANSCRIPTIONAL REGULATORY PROTEIN (POSSIBLY ARSR-FAMILY).

Mol	Chain	Residues	Atoms						Trace
1	A	108	Total	C	H	N	O	S	0
			1664	505	839	165	153	2	
1	B	108	Total	C	H	N	O	S	0
			1664	505	839	165	153	2	

There are 16 discrepancies between the modelled and reference sequences:

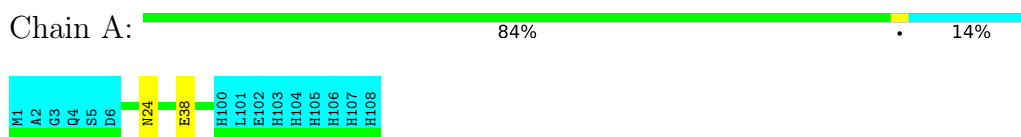
Chain	Residue	Modelled	Actual	Comment	Reference
A	101	LEU	-	EXPRESSION TAG	UNP Q7U294
A	102	GLU	-	EXPRESSION TAG	UNP Q7U294
A	103	HIS	-	EXPRESSION TAG	UNP Q7U294
A	104	HIS	-	EXPRESSION TAG	UNP Q7U294
A	105	HIS	-	EXPRESSION TAG	UNP Q7U294
A	106	HIS	-	EXPRESSION TAG	UNP Q7U294
A	107	HIS	-	EXPRESSION TAG	UNP Q7U294
A	108	HIS	-	EXPRESSION TAG	UNP Q7U294
B	101	LEU	-	EXPRESSION TAG	UNP Q7U294
B	102	GLU	-	EXPRESSION TAG	UNP Q7U294
B	103	HIS	-	EXPRESSION TAG	UNP Q7U294
B	104	HIS	-	EXPRESSION TAG	UNP Q7U294
B	105	HIS	-	EXPRESSION TAG	UNP Q7U294
B	106	HIS	-	EXPRESSION TAG	UNP Q7U294
B	107	HIS	-	EXPRESSION TAG	UNP Q7U294
B	108	HIS	-	EXPRESSION TAG	UNP Q7U294

## 4 Residue-property plots [i](#)

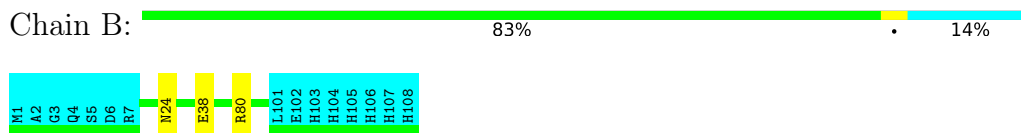
### 4.1 Average score per residue in the NMR ensemble

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: POSSIBLE TRANSCRIPTIONAL REGULATORY PROTEIN (POSSIBLY ARSR-FAMILY)



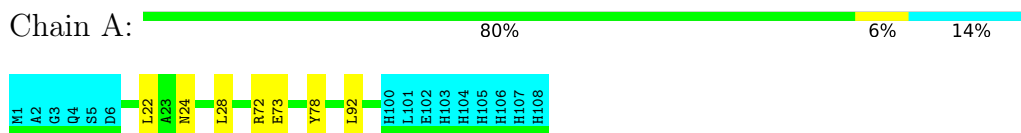
- Molecule 1: POSSIBLE TRANSCRIPTIONAL REGULATORY PROTEIN (POSSIBLY ARSR-FAMILY)



### 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: POSSIBLE TRANSCRIPTIONAL REGULATORY PROTEIN (POSSIBLY ARSR-FAMILY)



- Molecule 1: POSSIBLE TRANSCRIPTIONAL REGULATORY PROTEIN (POSSIBLY ARSR-FAMILY)





## 5 Refinement protocol and experimental data overview

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

Of the 150 calculated structures, 20 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
X-PLOR NIH	structure solution	2.20
CNS	refinement	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)	2kko_nmr.cif
Number of chemical shift lists	1
Total number of shifts	2501
Number of shifts mapped to atoms	1563
Number of unparsed shifts	386
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	552
Assignment completeness (well-defined parts)	63%

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

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [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	697	730	730	6±3
1	B	696	725	724	6±3
All	All	27860	29100	29080	198

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 3.

5 of 150 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:38:GLU:HG2	1:B:80:ARG:HB3	0.86	1.48	12	2
1:A:24:ASN:HB2	1:B:16:ALA:HA	0.71	1.60	4	1
1:A:62:LEU:HA	1:A:66:GLY:HA3	0.68	1.62	15	2
1:A:69:GLU:HB2	1:A:82:ALA:HA	0.66	1.65	13	3
1:B:22:LEU:HG	1:B:28:LEU:HD21	0.66	1.68	2	1

### 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	93/108 (86%)	91±1 (97±1%)	2±1 (2±1%)	0±0 (0±0%)	47	81
1	B	93/108 (86%)	91±1 (98±1%)	2±1 (2±1%)	0±0 (0±1%)	40	79
All	All	3720/4320 (86%)	3630 (98%)	77 (2%)	13 (0%)	47	81

All 5 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	24	ASN	5
1	B	24	ASN	5
1	B	25	GLY	1
1	B	23	ALA	1
1	A	74	GLY	1

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	67/80 (84%)	65±2 (97±3%)	2±2 (3±3%)	45	88
1	B	67/80 (84%)	65±1 (97±2%)	2±1 (3±2%)	47	89
All	All	2680/3200 (84%)	2594 (97%)	86 (3%)	46	89

5 of 37 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	38	GLU	6
1	A	24	ASN	6
1	A	38	GLU	5
1	A	69	GLU	5
1	B	69	GLU	4

### 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 63% for the well-defined parts and 59% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2kko\_nmr.cif

Chemical shift list name: *nef\_chemical\_shift\_list\_2kko.mr*

#### 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	2501
Number of shifts mapped to atoms	1563
Number of unparsed shifts	386
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	552
Number of shift outliers (ShiftChecker)	4

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

- Chemical shift has been reported more than once. First 5 (of 386) occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
7	A	2	ALA	HB%	1.410	0.020	1
8	A	2	ALA	HB%	1.410	0.020	1
15	A	3	GLY	HA%	4.030	0.020	1
26	A	4	GLN	HG%	2.390	0.020	1
45	A	6	ASP	HB%	2.710	0.020	1

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

- No matching atoms found in structure. First 5 (of 552) occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	100	HIS	HBy	3.42	0.02	2
B	58	ASN	HD2y	6.68	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	62	LEU	HBx	1.19	0.02	2
A	45	ALA	HB%	1.4	0.02	1
A	84	GLU	HG%	2.35	0.02	1

### 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
$^{13}\text{C}_\alpha$	210	$-0.46 \pm 0.04$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	192	$0.10 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	205	$-0.28 \pm 0.06$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	206	$0.05 \pm 0.23$	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 63%, i.e. 1406 atoms were assigned a chemical shift out of a possible 2231. 42 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	914/930 (98%)	356/372 (96%)	372/372 (100%)	186/186 (100%)
Sidechain	466/1243 (37%)	68/713 (10%)	374/449 (83%)	24/81 (30%)
Aromatic	26/58 (45%)	13/30 (43%)	13/26 (50%)	0/2 (0%)
Overall	1406/2231 (63%)	437/1115 (39%)	759/847 (90%)	210/269 (78%)

### 7.1.4 Statistically unusual chemical shifts [i](#)

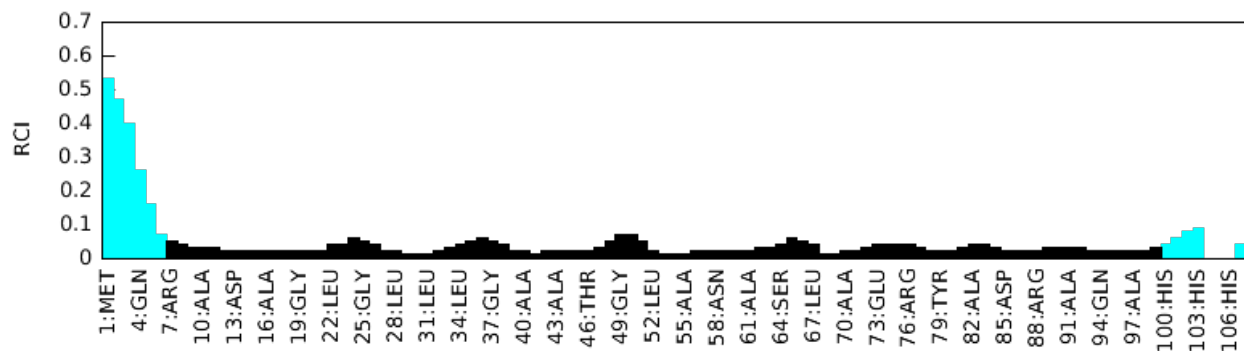
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	1	MET	CB	76.00	44.20 – 21.80	19.2
1	A	1	MET	CB	76.00	44.20 – 21.80	19.2
1	B	1	MET	CA	73.50	67.38 – 44.88	7.7
1	A	1	MET	CA	73.50	67.38 – 44.88	7.7

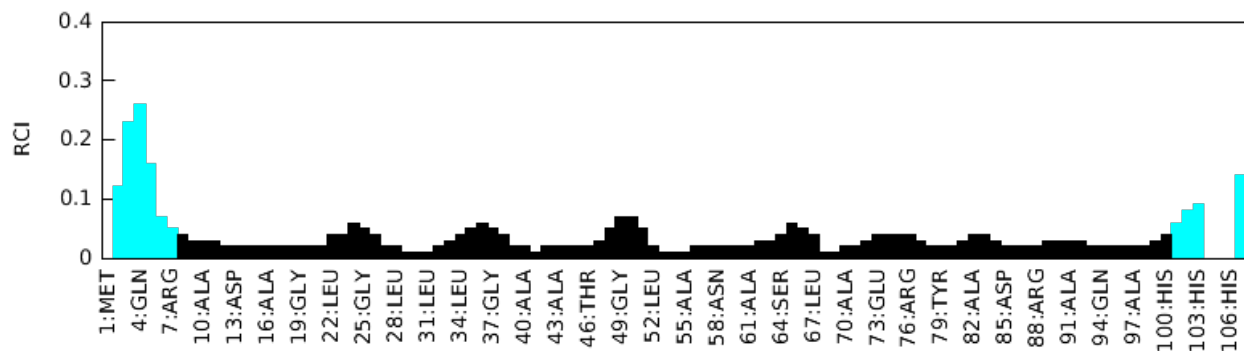
### 7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



## 8 Distance restraints analysis

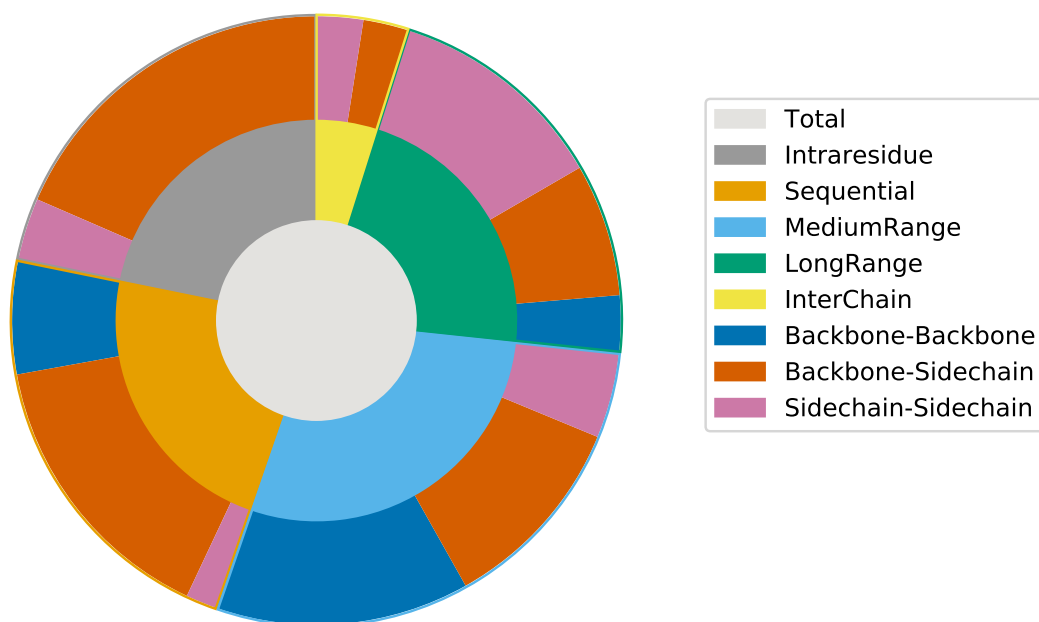
### 8.1 Distance restraints summary

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

Restraints type	B-B <sup>1</sup> (H <sup>4</sup> )	B-S <sup>2</sup> (H <sup>4</sup> )	S-S <sup>3</sup> (H <sup>4</sup> )	Total		
				Total(H <sup>4</sup> )	RR <sup>5</sup>	% <sup>6</sup>
Intraresidue ( $ i-j =0$ )	0(0)	478(0)	86(0)	564(0)	2.8	21.8
Sequential ( $ i-j =1$ )	156(0)	392(0)	44(0)	592(0)	3.0	22.9
Medium range ( $ i-j >1$ and $ i-j <5$ )	348(188)	274(0)	118(0)	740(188)	3.7	28.6
Long range ( $ i-j \geq 5$ )	78(40)	182(0)	304(0)	564(40)	2.8	21.8
Inter chain	0(0)	62(0)	64(0)	126(0)	0.6	4.9
Total	582(228)	1388(0)	616(0)	2586(228)	12.9	100.0

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

#### 8.1.1 Pie chart : Distance restraints summary



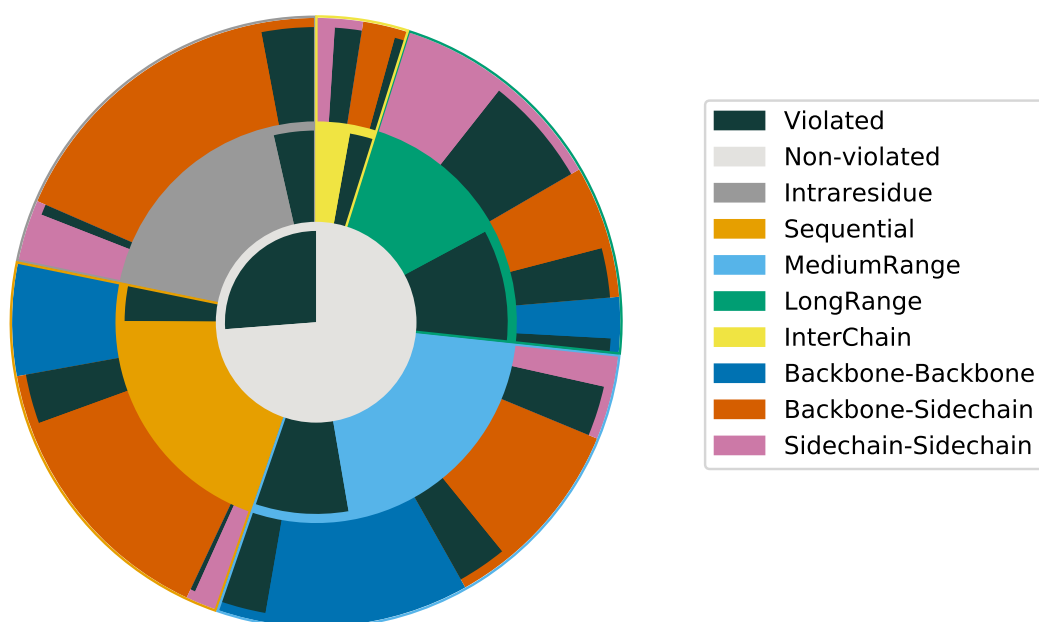
## 8.2 Distance violations summary

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

Restrains type	B-B <sup>1</sup> (% <sup>4</sup> )	B-S <sup>2</sup> (% <sup>4</sup> )	S-S <sup>3</sup> (% <sup>4</sup> )	Total		
				Total(% <sup>4</sup> )	RR <sup>5</sup>	% <sup>6</sup>
Intraresidue ( $ i-j =0$ )	0(0.0)	77(16.1)	15(17.4)	92(16.3)	0.5	13.6
Sequential ( $ i-j =1$ )	3(1.9)	70(17.9)	7(15.9)	80(13.5)	0.4	11.8
Medium range ( $ i-j >1$ and $ i-j <5$ )	66(19.0)	70(25.5)	71(60.2)	207(28.0)	1.0	30.5
Long range ( $ i-j \geq 5$ )	21(26.9)	70(38.5)	155(51.0)	246(43.6)	1.2	36.3
Inter chain	0(0.0)	15(24.2)	38(59.4)	53(42.1)	0.3	7.8
Total	90(15.5)	302(21.8)	286(46.4)	678(26.2)	3.4	100.0

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

### 8.2.1 Pie-chart : Distance violations summary



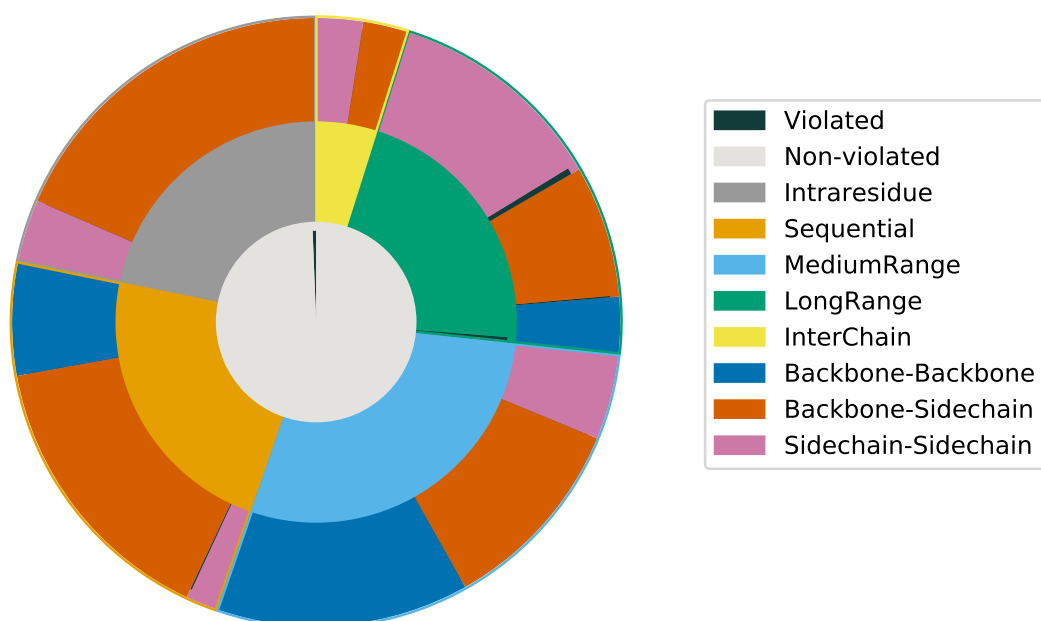
### 8.3 Consistent distance violations summary

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

Restrains type	B-B <sup>1</sup> (% <sup>4</sup> )	B-S <sup>2</sup> (% <sup>4</sup> )	S-S <sup>3</sup> (% <sup>4</sup> )	Total		
				Total(% <sup>4</sup> )	RR <sup>5</sup>	% <sup>6</sup>
Intraresidue ( $ i-j =0$ )	0(0.0)	0(0.0)	0(0.0)	0(0.0)	0.0	0.0
Sequential ( $ i-j =1$ )	0(0.0)	0(0.0)	2(4.5)	2(0.3)	0.0	12.5
Medium range ( $ i-j >1$ and $ i-j <5$ )	3(0.9)	0(0.0)	0(0.0)	3(0.4)	0.0	18.8
Long range ( $ i-j \geq 5$ )	0(0.0)	2(1.1)	9(3.0)	11(2.0)	0.1	68.8
Inter chain	0(0.0)	0(0.0)	0(0.0)	0(0.0)	0.0	0.0
Total	3(0.5)	2(0.1)	11(1.8)	16(0.6)	0.1	100.0

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

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





## 8.4 Residual distance violations

Violations are counted in different bin sizes and listed below

Range (Å)	No. of violated restraints per model	Max violation (Å)
0-0.2	83.8	0.2
0.2-0.5	36.2	0.5
0.5-1.0	29.2	1.0
1.0-2.0	22.4	2.0
2.0-5.0	10.1	4.14
5.0<	None	None

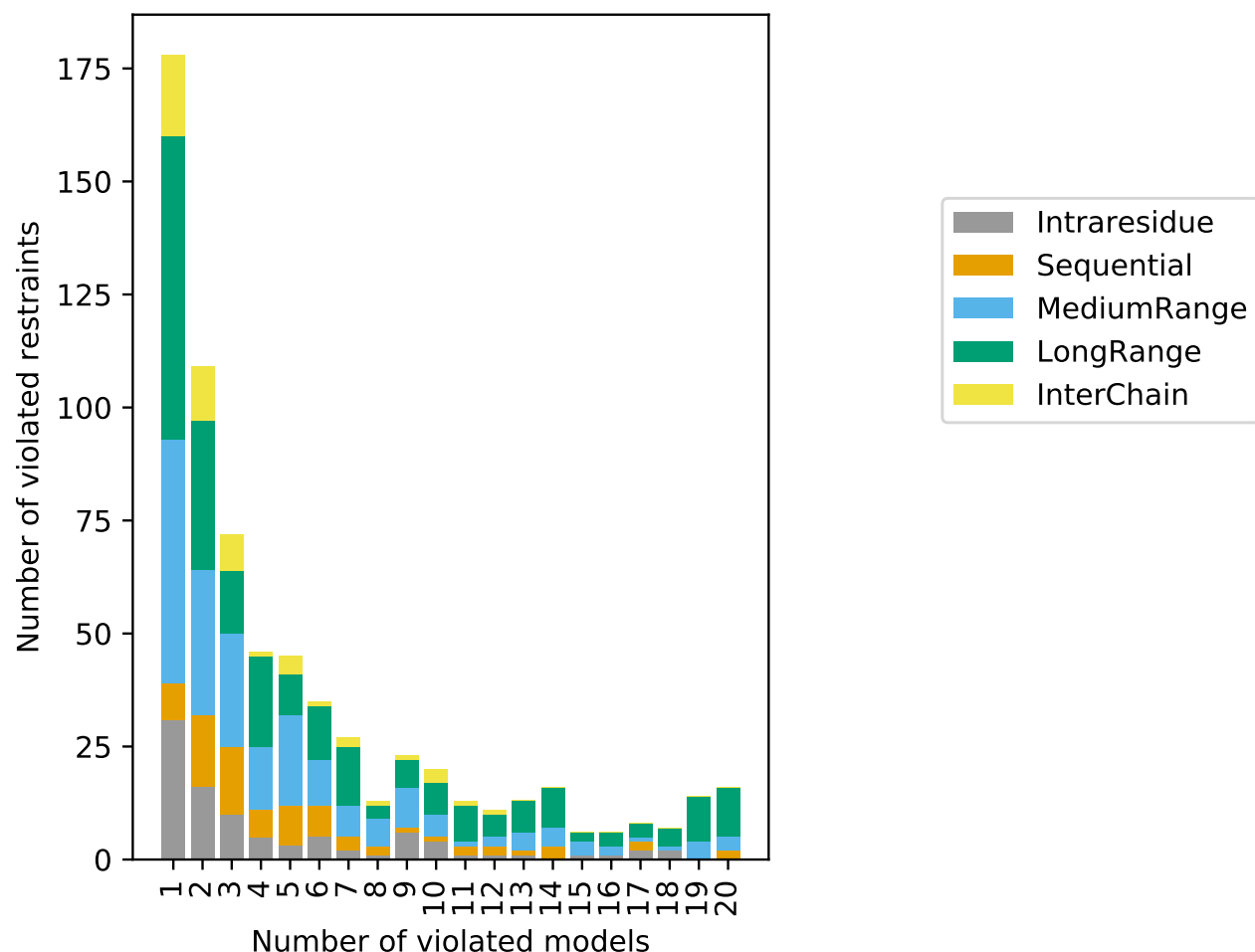
## 8.5 Distance violations in ensemble

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

No. of violated restraints						No. of violated models
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	
31	8	54	67	18	178	1
16	16	32	33	12	109	2
10	15	25	14	8	72	3
5	6	14	20	1	46	4
3	9	20	9	4	45	5
5	7	10	12	1	35	6
2	3	7	13	2	27	7
1	2	6	3	1	13	8
6	1	9	6	1	23	9
4	1	5	7	3	20	10
1	2	1	8	1	13	11
1	2	2	5	1	11	12
1	1	4	7	0	13	13
0	3	4	9	0	16	14
1	0	3	2	0	6	15
1	0	2	3	0	6	16
2	2	1	3	0	8	17
2	0	1	4	0	7	18
0	0	4	10	0	14	19
0	2	3	11	0	16	20

<sup>1</sup>intraresidue restraints, <sup>2</sup>sequential restraints, <sup>3</sup>medium range restraints, <sup>4</sup>long range restraints, <sup>5</sup>inter chain restraints

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



472 intraresidue restraints, 512 sequential restraints, 533 medium range restraints, 318 long range restraints and 73 inter chain restraints are not violated. There are totally 1908 restrains not violated in any of the models

## 8.6 Violations in each model

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

Model ID	No. of violations					Total	Mean (Å)	Max (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>			
1	22	32	51	79	5	189	0.55	2.8
2	23	17	57	88	6	191	0.58	3.81
3	13	21	59	80	3	176	0.55	2.96
4	23	20	53	85	11	192	0.47	3.37
5	16	18	49	83	6	172	0.51	3.4

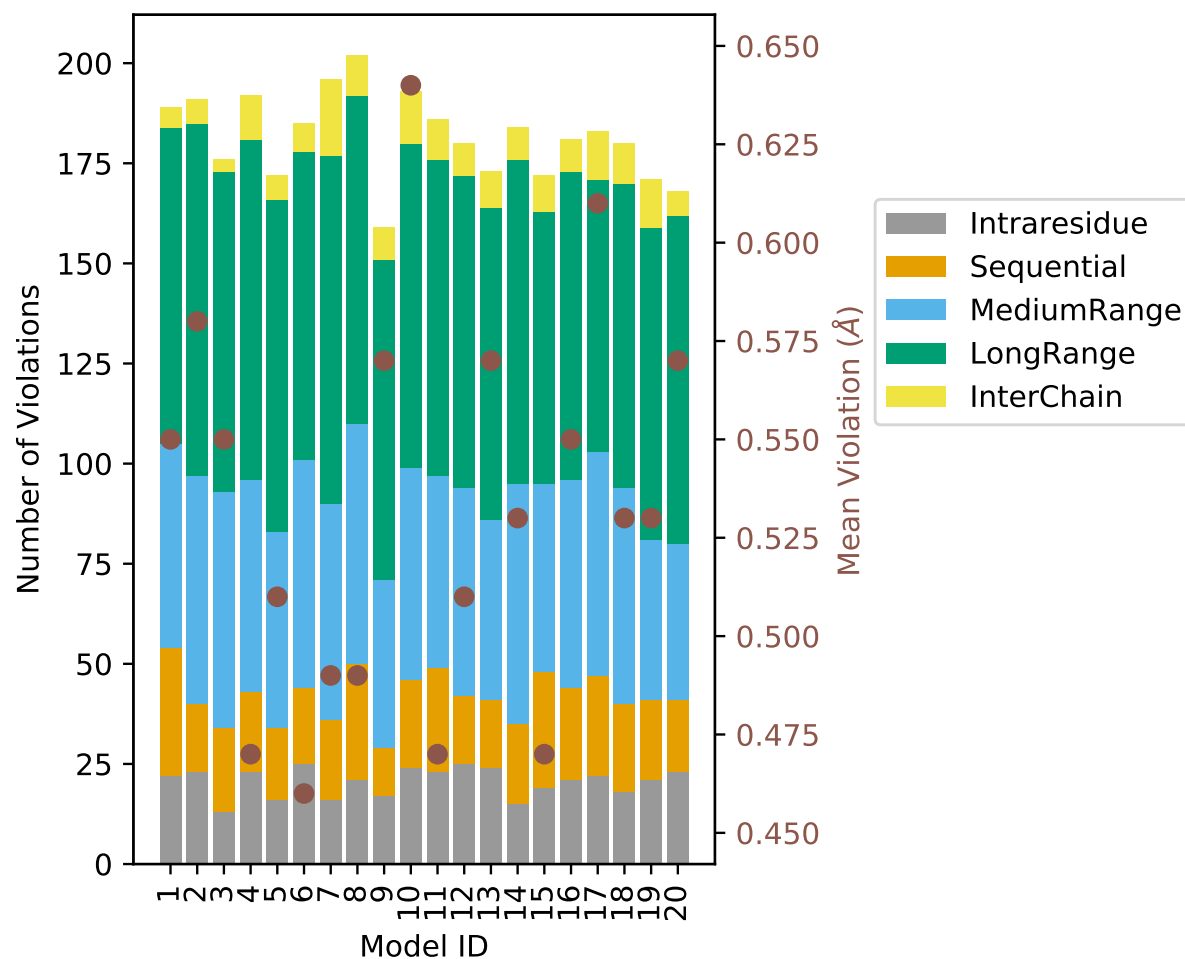
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Model ID	No. of violations						Mean (Å)	Max (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total		
6	25	19	57	77	7	185	0.46	3.35
7	16	20	54	87	19	196	0.49	3.45
8	21	29	60	82	10	202	0.49	3.33
9	17	12	42	80	8	159	0.57	3.1
10	24	22	53	81	13	193	0.64	3.57
11	23	26	48	79	10	186	0.47	4.14
12	25	17	52	78	8	180	0.51	2.98
13	24	17	45	78	9	173	0.57	3.26
14	15	20	60	81	8	184	0.53	2.83
15	19	29	47	68	9	172	0.47	2.71
16	21	23	52	77	8	181	0.55	2.87
17	22	25	56	68	12	183	0.61	3.68
18	18	22	54	76	10	180	0.53	3.65
19	21	20	40	78	12	171	0.53	2.74
20	23	18	39	82	6	168	0.57	3.2

<sup>1</sup>intraresidue restraints, <sup>2</sup>iequential restraints, <sup>3</sup>iedium range restraints, <sup>4</sup>long range restraints,  
<sup>5</sup>inter chain restraints

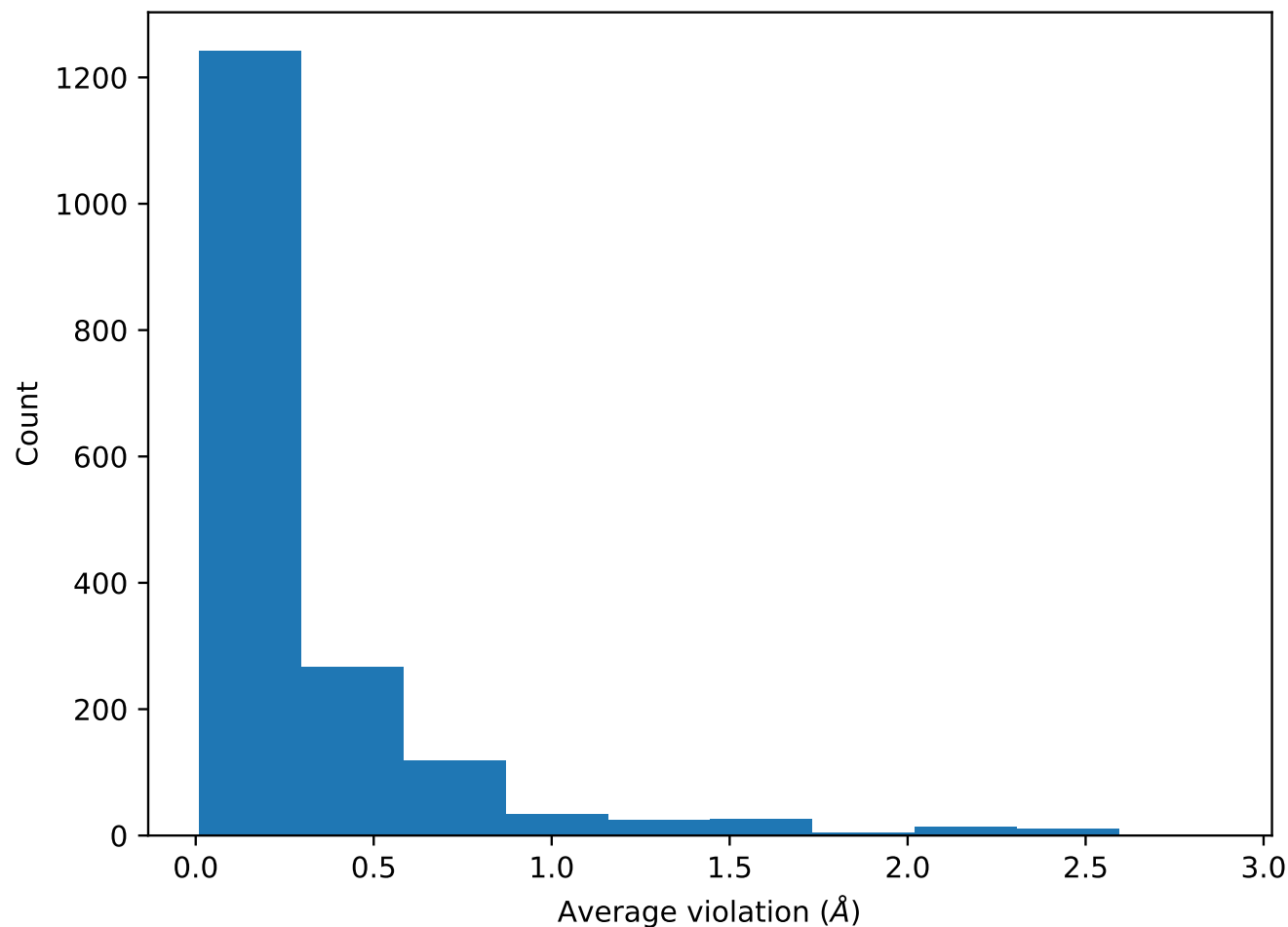
## 8.6.1 Bar graph : Violations in each model



## 8.7 Most violated distance restraints

### 8.7.1 Histogram : Distribution of mean distance violation

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



### 8.7.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	20	2.21	3.33
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	20	2.21	3.33
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	20	2.21	3.33
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	20	1.64	2.57
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	20	0.03	0.05
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	20	0.03	0.06

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	20	0.03	0.05
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	20	0.68	0.77
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	20	0.68	0.77
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	20	0.68	0.77
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	20	1.5	2.09
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	20	1.5	2.09
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	20	1.5	2.09
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	20	1.71	2.08
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	20	1.71	2.08
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	20	1.71	2.08
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	20	2.35	3.4
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	20	2.35	3.4
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	20	2.22	3.14
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	20	2.22	3.14
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	20	1.65	3.44
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	20	1.65	3.44
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	20	2.84	3.81
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	20	2.19	2.79
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	20	2.19	2.79
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	20	2.19	2.79
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	20	1.65	2.62
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	20	0.19	0.4
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	20	0.19	0.4
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	20	0.19	0.4
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	20	0.67	0.73
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	20	0.67	0.73
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	20	0.67	0.73
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	19	1.52	1.9
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	19	1.52	1.9
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	19	1.52	1.9
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	19	1.7	2.08
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	19	1.7	2.08
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	19	1.7	2.08
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	19	0.35	0.72
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	19	0.35	0.72
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	19	2.4	3.59
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	19	2.4	3.59
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	19	2.01	3.22
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	19	2.01	3.22
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	19	1.6	2.73
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	19	1.6	2.73
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	19	2.88	3.68

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	19	2.08	2.74
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	19	1.72	2.3
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	19	0.02	0.04
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	19	0.41	0.72
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	19	0.41	0.72
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	19	1.31	2.06
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	19	1.31	2.06
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	19	1.31	2.06
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	19	0.72	1.18
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	19	0.72	1.18
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	19	0.72	1.18
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	19	0.48	1.47
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	18	1.62	3.1
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	18	0.4	0.96
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	18	0.26	0.91
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	18	0.57	1.06
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	18	0.57	1.06
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	18	0.57	1.06
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	18	0.36	1.17
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	18	0.36	1.17
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	18	0.36	1.17
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	18	0.55	1.17
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	18	0.55	1.17
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	18	0.55	1.17
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	18	0.42	0.5
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	17	1.15	2.44
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	17	1.15	2.44
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	17	0.24	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	17	0.24	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	17	0.24	0.25
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	17	0.41	0.47
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	17	0.71	1.3
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	17	0.72	1.16
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	17	0.72	1.16
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	17	0.72	1.16
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	17	0.83	1.53
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	17	0.83	1.53
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	17	0.83	1.53
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	17	0.54	1.15
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	17	0.54	1.15
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	17	0.54	1.15
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	17	0.54	1.15

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	17	0.54	1.15
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	17	0.54	1.15
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	17	0.54	1.15
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	17	0.54	1.15
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	17	0.54	1.15
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	17	0.91	1.49
(1,471)	1:A:33:LEU:HD11	1:A:44:ILE:H	16	1.21	1.88
(1,471)	1:A:33:LEU:HD12	1:A:44:ILE:H	16	1.21	1.88
(1,471)	1:A:33:LEU:HD13	1:A:44:ILE:H	16	1.21	1.88
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	16	0.06	0.13
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	16	0.06	0.13
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	16	0.06	0.13
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	16	0.46	1.04
(1,1934)	1:B:59:LEU:HB2	1:B:79:TYR:HE1	16	0.39	1.07
(1,1596)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	16	0.7	1.09
(1,1596)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	16	0.7	1.09
(1,1596)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	16	0.7	1.09
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG11	16	0.24	0.25
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG12	16	0.24	0.25
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG13	16	0.24	0.25
(1,742)	1:A:52:LEU:HD11	1:A:56:SER:H	15	0.6	1.06
(1,742)	1:A:52:LEU:HD12	1:A:56:SER:H	15	0.6	1.06
(1,742)	1:A:52:LEU:HD13	1:A:56:SER:H	15	0.6	1.06
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD11	15	0.95	1.64
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD12	15	0.95	1.64
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD13	15	0.95	1.64
(1,473)	1:A:33:LEU:HD11	1:A:47:ALA:H	15	0.6	1.6
(1,473)	1:A:33:LEU:HD12	1:A:47:ALA:H	15	0.6	1.6
(1,473)	1:A:33:LEU:HD13	1:A:47:ALA:H	15	0.6	1.6
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB1	15	0.69	1.44
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB2	15	0.69	1.44
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB3	15	0.69	1.44
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB1	15	0.69	1.44
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB2	15	0.69	1.44
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB3	15	0.69	1.44
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB1	15	0.69	1.44
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB2	15	0.69	1.44
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB3	15	0.69	1.44
(1,1849)	1:B:50:MET:H	1:B:50:MET:HG2	15	0.32	0.89
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	15	0.56	1.31
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	15	0.56	1.31
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	15	0.56	1.31

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	14	0.74	1.38
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	14	0.74	1.38
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	14	0.74	1.38
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	14	0.89	1.25
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	14	0.89	1.25
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	14	0.89	1.25
(1,558)	1:A:40:ALA:HB1	1:A:78:TYR:HD1	14	0.42	0.77
(1,558)	1:A:40:ALA:HB2	1:A:78:TYR:HD1	14	0.42	0.77
(1,558)	1:A:40:ALA:HB3	1:A:78:TYR:HD1	14	0.42	0.77
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD11	14	0.52	1.02
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD12	14	0.52	1.02
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD13	14	0.52	1.02
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD11	14	0.52	1.02
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD12	14	0.52	1.02
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD13	14	0.52	1.02
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD11	14	0.52	1.02
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD12	14	0.52	1.02
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD13	14	0.52	1.02
(1,470)	1:A:33:LEU:HD11	1:A:44:ILE:HA	14	0.76	1.18
(1,470)	1:A:33:LEU:HD12	1:A:44:ILE:HA	14	0.76	1.18
(1,470)	1:A:33:LEU:HD13	1:A:44:ILE:HA	14	0.76	1.18
(1,464)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	14	1.33	2.7
(1,464)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	14	1.33	2.7
(1,464)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	14	1.33	2.7
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	14	0.43	0.65
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	14	0.43	0.65
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	14	0.43	0.65
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	14	0.39	0.82
(1,2134)	1:B:74:GLY:HA2	1:B:75:THR:HB	14	0.71	1.05
(1,2125)	1:B:73:GLU:HB2	1:B:76:ARG:HG2	14	1.43	3.01
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	14	0.54	1.43
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	14	0.54	1.43
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	14	0.54	1.43
(1,1695)	1:B:40:ALA:H	1:B:78:TYR:HE1	14	2.02	2.4
(1,1694)	1:B:40:ALA:H	1:B:78:TYR:HD1	14	1.67	1.95
(1,1681)	1:B:40:ALA:HB1	1:B:42:GLU:HG2	14	0.39	0.81
(1,1681)	1:B:40:ALA:HB2	1:B:42:GLU:HG2	14	0.39	0.81
(1,1681)	1:B:40:ALA:HB3	1:B:42:GLU:HG2	14	0.39	0.81
(1,1645)	1:B:36:GLN:HG2	1:B:37:GLY:H	14	0.55	0.66
(1,1002)	1:A:74:GLY:HA2	1:A:75:THR:HB	14	0.65	1.14
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB2	13	0.4	1.0
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB3	13	0.4	1.0

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB2	13	0.4	1.0
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB3	13	0.4	1.0
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB2	13	0.4	1.0
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB3	13	0.4	1.0
(1,559)	1:A:40:ALA:HB1	1:A:78:TYR:HE1	13	0.42	0.91
(1,559)	1:A:40:ALA:HB2	1:A:78:TYR:HE1	13	0.42	0.91
(1,559)	1:A:40:ALA:HB3	1:A:78:TYR:HE1	13	0.42	0.91
(1,513)	1:A:36:GLN:HG2	1:A:37:GLY:H	13	0.5	0.72
(1,2521)	1:B:21:ALA:H	1:B:17:ARG:O	13	0.03	0.06
(1,2298)	1:B:91:ALA:HA	1:B:94:GLN:HG2	13	0.25	0.45
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB1	13	0.63	0.85
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB2	13	0.63	0.85
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB3	13	0.63	0.85
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD11	13	0.19	0.25
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD12	13	0.19	0.25
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD13	13	0.19	0.25
(1,1658)	1:B:38:GLU:HG2	1:B:78:TYR:HD1	13	1.31	2.27
(1,1658)	1:B:38:GLU:HG3	1:B:78:TYR:HD1	13	1.31	2.27
(1,1657)	1:B:38:GLU:HG2	1:B:78:TYR:HB2	13	0.66	1.37
(1,1657)	1:B:38:GLU:HG3	1:B:78:TYR:HB2	13	0.66	1.37
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB1	13	0.49	1.15
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB2	13	0.49	1.15
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB3	13	0.49	1.15
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB1	13	0.49	1.15
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB2	13	0.49	1.15
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB3	13	0.49	1.15
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB1	13	0.49	1.15
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB2	13	0.49	1.15
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB3	13	0.49	1.15
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG21	13	0.33	0.63
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG22	13	0.33	0.63
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG23	13	0.33	0.63
(1,1361)	1:B:17:ARG:HA	1:B:65:GLY:HA2	13	0.26	0.83
(1,1166)	1:A:91:ALA:HA	1:A:94:GLN:HG2	13	0.24	0.53
(1,525)	1:A:38:GLU:HG2	1:A:78:TYR:HB2	12	0.61	1.51
(1,525)	1:A:38:GLU:HG3	1:A:78:TYR:HB2	12	0.61	1.51
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB1	12	0.49	1.13
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB2	12	0.49	1.13
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB3	12	0.49	1.13
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB1	12	0.49	1.13
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB2	12	0.49	1.13
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB3	12	0.49	1.13

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB1	12	0.49	1.13
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB2	12	0.49	1.13
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB3	12	0.49	1.13
(1,4)	1:A:11:LEU:HD11	1:B:98:ASP:H	12	0.43	1.42
(1,4)	1:A:11:LEU:HD12	1:B:98:ASP:H	12	0.43	1.42
(1,4)	1:A:11:LEU:HD13	1:B:98:ASP:H	12	0.43	1.42
(1,2407)	1:A:21:ALA:H	1:A:17:ARG:O	12	0.03	0.06
(1,2191)	1:B:81:ILE:HG12	1:B:87:ALA:HA	12	0.53	1.22
(1,2151)	1:B:76:ARG:HD2	1:B:77:GLN:H	12	0.06	0.16
(1,2151)	1:B:76:ARG:HD3	1:B:77:GLN:H	12	0.06	0.16
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	12	0.02	0.06
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	12	0.02	0.06
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	12	0.02	0.06
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	12	0.02	0.06
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	12	0.02	0.06
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	12	0.02	0.06
(1,1492)	1:B:29:GLN:HG2	1:B:48:THR:HB	12	0.38	0.86
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD21	12	0.79	1.15
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD22	12	0.79	1.15
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD23	12	0.79	1.15
(1,1047)	1:A:80:ARG:H	1:A:80:ARG:HG2	12	0.29	0.66
(1,1041)	1:A:79:TYR:HA	1:A:80:ARG:HG2	12	0.55	0.68
(1,987)	1:A:72:ARG:HD2	1:A:77:GLN:HG2	11	0.96	1.71
(1,987)	1:A:72:ARG:HD3	1:A:77:GLN:HG2	11	0.96	1.71
(1,899)	1:A:67:LEU:HD11	1:A:86:VAL:HA	11	0.06	0.11
(1,899)	1:A:67:LEU:HD12	1:A:86:VAL:HA	11	0.06	0.11
(1,899)	1:A:67:LEU:HD13	1:A:86:VAL:HA	11	0.06	0.11
(1,615)	1:A:42:GLU:HG2	1:A:52:LEU:HG	11	0.42	1.2
(1,245)	1:A:18:VAL:HG11	1:A:65:GLY:HA2	11	0.41	0.77
(1,245)	1:A:18:VAL:HG12	1:A:65:GLY:HA2	11	0.41	0.77
(1,245)	1:A:18:VAL:HG13	1:A:65:GLY:HA2	11	0.41	0.77
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	11	1.16	1.84
(1,2179)	1:B:80:ARG:H	1:B:80:ARG:HG2	11	0.28	0.47
(1,2173)	1:B:79:TYR:HA	1:B:80:ARG:HG2	11	0.49	0.67
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB2	11	0.45	1.12
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB3	11	0.45	1.12
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB2	11	0.45	1.12
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB3	11	0.45	1.12
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB2	11	0.45	1.12
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB3	11	0.45	1.12
(1,1690)	1:B:40:ALA:HB1	1:B:78:TYR:HD1	11	0.3	0.86
(1,1690)	1:B:40:ALA:HB2	1:B:78:TYR:HD1	11	0.3	0.86

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1690)	1:B:40:ALA:HB3	1:B:78:TYR:HD1	11	0.3	0.86
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	11	0.03	0.07
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	11	0.03	0.07
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	11	0.03	0.07
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	11	0.03	0.07
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	11	0.03	0.07
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	11	0.03	0.07
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB1	11	0.53	1.12
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB2	11	0.53	1.12
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB3	11	0.53	1.12
(1,1059)	1:A:81:ILE:HG12	1:A:87:ALA:HA	11	0.42	0.96
(1,1019)	1:A:76:ARG:HD2	1:A:77:GLN:H	11	0.03	0.07
(1,1019)	1:A:76:ARG:HD3	1:A:77:GLN:H	11	0.03	0.07
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG2	10	1.01	1.83
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	10	0.04	0.08
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	10	0.04	0.08
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	10	0.04	0.08
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	10	0.04	0.08
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	10	0.04	0.08
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	10	0.04	0.08
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	10	0.03	0.06
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	10	0.03	0.06
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	10	0.03	0.06
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	10	0.03	0.06
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	10	0.03	0.06
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	10	0.03	0.06
(1,2533)	1:B:39:ARG:H	1:B:79:TYR:O	10	0.02	0.06
(1,2515)	1:B:18:VAL:H	1:B:14:GLN:O	10	0.03	0.07
(1,2449)	1:A:61:ALA:H	1:A:57:ALA:O	10	0.02	0.04
(1,231)	1:A:17:ARG:H	1:A:17:ARG:HG2	10	0.07	0.16
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA2	10	0.33	1.07
(1,2169)	1:B:77:GLN:H	1:B:77:GLN:HG2	10	0.39	0.67
(1,2154)	1:B:76:ARG:HG2	1:B:78:TYR:HE1	10	0.62	1.18
(1,2095)	1:B:70:ALA:HB1	1:B:79:TYR:HE1	10	0.3	0.82
(1,2095)	1:B:70:ALA:HB2	1:B:79:TYR:HE1	10	0.3	0.82
(1,2095)	1:B:70:ALA:HB3	1:B:79:TYR:HE1	10	0.3	0.82
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE2	10	0.11	0.2
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE3	10	0.11	0.2
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	10	0.04	0.07
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	10	0.04	0.07
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	10	0.04	0.07
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	10	0.04	0.07

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	10	0.04	0.07
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	10	0.04	0.07
(1,1747)	1:B:42:GLU:HG2	1:B:52:LEU:HG	10	0.77	1.5
(1,1691)	1:B:40:ALA:HB1	1:B:78:TYR:HE1	10	0.36	0.96
(1,1691)	1:B:40:ALA:HB2	1:B:78:TYR:HE1	10	0.36	0.96
(1,1691)	1:B:40:ALA:HB3	1:B:78:TYR:HE1	10	0.36	0.96
(1,141)	1:A:7:ARG:HB2	1:A:8:LYS:H	10	0.33	0.62
(1,1377)	1:B:18:VAL:HG11	1:B:65:GLY:HA2	10	0.42	0.91
(1,1377)	1:B:18:VAL:HG12	1:B:65:GLY:HA2	10	0.42	0.91
(1,1377)	1:B:18:VAL:HG13	1:B:65:GLY:HA2	10	0.42	0.91
(1,1296)	1:B:10:ALA:HB1	1:B:13:ASP:HB2	10	0.24	0.67
(1,1296)	1:B:10:ALA:HB2	1:B:13:ASP:HB2	10	0.24	0.67
(1,1296)	1:B:10:ALA:HB3	1:B:13:ASP:HB2	10	0.24	0.67
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD21	10	0.02	0.04
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD22	10	0.02	0.04
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD23	10	0.02	0.04
(1,1037)	1:A:77:GLN:H	1:A:77:GLN:HG2	10	0.37	0.52
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE2	9	0.09	0.22
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE3	9	0.09	0.22
(1,8)	1:A:12:LEU:HD11	1:B:29:GLN:HE21	9	0.38	0.55
(1,8)	1:A:12:LEU:HD12	1:B:29:GLN:HE21	9	0.38	0.55
(1,8)	1:A:12:LEU:HD13	1:B:29:GLN:HE21	9	0.38	0.55
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB1	9	0.61	1.21
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB2	9	0.61	1.21
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB3	9	0.61	1.21
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB1	9	0.61	1.21
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB2	9	0.61	1.21
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB3	9	0.61	1.21
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB1	9	0.61	1.21
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB2	9	0.61	1.21
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB3	9	0.61	1.21
(1,549)	1:A:40:ALA:HB1	1:A:42:GLU:HG2	9	0.41	0.87
(1,549)	1:A:40:ALA:HB2	1:A:42:GLU:HG2	9	0.41	0.87
(1,549)	1:A:40:ALA:HB3	1:A:42:GLU:HG2	9	0.41	0.87
(1,467)	1:A:33:LEU:HD11	1:A:39:ARG:HD2	9	0.65	1.62
(1,467)	1:A:33:LEU:HD12	1:A:39:ARG:HD2	9	0.65	1.62
(1,467)	1:A:33:LEU:HD13	1:A:39:ARG:HD2	9	0.65	1.62
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	9	0.06	0.15
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	9	0.06	0.15
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	9	0.06	0.15
(1,2613)	1:B:97:ALA:H	1:B:93:VAL:O	9	0.03	0.06
(1,2563)	1:B:61:ALA:H	1:B:57:ALA:O	9	0.02	0.03

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2507)	1:B:14:GLN:H	1:B:10:ALA:O	9	0.03	0.06
(1,2459)	1:A:66:GLY:H	1:A:63:LYS:O	9	0.03	0.1
(1,2393)	1:A:14:GLN:H	1:A:10:ALA:O	9	0.02	0.04
(1,2031)	1:B:67:LEU:HD11	1:B:86:VAL:HA	9	0.06	0.12
(1,2031)	1:B:67:LEU:HD12	1:B:86:VAL:HA	9	0.06	0.12
(1,2031)	1:B:67:LEU:HD13	1:B:86:VAL:HA	9	0.06	0.12
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD11	9	0.16	0.18
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD12	9	0.16	0.18
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD13	9	0.16	0.18
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD11	9	1.08	1.31
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD12	9	1.08	1.31
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD13	9	1.08	1.31
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD11	9	0.48	0.81
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD12	9	0.48	0.81
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD13	9	0.48	0.81
(1,1726)	1:B:41:VAL:HG21	1:B:77:GLN:HG2	9	0.25	0.56
(1,1726)	1:B:41:VAL:HG22	1:B:77:GLN:HG2	9	0.25	0.56
(1,1726)	1:B:41:VAL:HG23	1:B:77:GLN:HG2	9	0.25	0.56
(1,1662)	1:B:39:ARG:HA	1:B:39:ARG:HD2	9	0.14	0.5
(1,1460)	1:B:27:ARG:HD2	1:B:58:ASN:HA	9	0.55	1.02
(1,144)	1:A:7:ARG:H	1:A:7:ARG:HG2	9	0.1	0.16
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD11	9	0.18	0.24
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD12	9	0.18	0.24
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD13	9	0.18	0.24
(1,1276)	1:B:7:ARG:H	1:B:7:ARG:HG2	9	0.13	0.24
(1,1273)	1:B:7:ARG:HB2	1:B:8:LYS:H	9	0.21	0.5
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG11	9	0.22	0.42
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG12	9	0.22	0.42
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG13	9	0.22	0.42
(1,999)	1:A:73:GLU:H	1:A:76:ARG:HG2	8	0.21	0.38
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	8	0.89	0.91
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	8	0.89	0.91
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	8	0.89	0.91
(1,67)	1:B:11:LEU:HD11	1:A:98:ASP:H	8	1.02	1.71
(1,67)	1:B:11:LEU:HD12	1:A:98:ASP:H	8	1.02	1.71
(1,67)	1:B:11:LEU:HD13	1:A:98:ASP:H	8	1.02	1.71
(1,594)	1:A:41:VAL:HG21	1:A:77:GLN:HG2	8	0.26	0.61
(1,594)	1:A:41:VAL:HG22	1:A:77:GLN:HG2	8	0.26	0.61
(1,594)	1:A:41:VAL:HG23	1:A:77:GLN:HG2	8	0.26	0.61
(1,486)	1:A:34:LEU:HB2	1:A:80:ARG:HA	8	0.61	1.38
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HE21	8	1.06	2.4
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HE21	8	1.06	2.4

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HE21	8	1.06	2.4
(1,2573)	1:B:66:GLY:H	1:B:63:LYS:O	8	0.03	0.1
(1,2527)	1:B:33:LEU:H	1:B:29:GLN:O	8	0.01	0.03
(1,2383)	1:B:101:LEU:HB2	1:B:102:GLU:H	8	0.3	0.41
(1,1411)	1:B:21:ALA:HB1	1:B:65:GLY:H	8	0.08	0.15
(1,1411)	1:B:21:ALA:HB2	1:B:65:GLY:H	8	0.08	0.15
(1,1411)	1:B:21:ALA:HB3	1:B:65:GLY:H	8	0.08	0.15
(1,1363)	1:B:17:ARG:H	1:B:17:ARG:HG2	8	0.07	0.16
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD11	8	0.88	1.59
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD12	8	0.88	1.59
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD13	8	0.88	1.59
(1,1035)	1:A:77:GLN:HG2	1:A:79:TYR:HE1	8	0.25	0.48
(1,972)	1:A:71:ARG:HG2	1:A:78:TYR:HB2	7	0.65	1.03
(1,9)	1:A:12:LEU:HD11	1:B:29:GLN:HG2	7	0.69	0.84
(1,9)	1:A:12:LEU:HD12	1:B:29:GLN:HG2	7	0.69	0.84
(1,9)	1:A:12:LEU:HD13	1:B:29:GLN:HG2	7	0.69	0.84
(1,749)	1:A:53:THR:HG21	1:A:54:THR:H	7	0.04	0.07
(1,749)	1:A:53:THR:HG22	1:A:54:THR:H	7	0.04	0.07
(1,749)	1:A:53:THR:HG23	1:A:54:THR:H	7	0.04	0.07
(1,7)	1:A:12:LEU:HD11	1:B:29:GLN:HB2	7	0.14	0.32
(1,7)	1:A:12:LEU:HD12	1:B:29:GLN:HB2	7	0.14	0.32
(1,7)	1:A:12:LEU:HD13	1:B:29:GLN:HB2	7	0.14	0.32
(1,691)	1:A:48:THR:HB	1:A:50:MET:HG2	7	0.13	0.34
(1,475)	1:A:33:LEU:HG	1:A:36:GLN:HE21	7	0.67	1.3
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD1	7	0.03	0.06
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD2	7	0.03	0.06
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD1	7	0.03	0.06
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD2	7	0.03	0.06
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD1	7	0.03	0.06
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD2	7	0.03	0.06
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB1	7	0.59	1.1
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB2	7	0.59	1.1
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB3	7	0.59	1.1
(1,328)	1:A:27:ARG:HD2	1:A:58:ASN:HA	7	0.63	1.58
(1,2535)	1:B:41:VAL:H	1:B:77:GLN:O	7	0.03	0.07
(1,2523)	1:B:22:LEU:H	1:B:18:VAL:O	7	0.02	0.03
(1,2469)	1:A:76:ARG:H	1:A:73:GLU:O	7	0.03	0.06
(1,2421)	1:A:41:VAL:H	1:A:77:GLN:O	7	0.02	0.04
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB2	7	0.06	0.13
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB3	7	0.06	0.13
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB2	7	0.06	0.13
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB3	7	0.06	0.13

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2167)	1:B:77:GLN:HG2	1:B:79:TYR:HE1	7	0.45	0.63
(1,2129)	1:B:73:GLU:HG2	1:B:78:TYR:HE1	7	1.21	2.14
(1,2129)	1:B:73:GLU:HG3	1:B:78:TYR:HE1	7	1.21	2.14
(1,2128)	1:B:73:GLU:HG2	1:B:78:TYR:HD1	7	1.44	2.38
(1,2128)	1:B:73:GLU:HG3	1:B:78:TYR:HD1	7	1.44	2.38
(1,2127)	1:B:73:GLU:HB2	1:B:78:TYR:HE1	7	1.91	3.12
(1,2126)	1:B:73:GLU:HB2	1:B:78:TYR:HD1	7	2.27	3.01
(1,2119)	1:B:72:ARG:HD2	1:B:77:GLN:HG2	7	0.74	1.44
(1,2119)	1:B:72:ARG:HD3	1:B:77:GLN:HG2	7	0.74	1.44
(1,1854)	1:B:51:ASN:HB2	1:B:53:THR:H	7	0.17	0.42
(1,1668)	1:B:39:ARG:HD2	1:B:40:ALA:H	7	0.59	1.07
(1,1494)	1:B:29:GLN:H	1:B:29:GLN:HG2	7	0.18	0.2
(1,1441)	1:B:24:ASN:H	1:B:24:ASN:HB2	7	0.22	0.33
(1,1367)	1:B:17:ARG:HD2	1:B:64:SER:HB2	7	0.05	0.1
(1,1367)	1:B:17:ARG:HD2	1:B:64:SER:HB3	7	0.05	0.1
(1,1367)	1:B:17:ARG:HD3	1:B:64:SER:HB2	7	0.05	0.1
(1,1367)	1:B:17:ARG:HD3	1:B:64:SER:HB3	7	0.05	0.1
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD11	7	0.45	0.55
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD12	7	0.45	0.55
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD13	7	0.45	0.55
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG11	7	0.03	0.05
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG12	7	0.03	0.05
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG13	7	0.03	0.05
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG11	7	0.03	0.05
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG12	7	0.03	0.05
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG13	7	0.03	0.05
(1,968)	1:A:71:ARG:HB2	1:A:72:ARG:H	6	0.05	0.1
(1,816)	1:A:60:GLN:HA	1:A:60:GLN:HE21	6	0.1	0.17
(1,70)	1:B:12:LEU:HD11	1:A:29:GLN:HB2	6	0.36	0.64
(1,70)	1:B:12:LEU:HD12	1:A:29:GLN:HB2	6	0.36	0.64
(1,70)	1:B:12:LEU:HD13	1:A:29:GLN:HB2	6	0.36	0.64
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD11	6	0.29	0.6
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD12	6	0.29	0.6
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD13	6	0.29	0.6
(1,516)	1:A:37:GLY:HA2	1:A:38:GLU:HB2	6	0.1	0.27
(1,516)	1:A:37:GLY:HA2	1:A:38:GLU:HB3	6	0.1	0.27
(1,514)	1:A:36:GLN:H	1:A:36:GLN:HB2	6	0.15	0.19
(1,460)	1:A:33:LEU:HB2	1:A:34:LEU:H	6	0.05	0.11
(1,362)	1:A:29:GLN:H	1:A:29:GLN:HG2	6	0.16	0.2
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG21	6	0.49	1.11
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG22	6	0.49	1.11
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG23	6	0.49	1.11

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,330)	1:A:27:ARG:HD2	1:A:62:LEU:H	6	0.5	1.12
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD21	6	0.06	0.09
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD22	6	0.06	0.09
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD23	6	0.06	0.09
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD21	6	0.06	0.09
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD22	6	0.06	0.09
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD23	6	0.06	0.09
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD21	6	0.06	0.09
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD22	6	0.06	0.09
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD23	6	0.06	0.09
(1,2583)	1:B:76:ARG:H	1:B:73:GLU:O	6	0.02	0.06
(1,2571)	1:B:65:GLY:H	1:B:61:ALA:O	6	0.02	0.03
(1,2493)	1:A:94:GLN:H	1:A:90:PHE:O	6	0.02	0.04
(1,2441)	1:A:57:ALA:H	1:A:53:THR:O	6	0.01	0.02
(1,2419)	1:A:39:ARG:H	1:A:79:TYR:O	6	0.02	0.04
(1,2417)	1:A:35:ALA:H	1:A:31:LEU:O	6	0.02	0.03
(1,2413)	1:A:33:LEU:H	1:A:29:GLN:O	6	0.01	0.03
(1,2401)	1:A:18:VAL:H	1:A:14:GLN:O	6	0.02	0.03
(1,2390)	1:B:107:HIS:HB2	1:B:108:HIS:H	6	0.08	0.13
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD21	6	0.71	0.84
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD22	6	0.71	0.84
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD23	6	0.71	0.84
(1,2133)	1:B:73:GLU:H	1:B:78:TYR:HD1	6	1.33	1.54
(1,2100)	1:B:71:ARG:HB2	1:B:72:ARG:H	6	0.09	0.18
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD21	6	0.87	0.93
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD22	6	0.87	0.93
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD23	6	0.87	0.93
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB1	6	0.34	0.58
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB2	6	0.34	0.58
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB3	6	0.34	0.58
(1,1675)	1:B:40:ALA:HA	1:B:78:TYR:HA	6	0.04	0.08
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD11	6	0.36	0.51
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD12	6	0.36	0.51
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD13	6	0.36	0.51
(1,1618)	1:B:34:LEU:HB2	1:B:80:ARG:HA	6	0.55	0.8
(1,1599)	1:B:33:LEU:HD11	1:B:39:ARG:HD2	6	0.5	1.36
(1,1599)	1:B:33:LEU:HD12	1:B:39:ARG:HD2	6	0.5	1.36
(1,1599)	1:B:33:LEU:HD13	1:B:39:ARG:HD2	6	0.5	1.36
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG21	6	0.6	0.95
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG22	6	0.6	0.95
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG23	6	0.6	0.95
(1,1462)	1:B:27:ARG:HD2	1:B:62:LEU:H	6	0.59	1.11

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD2	6	0.04	0.13
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD3	6	0.04	0.13
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD11	6	0.02	0.05
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD12	6	0.02	0.05
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD13	6	0.02	0.05
(1,1278)	1:B:8:LYS:HA	1:B:8:LYS:HD2	6	0.11	0.21
(1,1278)	1:B:8:LYS:HA	1:B:8:LYS:HD3	6	0.11	0.21
(1,1095)	1:A:84:GLU:HG2	1:A:88:ARG:HG2	6	0.38	0.96
(1,1095)	1:A:84:GLU:HG3	1:A:88:ARG:HG2	6	0.38	0.96
(1,969)	1:A:71:ARG:HB2	1:A:79:TYR:HA	5	0.08	0.19
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD11	5	0.57	1.3
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD12	5	0.57	1.3
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD13	5	0.57	1.3
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG21	5	0.05	0.07
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG22	5	0.05	0.07
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG23	5	0.05	0.07
(1,722)	1:A:51:ASN:HB2	1:A:53:THR:H	5	0.14	0.24
(1,72)	1:B:12:LEU:HD11	1:A:29:GLN:HG2	5	0.63	0.75
(1,72)	1:B:12:LEU:HD12	1:A:29:GLN:HG2	5	0.63	0.75
(1,72)	1:B:12:LEU:HD13	1:A:29:GLN:HG2	5	0.63	0.75
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD11	5	0.27	0.68
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD12	5	0.27	0.68
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD13	5	0.27	0.68
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB1	5	0.06	0.1
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB2	5	0.06	0.1
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB3	5	0.06	0.1
(1,462)	1:A:33:LEU:HD11	1:A:36:GLN:HB2	5	0.17	0.45
(1,462)	1:A:33:LEU:HD12	1:A:36:GLN:HB2	5	0.17	0.45
(1,462)	1:A:33:LEU:HD13	1:A:36:GLN:HB2	5	0.17	0.45
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD21	5	0.01	0.02
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD22	5	0.01	0.02
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD23	5	0.01	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD21	5	0.01	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD22	5	0.01	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD23	5	0.01	0.02
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD21	5	0.01	0.02
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD22	5	0.01	0.02
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD23	5	0.01	0.02
(1,318)	1:A:26:ARG:HA	1:A:29:GLN:HG2	5	0.47	0.79
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD21	5	0.74	1.22
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD22	5	0.74	1.22
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD23	5	0.74	1.22

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,312)	1:A:25:GLY:HA2	1:A:28:LEU:HB2	5	0.67	1.31
(1,2579)	1:B:71:ARG:H	1:B:78:TYR:O	5	0.01	0.02
(1,2531)	1:B:35:ALA:H	1:B:31:LEU:O	5	0.01	0.01
(1,2513)	1:B:17:ARG:H	1:B:13:ASP:O	5	0.03	0.05
(1,2483)	1:A:89:LEU:H	1:A:85:ASP:O	5	0.02	0.03
(1,2461)	1:A:67:LEU:H	1:A:62:LEU:O	5	0.04	0.06
(1,2457)	1:A:65:GLY:H	1:A:61:ALA:O	5	0.01	0.02
(1,2443)	1:A:58:ASN:H	1:A:54:THR:O	5	0.02	0.04
(1,2399)	1:A:17:ARG:H	1:A:13:ASP:O	5	0.02	0.04
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD21	5	0.07	0.12
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD22	5	0.07	0.12
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD23	5	0.07	0.12
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD21	5	0.07	0.12
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD22	5	0.07	0.12
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD23	5	0.07	0.12
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD21	5	0.07	0.12
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD22	5	0.07	0.12
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD23	5	0.07	0.12
(1,2343)	1:B:95:VAL:HG11	1:B:99:GLU:HG2	5	0.37	0.81
(1,2343)	1:B:95:VAL:HG12	1:B:99:GLU:HG2	5	0.37	0.81
(1,2343)	1:B:95:VAL:HG13	1:B:99:GLU:HG2	5	0.37	0.81
(1,2227)	1:B:84:GLU:HG2	1:B:88:ARG:HG2	5	0.48	0.99
(1,2227)	1:B:84:GLU:HG3	1:B:88:ARG:HG2	5	0.48	0.99
(1,2171)	1:B:78:TYR:H	1:B:78:TYR:HD1	5	0.24	0.38
(1,2153)	1:B:76:ARG:HG2	1:B:77:GLN:H	5	0.42	0.74
(1,2152)	1:B:76:ARG:HD2	1:B:78:TYR:HE1	5	0.1	0.18
(1,2152)	1:B:76:ARG:HD3	1:B:78:TYR:HE1	5	0.1	0.18
(1,2113)	1:B:72:ARG:HA	1:B:77:GLN:HG2	5	0.55	0.86
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD21	5	0.02	0.04
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD22	5	0.02	0.04
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD23	5	0.02	0.04
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD21	5	0.02	0.04
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD22	5	0.02	0.04
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD23	5	0.02	0.04
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD21	5	0.02	0.04
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD22	5	0.02	0.04
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD23	5	0.02	0.04
(1,1706)	1:B:41:VAL:HB	1:B:79:TYR:HE1	5	0.06	0.11
(1,1646)	1:B:36:GLN:H	1:B:36:GLN:HB2	5	0.17	0.19
(1,164)	1:A:10:ALA:HB1	1:A:13:ASP:HB2	5	0.32	0.65
(1,164)	1:A:10:ALA:HB2	1:A:13:ASP:HB2	5	0.32	0.65
(1,164)	1:A:10:ALA:HB3	1:A:13:ASP:HB2	5	0.32	0.65

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB1	5	0.07	0.19
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB2	5	0.07	0.19
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB3	5	0.07	0.19
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB1	5	0.07	0.19
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB2	5	0.07	0.19
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB3	5	0.07	0.19
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB1	5	0.07	0.19
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB2	5	0.07	0.19
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB3	5	0.07	0.19
(1,1592)	1:B:33:LEU:HB2	1:B:34:LEU:H	5	0.05	0.09
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD11	5	0.05	0.13
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD12	5	0.05	0.13
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD13	5	0.05	0.13
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD11	5	0.05	0.13
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD12	5	0.05	0.13
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD13	5	0.05	0.13
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD11	5	0.8	1.36
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD12	5	0.8	1.36
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD13	5	0.8	1.36
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD21	5	0.64	1.11
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD22	5	0.64	1.11
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD23	5	0.64	1.11
(1,130)	1:A:5:SER:HB2	1:A:6:ASP:H	5	0.13	0.24
(1,1262)	1:B:5:SER:HB2	1:B:6:ASP:H	5	0.1	0.17
(1,1258)	1:A:107:HIS:HB2	1:A:108:HIS:H	5	0.13	0.22
(1,1252)	1:A:101:LEU:HD21	1:A:102:GLU:H	5	0.05	0.13
(1,1252)	1:A:101:LEU:HD22	1:A:102:GLU:H	5	0.05	0.13
(1,1252)	1:A:101:LEU:HD23	1:A:102:GLU:H	5	0.05	0.13
(1,1242)	1:A:99:GLU:HG2	1:A:100:HIS:H	5	0.09	0.12
(1,1052)	1:A:81:ILE:HD11	1:A:82:ALA:H	5	0.03	0.05
(1,1052)	1:A:81:ILE:HD12	1:A:82:ALA:H	5	0.03	0.05
(1,1052)	1:A:81:ILE:HD13	1:A:82:ALA:H	5	0.03	0.05
(1,1033)	1:A:77:GLN:HG2	1:A:77:GLN:HE21	5	0.05	0.07
(1,1022)	1:A:76:ARG:HG2	1:A:78:TYR:HE1	5	0.43	1.0
(1,1021)	1:A:76:ARG:HG2	1:A:77:GLN:H	5	0.38	0.55
(1,963)	1:A:70:ALA:HB1	1:A:79:TYR:HE1	4	0.11	0.22
(1,963)	1:A:70:ALA:HB2	1:A:79:TYR:HE1	4	0.11	0.22
(1,963)	1:A:70:ALA:HB3	1:A:79:TYR:HE1	4	0.11	0.22
(1,944)	1:A:69:GLU:HG3	1:A:82:ALA:HB1	4	0.06	0.09
(1,944)	1:A:69:GLU:HG3	1:A:82:ALA:HB2	4	0.06	0.09
(1,944)	1:A:69:GLU:HG3	1:A:82:ALA:HB3	4	0.06	0.09
(1,839)	1:A:62:LEU:HB2	1:A:67:LEU:HD21	4	1.14	1.65

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,839)	1:A:62:LEU:HB2	1:A:67:LEU:HD22	4	1.14	1.65
(1,839)	1:A:62:LEU:HB2	1:A:67:LEU:HD23	4	1.14	1.65
(1,810)	1:A:59:LEU:HD21	1:A:79:TYR:HE1	4	0.18	0.42
(1,810)	1:A:59:LEU:HD22	1:A:79:TYR:HE1	4	0.18	0.42
(1,810)	1:A:59:LEU:HD23	1:A:79:TYR:HE1	4	0.18	0.42
(1,729)	1:A:52:LEU:HA	1:A:52:LEU:HD11	4	0.17	0.19
(1,729)	1:A:52:LEU:HA	1:A:52:LEU:HD12	4	0.17	0.19
(1,729)	1:A:52:LEU:HA	1:A:52:LEU:HD13	4	0.17	0.19
(1,71)	1:B:12:LEU:HD11	1:A:29:GLN:HE21	4	0.27	0.44
(1,71)	1:B:12:LEU:HD12	1:A:29:GLN:HE21	4	0.27	0.44
(1,71)	1:B:12:LEU:HD13	1:A:29:GLN:HE21	4	0.27	0.44
(1,672)	1:A:45:ALA:H	1:A:52:LEU:HD11	4	1.04	1.33
(1,672)	1:A:45:ALA:H	1:A:52:LEU:HD12	4	1.04	1.33
(1,672)	1:A:45:ALA:H	1:A:52:LEU:HD13	4	1.04	1.33
(1,621)	1:A:42:GLU:H	1:A:42:GLU:HG2	4	0.36	0.49
(1,616)	1:A:42:GLU:HG3	1:A:52:LEU:HD11	4	0.02	0.03
(1,616)	1:A:42:GLU:HG3	1:A:52:LEU:HD12	4	0.02	0.03
(1,616)	1:A:42:GLU:HG3	1:A:52:LEU:HD13	4	0.02	0.03
(1,592)	1:A:41:VAL:HG21	1:A:59:LEU:HD21	4	0.02	0.03
(1,592)	1:A:41:VAL:HG21	1:A:59:LEU:HD22	4	0.02	0.03
(1,592)	1:A:41:VAL:HG21	1:A:59:LEU:HD23	4	0.02	0.03
(1,592)	1:A:41:VAL:HG22	1:A:59:LEU:HD21	4	0.02	0.03
(1,592)	1:A:41:VAL:HG22	1:A:59:LEU:HD22	4	0.02	0.03
(1,592)	1:A:41:VAL:HG22	1:A:59:LEU:HD23	4	0.02	0.03
(1,592)	1:A:41:VAL:HG23	1:A:59:LEU:HD21	4	0.02	0.03
(1,592)	1:A:41:VAL:HG23	1:A:59:LEU:HD22	4	0.02	0.03
(1,592)	1:A:41:VAL:HG23	1:A:59:LEU:HD23	4	0.02	0.03
(1,543)	1:A:40:ALA:HA	1:A:78:TYR:HA	4	0.03	0.05
(1,538)	1:A:39:ARG:HG2	1:A:40:ALA:H	4	0.04	0.08
(1,536)	1:A:39:ARG:HD2	1:A:40:ALA:H	4	0.43	0.65
(1,530)	1:A:39:ARG:HA	1:A:39:ARG:HD2	4	0.1	0.12
(1,476)	1:A:33:LEU:HG	1:A:39:ARG:HE	4	0.04	0.07
(1,472)	1:A:33:LEU:HD11	1:A:47:ALA:HB1	4	0.4	0.81
(1,472)	1:A:33:LEU:HD11	1:A:47:ALA:HB2	4	0.4	0.81
(1,472)	1:A:33:LEU:HD11	1:A:47:ALA:HB3	4	0.4	0.81
(1,472)	1:A:33:LEU:HD12	1:A:47:ALA:HB1	4	0.4	0.81
(1,472)	1:A:33:LEU:HD12	1:A:47:ALA:HB2	4	0.4	0.81
(1,472)	1:A:33:LEU:HD12	1:A:47:ALA:HB3	4	0.4	0.81
(1,472)	1:A:33:LEU:HD13	1:A:47:ALA:HB1	4	0.4	0.81
(1,472)	1:A:33:LEU:HD13	1:A:47:ALA:HB2	4	0.4	0.81
(1,472)	1:A:33:LEU:HD13	1:A:47:ALA:HB3	4	0.4	0.81
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD21	4	0.07	0.11

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD22	4	0.07	0.11
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD23	4	0.07	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD21	4	0.07	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD22	4	0.07	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD23	4	0.07	0.11
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD21	4	0.07	0.11
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD22	4	0.07	0.11
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD23	4	0.07	0.11
(1,2607)	1:B:94:GLN:H	1:B:90:PHE:O	4	0.01	0.02
(1,2589)	1:B:80:ARG:H	1:B:69:GLU:O	4	0.02	0.03
(1,2555)	1:B:57:ALA:H	1:B:53:THR:O	4	0.02	0.03
(1,2511)	1:B:16:ALA:H	1:B:12:LEU:O	4	0.01	0.02
(1,2499)	1:A:97:ALA:H	1:A:93:VAL:O	4	0.02	0.03
(1,2475)	1:A:80:ARG:H	1:A:69:GLU:O	4	0.02	0.03
(1,2409)	1:A:22:LEU:H	1:A:18:VAL:O	4	0.03	0.05
(1,2287)	1:B:90:PHE:HB2	1:B:93:VAL:HG11	4	0.3	0.42
(1,2287)	1:B:90:PHE:HB2	1:B:93:VAL:HG12	4	0.3	0.42
(1,2287)	1:B:90:PHE:HB2	1:B:93:VAL:HG13	4	0.3	0.42
(1,2276)	1:B:89:LEU:HD21	1:B:93:VAL:HB	4	0.06	0.12
(1,2276)	1:B:89:LEU:HD22	1:B:93:VAL:HB	4	0.06	0.12
(1,2276)	1:B:89:LEU:HD23	1:B:93:VAL:HB	4	0.06	0.12
(1,2269)	1:B:89:LEU:HA	1:B:92:LEU:HD21	4	0.02	0.04
(1,2269)	1:B:89:LEU:HA	1:B:92:LEU:HD22	4	0.02	0.04
(1,2269)	1:B:89:LEU:HA	1:B:92:LEU:HD23	4	0.02	0.04
(1,2162)	1:B:77:GLN:HB2	1:B:77:GLN:HE21	4	0.02	0.03
(1,2162)	1:B:77:GLN:HB3	1:B:77:GLN:HE21	4	0.02	0.03
(1,2131)	1:B:73:GLU:H	1:B:76:ARG:HG2	4	0.21	0.43
(1,2024)	1:B:67:LEU:HA	1:B:86:VAL:HG21	4	0.02	0.03
(1,2024)	1:B:67:LEU:HA	1:B:86:VAL:HG22	4	0.02	0.03
(1,2024)	1:B:67:LEU:HA	1:B:86:VAL:HG23	4	0.02	0.03
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD2	4	0.04	0.07
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD3	4	0.04	0.07
(1,1991)	1:B:63:LYS:HB2	1:B:69:GLU:HA	4	0.18	0.29
(1,1837)	1:B:50:MET:HB2	1:B:55:ALA:H	4	0.38	1.01
(1,1753)	1:B:42:GLU:H	1:B:42:GLU:HG2	4	0.41	0.47
(1,1748)	1:B:42:GLU:HG3	1:B:52:LEU:HD11	4	0.01	0.03
(1,1748)	1:B:42:GLU:HG3	1:B:52:LEU:HD12	4	0.01	0.03
(1,1748)	1:B:42:GLU:HG3	1:B:52:LEU:HD13	4	0.01	0.03
(1,1648)	1:B:37:GLY:HA2	1:B:38:GLU:HB2	4	0.29	0.57
(1,1648)	1:B:37:GLY:HA2	1:B:38:GLU:HB3	4	0.29	0.57
(1,1607)	1:B:33:LEU:HG	1:B:36:GLN:HE21	4	0.51	1.15
(1,1567)	1:B:31:LEU:HD21	1:B:81:ILE:HD11	4	0.03	0.05

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1567)	1:B:31:LEU:HD21	1:B:81:ILE:HD12	4	0.03	0.05
(1,1567)	1:B:31:LEU:HD21	1:B:81:ILE:HD13	4	0.03	0.05
(1,1567)	1:B:31:LEU:HD22	1:B:81:ILE:HD11	4	0.03	0.05
(1,1567)	1:B:31:LEU:HD22	1:B:81:ILE:HD12	4	0.03	0.05
(1,1567)	1:B:31:LEU:HD22	1:B:81:ILE:HD13	4	0.03	0.05
(1,1567)	1:B:31:LEU:HD23	1:B:81:ILE:HD11	4	0.03	0.05
(1,1567)	1:B:31:LEU:HD23	1:B:81:ILE:HD12	4	0.03	0.05
(1,1567)	1:B:31:LEU:HD23	1:B:81:ILE:HD13	4	0.03	0.05
(1,1486)	1:B:29:GLN:HB2	1:B:48:THR:HB	4	0.64	0.82
(1,1450)	1:B:26:ARG:HA	1:B:29:GLN:HG2	4	0.61	0.95
(1,1425)	1:B:22:LEU:HD11	1:B:89:LEU:HD21	4	0.03	0.05
(1,1425)	1:B:22:LEU:HD11	1:B:89:LEU:HD22	4	0.03	0.05
(1,1425)	1:B:22:LEU:HD11	1:B:89:LEU:HD23	4	0.03	0.05
(1,1425)	1:B:22:LEU:HD12	1:B:89:LEU:HD21	4	0.03	0.05
(1,1425)	1:B:22:LEU:HD12	1:B:89:LEU:HD22	4	0.03	0.05
(1,1425)	1:B:22:LEU:HD12	1:B:89:LEU:HD23	4	0.03	0.05
(1,1425)	1:B:22:LEU:HD13	1:B:89:LEU:HD21	4	0.03	0.05
(1,1425)	1:B:22:LEU:HD13	1:B:89:LEU:HD22	4	0.03	0.05
(1,1425)	1:B:22:LEU:HD13	1:B:89:LEU:HD23	4	0.03	0.05
(1,1421)	1:B:22:LEU:HB2	1:B:23:ALA:H	4	0.12	0.18
(1,1333)	1:B:14:GLN:HA	1:B:17:ARG:HD2	4	0.05	0.07
(1,1333)	1:B:14:GLN:HA	1:B:17:ARG:HD3	4	0.05	0.07
(1,1304)	1:B:11:LEU:HA	1:B:14:GLN:HG2	4	0.16	0.37
(1,1282)	1:B:8:LYS:HB2	1:B:9:ALA:H	4	0.02	0.03
(1,1282)	1:B:8:LYS:HB3	1:B:9:ALA:H	4	0.02	0.03
(1,1183)	1:A:93:VAL:HG11	1:A:94:GLN:H	4	0.02	0.05
(1,1183)	1:A:93:VAL:HG12	1:A:94:GLN:H	4	0.02	0.05
(1,1183)	1:A:93:VAL:HG13	1:A:94:GLN:H	4	0.02	0.05
(1,996)	1:A:73:GLU:HG2	1:A:78:TYR:HD1	3	0.59	1.65
(1,996)	1:A:73:GLU:HG3	1:A:78:TYR:HD1	3	0.59	1.65
(1,995)	1:A:73:GLU:HB2	1:A:78:TYR:HE1	3	1.04	1.97
(1,989)	1:A:72:ARG:H	1:A:72:ARG:HB2	3	0.39	0.41
(1,981)	1:A:72:ARG:HA	1:A:77:GLN:HG2	3	0.42	0.56
(1,965)	1:A:71:ARG:HA	1:A:72:ARG:HB2	3	0.63	0.66
(1,943)	1:A:69:GLU:HG3	1:A:82:ALA:HA	3	0.03	0.03
(1,897)	1:A:67:LEU:HB2	1:A:68:VAL:HG21	3	0.07	0.1
(1,897)	1:A:67:LEU:HB2	1:A:68:VAL:HG22	3	0.07	0.1
(1,897)	1:A:67:LEU:HB2	1:A:68:VAL:HG23	3	0.07	0.1
(1,897)	1:A:67:LEU:HB3	1:A:68:VAL:HG21	3	0.07	0.1
(1,897)	1:A:67:LEU:HB3	1:A:68:VAL:HG22	3	0.07	0.1
(1,897)	1:A:67:LEU:HB3	1:A:68:VAL:HG23	3	0.07	0.1
(1,891)	1:A:67:LEU:HA	1:A:86:VAL:HG11	3	0.02	0.05

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,891)	1:A:67:LEU:HA	1:A:86:VAL:HG12	3	0.02	0.05
(1,891)	1:A:67:LEU:HA	1:A:86:VAL:HG13	3	0.02	0.05
(1,864)	1:A:63:LYS:HE2	1:A:70:ALA:HB1	3	0.02	0.03
(1,864)	1:A:63:LYS:HE2	1:A:70:ALA:HB2	3	0.02	0.03
(1,864)	1:A:63:LYS:HE2	1:A:70:ALA:HB3	3	0.02	0.03
(1,864)	1:A:63:LYS:HE3	1:A:70:ALA:HB1	3	0.02	0.03
(1,864)	1:A:63:LYS:HE3	1:A:70:ALA:HB2	3	0.02	0.03
(1,864)	1:A:63:LYS:HE3	1:A:70:ALA:HB3	3	0.02	0.03
(1,859)	1:A:63:LYS:HB2	1:A:69:GLU:HA	3	0.2	0.36
(1,819)	1:A:60:GLN:HA	1:A:63:LYS:HG2	3	0.06	0.1
(1,819)	1:A:60:GLN:HA	1:A:63:LYS:HG3	3	0.06	0.1
(1,705)	1:A:50:MET:HB2	1:A:55:ALA:H	3	0.17	0.4
(1,65)	1:B:11:LEU:HD11	1:A:98:ASP:HB3	3	0.2	0.27
(1,65)	1:B:11:LEU:HD12	1:A:98:ASP:HB3	3	0.2	0.27
(1,65)	1:B:11:LEU:HD13	1:A:98:ASP:HB3	3	0.2	0.27
(1,64)	1:B:11:LEU:HD11	1:A:98:ASP:HA	3	0.47	0.71
(1,64)	1:B:11:LEU:HD12	1:A:98:ASP:HA	3	0.47	0.71
(1,64)	1:B:11:LEU:HD13	1:A:98:ASP:HA	3	0.47	0.71
(1,612)	1:A:42:GLU:HG2	1:A:43:ALA:H	3	0.05	0.07
(1,602)	1:A:42:GLU:HA	1:A:42:GLU:HG2	3	0.05	0.05
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD21	3	0.15	0.32
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD22	3	0.15	0.32
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD23	3	0.15	0.32
(1,574)	1:A:41:VAL:HB	1:A:79:TYR:HE1	3	1.41	4.14
(1,528)	1:A:38:GLU:H	1:A:38:GLU:HG2	3	0.02	0.03
(1,528)	1:A:38:GLU:H	1:A:38:GLU:HG3	3	0.02	0.03
(1,511)	1:A:36:GLN:HB2	1:A:37:GLY:H	3	0.08	0.12
(1,465)	1:A:33:LEU:HD11	1:A:36:GLN:H	3	0.26	0.43
(1,465)	1:A:33:LEU:HD12	1:A:36:GLN:H	3	0.26	0.43
(1,465)	1:A:33:LEU:HD13	1:A:36:GLN:H	3	0.26	0.43
(1,455)	1:A:33:LEU:HA	1:A:33:LEU:HD11	3	0.2	0.28
(1,455)	1:A:33:LEU:HA	1:A:33:LEU:HD12	3	0.2	0.28
(1,455)	1:A:33:LEU:HA	1:A:33:LEU:HD13	3	0.2	0.28
(1,42)	1:A:16:ALA:HB1	1:B:25:GLY:HA2	3	0.32	0.56
(1,42)	1:A:16:ALA:HB2	1:B:25:GLY:HA2	3	0.32	0.56
(1,42)	1:A:16:ALA:HB3	1:B:25:GLY:HA2	3	0.32	0.56
(1,354)	1:A:29:GLN:HB2	1:A:48:THR:HB	3	0.41	0.85
(1,308)	1:A:23:ALA:H	1:A:24:ASN:H	3	0.05	0.08
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD11	3	0.25	0.36
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD12	3	0.25	0.36
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD13	3	0.25	0.36
(1,2597)	1:B:89:LEU:H	1:B:85:ASP:O	3	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2593)	1:B:87:ALA:H	1:B:83:GLY:O	3	0.02	0.04
(1,2557)	1:B:58:ASN:H	1:B:54:THR:O	3	0.02	0.03
(1,2479)	1:A:87:ALA:H	1:A:83:GLY:O	3	0.01	0.02
(1,2465)	1:A:71:ARG:H	1:A:78:TYR:O	3	0.01	0.02
(1,2427)	1:A:46:THR:H	1:A:42:GLU:O	3	0.01	0.01
(1,241)	1:A:18:VAL:HG11	1:A:19:GLY:HA2	3	0.57	0.58
(1,241)	1:A:18:VAL:HG11	1:A:19:GLY:HA3	3	0.57	0.58
(1,241)	1:A:18:VAL:HG12	1:A:19:GLY:HA2	3	0.57	0.58
(1,241)	1:A:18:VAL:HG12	1:A:19:GLY:HA3	3	0.57	0.58
(1,241)	1:A:18:VAL:HG13	1:A:19:GLY:HA2	3	0.57	0.58
(1,241)	1:A:18:VAL:HG13	1:A:19:GLY:HA3	3	0.57	0.58
(1,2384)	1:B:101:LEU:HD21	1:B:102:GLU:H	3	0.11	0.21
(1,2384)	1:B:101:LEU:HD22	1:B:102:GLU:H	3	0.11	0.21
(1,2384)	1:B:101:LEU:HD23	1:B:102:GLU:H	3	0.11	0.21
(1,2374)	1:B:99:GLU:HG2	1:B:100:HIS:H	3	0.2	0.41
(1,2362)	1:B:97:ALA:HA	1:B:101:LEU:HD21	3	0.04	0.05
(1,2362)	1:B:97:ALA:HA	1:B:101:LEU:HD22	3	0.04	0.05
(1,2362)	1:B:97:ALA:HA	1:B:101:LEU:HD23	3	0.04	0.05
(1,2357)	1:B:96:VAL:HG21	1:B:100:HIS:HD2	3	0.04	0.07
(1,2357)	1:B:96:VAL:HG22	1:B:100:HIS:HD2	3	0.04	0.07
(1,2357)	1:B:96:VAL:HG23	1:B:100:HIS:HD2	3	0.04	0.07
(1,2318)	1:B:93:VAL:H	1:B:93:VAL:HG11	3	0.07	0.07
(1,2318)	1:B:93:VAL:H	1:B:93:VAL:HG12	3	0.07	0.07
(1,2318)	1:B:93:VAL:H	1:B:93:VAL:HG13	3	0.07	0.07
(1,2165)	1:B:77:GLN:HG2	1:B:77:GLN:HE21	3	0.04	0.05
(1,1971)	1:B:62:LEU:HB2	1:B:67:LEU:HD21	3	1.29	1.6
(1,1971)	1:B:62:LEU:HB2	1:B:67:LEU:HD22	3	1.29	1.6
(1,1971)	1:B:62:LEU:HB2	1:B:67:LEU:HD23	3	1.29	1.6
(1,1967)	1:B:62:LEU:HA	1:B:67:LEU:HD21	3	0.05	0.08
(1,1967)	1:B:62:LEU:HA	1:B:67:LEU:HD22	3	0.05	0.08
(1,1967)	1:B:62:LEU:HA	1:B:67:LEU:HD23	3	0.05	0.08
(1,1951)	1:B:60:GLN:HA	1:B:63:LYS:HG2	3	0.04	0.08
(1,1951)	1:B:60:GLN:HA	1:B:63:LYS:HG3	3	0.04	0.08
(1,1881)	1:B:53:THR:HG21	1:B:54:THR:H	3	0.05	0.06
(1,1881)	1:B:53:THR:HG22	1:B:54:THR:H	3	0.05	0.06
(1,1881)	1:B:53:THR:HG23	1:B:54:THR:H	3	0.05	0.06
(1,1847)	1:B:50:MET:H	1:B:50:MET:HB2	3	0.02	0.02
(1,1845)	1:B:50:MET:HG2	1:B:54:THR:HG21	3	0.15	0.22
(1,1845)	1:B:50:MET:HG2	1:B:54:THR:HG22	3	0.15	0.22
(1,1845)	1:B:50:MET:HG2	1:B:54:THR:HG23	3	0.15	0.22
(1,1823)	1:B:48:THR:HB	1:B:50:MET:HG2	3	0.24	0.51
(1,1782)	1:B:44:ILE:HG21	1:B:47:ALA:HB1	3	0.03	0.05

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1782)	1:B:44:ILE:HG21	1:B:47:ALA:HB2	3	0.03	0.05
(1,1782)	1:B:44:ILE:HG21	1:B:47:ALA:HB3	3	0.03	0.05
(1,1782)	1:B:44:ILE:HG22	1:B:47:ALA:HB1	3	0.03	0.05
(1,1782)	1:B:44:ILE:HG22	1:B:47:ALA:HB2	3	0.03	0.05
(1,1782)	1:B:44:ILE:HG22	1:B:47:ALA:HB3	3	0.03	0.05
(1,1782)	1:B:44:ILE:HG23	1:B:47:ALA:HB1	3	0.03	0.05
(1,1782)	1:B:44:ILE:HG23	1:B:47:ALA:HB2	3	0.03	0.05
(1,1782)	1:B:44:ILE:HG23	1:B:47:ALA:HB3	3	0.03	0.05
(1,1744)	1:B:42:GLU:HG2	1:B:43:ALA:H	3	0.08	0.16
(1,1670)	1:B:39:ARG:HG2	1:B:40:ALA:H	3	0.06	0.08
(1,1669)	1:B:39:ARG:HD2	1:B:43:ALA:HB1	3	0.3	0.39
(1,1669)	1:B:39:ARG:HD2	1:B:43:ALA:HB2	3	0.3	0.39
(1,1669)	1:B:39:ARG:HD2	1:B:43:ALA:HB3	3	0.3	0.39
(1,1643)	1:B:36:GLN:HB2	1:B:37:GLY:H	3	0.06	0.09
(1,1634)	1:B:35:ALA:HB1	1:B:36:GLN:HE21	3	0.42	0.51
(1,1634)	1:B:35:ALA:HB2	1:B:36:GLN:HE21	3	0.42	0.51
(1,1634)	1:B:35:ALA:HB3	1:B:36:GLN:HE21	3	0.42	0.51
(1,1595)	1:B:33:LEU:HD11	1:B:36:GLN:HE21	3	0.8	1.14
(1,1595)	1:B:33:LEU:HD12	1:B:36:GLN:HE21	3	0.8	1.14
(1,1595)	1:B:33:LEU:HD13	1:B:36:GLN:HE21	3	0.8	1.14
(1,1527)	1:B:30:ILE:HG21	1:B:59:LEU:HD21	3	0.02	0.02
(1,1527)	1:B:30:ILE:HG21	1:B:59:LEU:HD22	3	0.02	0.02
(1,1527)	1:B:30:ILE:HG21	1:B:59:LEU:HD23	3	0.02	0.02
(1,1527)	1:B:30:ILE:HG22	1:B:59:LEU:HD21	3	0.02	0.02
(1,1527)	1:B:30:ILE:HG22	1:B:59:LEU:HD22	3	0.02	0.02
(1,1527)	1:B:30:ILE:HG22	1:B:59:LEU:HD23	3	0.02	0.02
(1,1527)	1:B:30:ILE:HG23	1:B:59:LEU:HD21	3	0.02	0.02
(1,1527)	1:B:30:ILE:HG23	1:B:59:LEU:HD22	3	0.02	0.02
(1,1527)	1:B:30:ILE:HG23	1:B:59:LEU:HD23	3	0.02	0.02
(1,1521)	1:B:30:ILE:HG21	1:B:33:LEU:HB2	3	0.09	0.19
(1,1521)	1:B:30:ILE:HG22	1:B:33:LEU:HB2	3	0.09	0.19
(1,1521)	1:B:30:ILE:HG23	1:B:33:LEU:HB2	3	0.09	0.19
(1,1499)	1:B:30:ILE:HA	1:B:33:LEU:HD11	3	0.09	0.17
(1,1499)	1:B:30:ILE:HA	1:B:33:LEU:HD12	3	0.09	0.17
(1,1499)	1:B:30:ILE:HA	1:B:33:LEU:HD13	3	0.09	0.17
(1,1451)	1:B:26:ARG:H	1:B:26:ARG:HG2	3	0.19	0.3
(1,1451)	1:B:26:ARG:H	1:B:26:ARG:HG3	3	0.19	0.3
(1,1444)	1:B:25:GLY:HA2	1:B:28:LEU:HB2	3	0.87	1.11
(1,1399)	1:B:20:LYS:HG2	1:B:20:LYS:HE2	3	0.2	0.21
(1,1399)	1:B:20:LYS:HG2	1:B:20:LYS:HE3	3	0.2	0.21
(1,1375)	1:B:18:VAL:HG11	1:B:22:LEU:H	3	0.31	0.42
(1,1375)	1:B:18:VAL:HG12	1:B:22:LEU:H	3	0.31	0.42

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1375)	1:B:18:VAL:HG13	1:B:22:LEU:H	3	0.31	0.42
(1,1373)	1:B:18:VAL:HG11	1:B:19:GLY:HA2	3	0.56	0.59
(1,1373)	1:B:18:VAL:HG11	1:B:19:GLY:HA3	3	0.56	0.59
(1,1373)	1:B:18:VAL:HG12	1:B:19:GLY:HA2	3	0.56	0.59
(1,1373)	1:B:18:VAL:HG12	1:B:19:GLY:HA3	3	0.56	0.59
(1,1373)	1:B:18:VAL:HG13	1:B:19:GLY:HA2	3	0.56	0.59
(1,1373)	1:B:18:VAL:HG13	1:B:19:GLY:HA3	3	0.56	0.59
(1,1283)	1:B:8:LYS:HE2	1:B:12:LEU:HD11	3	0.07	0.09
(1,1283)	1:B:8:LYS:HE2	1:B:12:LEU:HD12	3	0.07	0.09
(1,1283)	1:B:8:LYS:HE2	1:B:12:LEU:HD13	3	0.07	0.09
(1,1283)	1:B:8:LYS:HE3	1:B:12:LEU:HD11	3	0.07	0.09
(1,1283)	1:B:8:LYS:HE3	1:B:12:LEU:HD12	3	0.07	0.09
(1,1283)	1:B:8:LYS:HE3	1:B:12:LEU:HD13	3	0.07	0.09
(1,1251)	1:A:101:LEU:HB2	1:A:102:GLU:H	3	0.03	0.05
(1,1234)	1:A:97:ALA:HB1	1:A:101:LEU:HD21	3	0.04	0.05
(1,1234)	1:A:97:ALA:HB1	1:A:101:LEU:HD22	3	0.04	0.05
(1,1234)	1:A:97:ALA:HB1	1:A:101:LEU:HD23	3	0.04	0.05
(1,1234)	1:A:97:ALA:HB2	1:A:101:LEU:HD21	3	0.04	0.05
(1,1234)	1:A:97:ALA:HB2	1:A:101:LEU:HD22	3	0.04	0.05
(1,1234)	1:A:97:ALA:HB2	1:A:101:LEU:HD23	3	0.04	0.05
(1,1234)	1:A:97:ALA:HB3	1:A:101:LEU:HD21	3	0.04	0.05
(1,1234)	1:A:97:ALA:HB3	1:A:101:LEU:HD22	3	0.04	0.05
(1,1234)	1:A:97:ALA:HB3	1:A:101:LEU:HD23	3	0.04	0.05
(1,1220)	1:A:96:VAL:HA	1:A:100:HIS:HD2	3	0.07	0.11
(1,1219)	1:A:96:VAL:HA	1:A:99:GLU:HB2	3	0.36	0.7
(1,120)	1:B:88:ARG:HB2	1:A:92:LEU:HD11	3	0.16	0.32
(1,120)	1:B:88:ARG:HB2	1:A:92:LEU:HD12	3	0.16	0.32
(1,120)	1:B:88:ARG:HB2	1:A:92:LEU:HD13	3	0.16	0.32
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB1	3	0.09	0.14
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB2	3	0.09	0.14
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB3	3	0.09	0.14
(1,1093)	1:A:84:GLU:HG2	1:A:88:ARG:HD2	3	0.04	0.05
(1,1093)	1:A:84:GLU:HG2	1:A:88:ARG:HD3	3	0.04	0.05
(1,1093)	1:A:84:GLU:HG3	1:A:88:ARG:HD2	3	0.04	0.05
(1,1093)	1:A:84:GLU:HG3	1:A:88:ARG:HD3	3	0.04	0.05
(1,1064)	1:A:81:ILE:HG21	1:A:83:GLY:H	3	0.01	0.02
(1,1064)	1:A:81:ILE:HG22	1:A:83:GLY:H	3	0.01	0.02
(1,1064)	1:A:81:ILE:HG23	1:A:83:GLY:H	3	0.01	0.02
(1,1030)	1:A:77:GLN:HB2	1:A:77:GLN:HE21	3	0.02	0.02
(1,1030)	1:A:77:GLN:HB3	1:A:77:GLN:HE21	3	0.02	0.02
(1,100)	1:B:15:VAL:HG11	1:A:94:GLN:HA	3	0.02	0.03
(1,100)	1:B:15:VAL:HG12	1:A:94:GLN:HA	3	0.02	0.03

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,100)	1:B:15:VAL:HG13	1:A:94:GLN:HA	3	0.02	0.03
(1,994)	1:A:73:GLU:HB2	1:A:78:TYR:HD1	2	1.53	2.66
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB1	2	0.15	0.27
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB2	2	0.15	0.27
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB3	2	0.15	0.27
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB1	2	0.15	0.27
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB2	2	0.15	0.27
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB3	2	0.15	0.27
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB1	2	0.15	0.27
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB2	2	0.15	0.27
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB3	2	0.15	0.27
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB1	2	0.03	0.03
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB2	2	0.03	0.03
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB3	2	0.03	0.03
(1,916)	1:A:68:VAL:HG11	1:A:69:GLU:HB2	2	0.72	0.77
(1,916)	1:A:68:VAL:HG12	1:A:69:GLU:HB2	2	0.72	0.77
(1,916)	1:A:68:VAL:HG13	1:A:69:GLU:HB2	2	0.72	0.77
(1,91)	1:B:14:GLN:HG2	1:A:101:LEU:HD21	2	0.14	0.26
(1,91)	1:B:14:GLN:HG2	1:A:101:LEU:HD22	2	0.14	0.26
(1,91)	1:B:14:GLN:HG2	1:A:101:LEU:HD23	2	0.14	0.26
(1,888)	1:A:67:LEU:HA	1:A:67:LEU:HD11	2	0.08	0.12
(1,888)	1:A:67:LEU:HA	1:A:67:LEU:HD12	2	0.08	0.12
(1,888)	1:A:67:LEU:HA	1:A:67:LEU:HD13	2	0.08	0.12
(1,865)	1:A:63:LYS:HE2	1:A:70:ALA:H	2	0.04	0.05
(1,865)	1:A:63:LYS:HE3	1:A:70:ALA:H	2	0.04	0.05
(1,863)	1:A:63:LYS:HE2	1:A:69:GLU:HA	2	0.04	0.05
(1,863)	1:A:63:LYS:HE3	1:A:69:GLU:HA	2	0.04	0.05
(1,855)	1:A:63:LYS:HB2	1:A:64:SER:H	2	0.03	0.05
(1,845)	1:A:62:LEU:HD11	1:A:63:LYS:H	2	0.01	0.01
(1,845)	1:A:62:LEU:HD12	1:A:63:LYS:H	2	0.01	0.01
(1,845)	1:A:62:LEU:HD13	1:A:63:LYS:H	2	0.01	0.01
(1,835)	1:A:62:LEU:HA	1:A:67:LEU:HD21	2	0.08	0.09
(1,835)	1:A:62:LEU:HA	1:A:67:LEU:HD22	2	0.08	0.09
(1,835)	1:A:62:LEU:HA	1:A:67:LEU:HD23	2	0.08	0.09
(1,824)	1:A:60:GLN:HG2	1:A:61:ALA:HA	2	0.04	0.04
(1,824)	1:A:60:GLN:HG3	1:A:61:ALA:HA	2	0.04	0.04
(1,809)	1:A:59:LEU:HD21	1:A:79:TYR:HD1	2	0.1	0.15
(1,809)	1:A:59:LEU:HD22	1:A:79:TYR:HD1	2	0.1	0.15
(1,809)	1:A:59:LEU:HD23	1:A:79:TYR:HD1	2	0.1	0.15
(1,78)	1:B:12:LEU:HD21	1:A:29:GLN:H	2	0.01	0.01
(1,78)	1:B:12:LEU:HD22	1:A:29:GLN:H	2	0.01	0.01
(1,78)	1:B:12:LEU:HD23	1:A:29:GLN:H	2	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,747)	1:A:53:THR:HB	1:A:54:THR:H	2	0.04	0.04
(1,715)	1:A:50:MET:H	1:A:50:MET:HB2	2	0.03	0.04
(1,713)	1:A:50:MET:HG2	1:A:54:THR:HG21	2	0.13	0.21
(1,713)	1:A:50:MET:HG2	1:A:54:THR:HG22	2	0.13	0.21
(1,713)	1:A:50:MET:HG2	1:A:54:THR:HG23	2	0.13	0.21
(1,704)	1:A:50:MET:HB2	1:A:55:ALA:HB1	2	0.3	0.34
(1,704)	1:A:50:MET:HB2	1:A:55:ALA:HB2	2	0.3	0.34
(1,704)	1:A:50:MET:HB2	1:A:55:ALA:HB3	2	0.3	0.34
(1,650)	1:A:44:ILE:HG21	1:A:47:ALA:HB1	2	0.03	0.03
(1,650)	1:A:44:ILE:HG21	1:A:47:ALA:HB2	2	0.03	0.03
(1,650)	1:A:44:ILE:HG21	1:A:47:ALA:HB3	2	0.03	0.03
(1,650)	1:A:44:ILE:HG22	1:A:47:ALA:HB1	2	0.03	0.03
(1,650)	1:A:44:ILE:HG22	1:A:47:ALA:HB2	2	0.03	0.03
(1,650)	1:A:44:ILE:HG22	1:A:47:ALA:HB3	2	0.03	0.03
(1,650)	1:A:44:ILE:HG23	1:A:47:ALA:HB1	2	0.03	0.03
(1,650)	1:A:44:ILE:HG23	1:A:47:ALA:HB2	2	0.03	0.03
(1,650)	1:A:44:ILE:HG23	1:A:47:ALA:HB3	2	0.03	0.03
(1,619)	1:A:42:GLU:HG2	1:A:52:LEU:HD21	2	0.03	0.05
(1,619)	1:A:42:GLU:HG2	1:A:52:LEU:HD22	2	0.03	0.05
(1,619)	1:A:42:GLU:HG2	1:A:52:LEU:HD23	2	0.03	0.05
(1,618)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	2	0.02	0.02
(1,618)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	2	0.02	0.02
(1,618)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	2	0.02	0.02
(1,524)	1:A:38:GLU:HG2	1:A:39:ARG:H	2	0.07	0.07
(1,524)	1:A:38:GLU:HG3	1:A:39:ARG:H	2	0.07	0.07
(1,522)	1:A:38:GLU:HB2	1:A:80:ARG:HE	2	0.07	0.11
(1,522)	1:A:38:GLU:HB3	1:A:80:ARG:HE	2	0.07	0.11
(1,502)	1:A:35:ALA:HB1	1:A:36:GLN:HE21	2	0.42	0.66
(1,502)	1:A:35:ALA:HB2	1:A:36:GLN:HE21	2	0.42	0.66
(1,502)	1:A:35:ALA:HB3	1:A:36:GLN:HE21	2	0.42	0.66
(1,431)	1:A:31:LEU:HD21	1:A:67:LEU:HD11	2	0.07	0.07
(1,431)	1:A:31:LEU:HD21	1:A:67:LEU:HD12	2	0.07	0.07
(1,431)	1:A:31:LEU:HD21	1:A:67:LEU:HD13	2	0.07	0.07
(1,431)	1:A:31:LEU:HD22	1:A:67:LEU:HD11	2	0.07	0.07
(1,431)	1:A:31:LEU:HD22	1:A:67:LEU:HD12	2	0.07	0.07
(1,431)	1:A:31:LEU:HD22	1:A:67:LEU:HD13	2	0.07	0.07
(1,431)	1:A:31:LEU:HD23	1:A:67:LEU:HD11	2	0.07	0.07
(1,431)	1:A:31:LEU:HD23	1:A:67:LEU:HD12	2	0.07	0.07
(1,431)	1:A:31:LEU:HD23	1:A:67:LEU:HD13	2	0.07	0.07
(1,420)	1:A:31:LEU:HD11	1:A:67:LEU:HB2	2	0.03	0.03
(1,420)	1:A:31:LEU:HD11	1:A:67:LEU:HB3	2	0.03	0.03
(1,420)	1:A:31:LEU:HD12	1:A:67:LEU:HB2	2	0.03	0.03

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,420)	1:A:31:LEU:HD12	1:A:67:LEU:HB3	2	0.03	0.03
(1,420)	1:A:31:LEU:HD13	1:A:67:LEU:HB2	2	0.03	0.03
(1,420)	1:A:31:LEU:HD13	1:A:67:LEU:HB3	2	0.03	0.03
(1,408)	1:A:31:LEU:HA	1:A:62:LEU:HD11	2	0.09	0.11
(1,408)	1:A:31:LEU:HA	1:A:62:LEU:HD12	2	0.09	0.11
(1,408)	1:A:31:LEU:HA	1:A:62:LEU:HD13	2	0.09	0.11
(1,36)	1:A:15:VAL:HG11	1:B:97:ALA:HB1	2	0.22	0.3
(1,36)	1:A:15:VAL:HG11	1:B:97:ALA:HB2	2	0.22	0.3
(1,36)	1:A:15:VAL:HG11	1:B:97:ALA:HB3	2	0.22	0.3
(1,36)	1:A:15:VAL:HG12	1:B:97:ALA:HB1	2	0.22	0.3
(1,36)	1:A:15:VAL:HG12	1:B:97:ALA:HB2	2	0.22	0.3
(1,36)	1:A:15:VAL:HG12	1:B:97:ALA:HB3	2	0.22	0.3
(1,36)	1:A:15:VAL:HG13	1:B:97:ALA:HB1	2	0.22	0.3
(1,36)	1:A:15:VAL:HG13	1:B:97:ALA:HB2	2	0.22	0.3
(1,36)	1:A:15:VAL:HG13	1:B:97:ALA:HB3	2	0.22	0.3
(1,314)	1:A:25:GLY:HA3	1:A:28:LEU:HD11	2	0.01	0.02
(1,314)	1:A:25:GLY:HA3	1:A:28:LEU:HD12	2	0.01	0.02
(1,314)	1:A:25:GLY:HA3	1:A:28:LEU:HD13	2	0.01	0.02
(1,30)	1:A:14:GLN:HG2	1:B:97:ALA:HA	2	0.04	0.06
(1,295)	1:A:22:LEU:HD11	1:A:93:VAL:HB	2	0.03	0.04
(1,295)	1:A:22:LEU:HD12	1:A:93:VAL:HB	2	0.03	0.04
(1,295)	1:A:22:LEU:HD13	1:A:93:VAL:HB	2	0.03	0.04
(1,289)	1:A:22:LEU:HB2	1:A:23:ALA:H	2	0.19	0.21
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD21	2	0.02	0.03
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD22	2	0.02	0.03
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD23	2	0.02	0.03
(1,277)	1:A:21:ALA:HB1	1:A:65:GLY:HA2	2	0.03	0.05
(1,277)	1:A:21:ALA:HB2	1:A:65:GLY:HA2	2	0.03	0.05
(1,277)	1:A:21:ALA:HB3	1:A:65:GLY:HA2	2	0.03	0.05
(1,2601)	1:B:91:ALA:H	1:B:87:ALA:O	2	0.02	0.02
(1,2585)	1:B:78:TYR:H	1:B:71:ARG:O	2	0.02	0.02
(1,2581)	1:B:73:GLU:H	1:B:76:ARG:O	2	0.02	0.02
(1,2575)	1:B:67:LEU:H	1:B:62:LEU:O	2	0.03	0.03
(1,2561)	1:B:60:GLN:H	1:B:56:SER:O	2	0.01	0.02
(1,2545)	1:B:48:THR:H	1:B:44:ILE:O	2	0.01	0.01
(1,2525)	1:B:32:ASP:H	1:B:28:LEU:O	2	0.03	0.03
(1,2517)	1:B:19:GLY:H	1:B:15:VAL:O	2	0.01	0.01
(1,2460)	1:A:66:GLY:N	1:A:63:LYS:O	2	0.06	0.06
(1,2431)	1:A:48:THR:H	1:A:44:ILE:O	2	0.01	0.01
(1,243)	1:A:18:VAL:HG11	1:A:22:LEU:H	2	0.27	0.31
(1,243)	1:A:18:VAL:HG12	1:A:22:LEU:H	2	0.27	0.31
(1,243)	1:A:18:VAL:HG13	1:A:22:LEU:H	2	0.27	0.31

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB1	2	0.01	0.02
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB2	2	0.01	0.02
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB3	2	0.01	0.02
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB1	2	0.01	0.02
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB2	2	0.01	0.02
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB3	2	0.01	0.02
(1,2397)	1:A:16:ALA:H	1:A:12:LEU:O	2	0.01	0.01
(1,2351)	1:B:96:VAL:HA	1:B:99:GLU:HB2	2	0.68	0.79
(1,2342)	1:B:95:VAL:HG11	1:B:99:GLU:HB2	2	0.34	0.56
(1,2342)	1:B:95:VAL:HG12	1:B:99:GLU:HB2	2	0.34	0.56
(1,2342)	1:B:95:VAL:HG13	1:B:99:GLU:HB2	2	0.34	0.56
(1,2285)	1:B:90:PHE:HA	1:B:93:VAL:HG11	2	0.05	0.06
(1,2285)	1:B:90:PHE:HA	1:B:93:VAL:HG12	2	0.05	0.06
(1,2285)	1:B:90:PHE:HA	1:B:93:VAL:HG13	2	0.05	0.06
(1,2225)	1:B:84:GLU:HG2	1:B:88:ARG:HD2	2	0.08	0.14
(1,2225)	1:B:84:GLU:HG2	1:B:88:ARG:HD3	2	0.08	0.14
(1,2225)	1:B:84:GLU:HG3	1:B:88:ARG:HD2	2	0.08	0.14
(1,2225)	1:B:84:GLU:HG3	1:B:88:ARG:HD3	2	0.08	0.14
(1,2196)	1:B:81:ILE:HG21	1:B:83:GLY:H	2	0.04	0.04
(1,2196)	1:B:81:ILE:HG22	1:B:83:GLY:H	2	0.04	0.04
(1,2196)	1:B:81:ILE:HG23	1:B:83:GLY:H	2	0.04	0.04
(1,2184)	1:B:81:ILE:HD11	1:B:82:ALA:H	2	0.02	0.02
(1,2184)	1:B:81:ILE:HD12	1:B:82:ALA:H	2	0.02	0.02
(1,2184)	1:B:81:ILE:HD13	1:B:82:ALA:H	2	0.02	0.02
(1,2176)	1:B:80:ARG:HB2	1:B:80:ARG:HE	2	0.1	0.13
(1,2157)	1:B:76:ARG:H	1:B:76:ARG:HG2	2	0.11	0.15
(1,2145)	1:B:76:ARG:HB2	1:B:78:TYR:HD1	2	0.09	0.09
(1,2139)	1:B:75:THR:H	1:B:76:ARG:HG2	2	0.2	0.3
(1,2135)	1:B:74:GLY:HA2	1:B:76:ARG:H	2	0.03	0.03
(1,2104)	1:B:71:ARG:HG2	1:B:78:TYR:HB2	2	1.34	1.43
(1,2101)	1:B:71:ARG:HB2	1:B:79:TYR:HA	2	1.37	1.61
(1,2094)	1:B:70:ALA:HB1	1:B:79:TYR:HD1	2	0.18	0.28
(1,2094)	1:B:70:ALA:HB2	1:B:79:TYR:HD1	2	0.18	0.28
(1,2094)	1:B:70:ALA:HB3	1:B:79:TYR:HD1	2	0.18	0.28
(1,2091)	1:B:70:ALA:HB1	1:B:77:GLN:HE22	2	0.04	0.05
(1,2091)	1:B:70:ALA:HB2	1:B:77:GLN:HE22	2	0.04	0.05
(1,2091)	1:B:70:ALA:HB3	1:B:77:GLN:HE22	2	0.04	0.05
(1,2076)	1:B:69:GLU:HG3	1:B:82:ALA:HB1	2	0.01	0.01
(1,2076)	1:B:69:GLU:HG3	1:B:82:ALA:HB2	2	0.01	0.01
(1,2076)	1:B:69:GLU:HG3	1:B:82:ALA:HB3	2	0.01	0.01
(1,203)	1:A:14:GLN:HB2	1:A:14:GLN:HE21	2	0.05	0.07
(1,203)	1:A:14:GLN:HB3	1:A:14:GLN:HE21	2	0.05	0.07

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2029)	1:B:67:LEU:HB2	1:B:68:VAL:HG21	2	0.07	0.12
(1,2029)	1:B:67:LEU:HB2	1:B:68:VAL:HG22	2	0.07	0.12
(1,2029)	1:B:67:LEU:HB2	1:B:68:VAL:HG23	2	0.07	0.12
(1,2029)	1:B:67:LEU:HB3	1:B:68:VAL:HG21	2	0.07	0.12
(1,2029)	1:B:67:LEU:HB3	1:B:68:VAL:HG22	2	0.07	0.12
(1,2029)	1:B:67:LEU:HB3	1:B:68:VAL:HG23	2	0.07	0.12
(1,2023)	1:B:67:LEU:HA	1:B:86:VAL:HG11	2	0.03	0.04
(1,2023)	1:B:67:LEU:HA	1:B:86:VAL:HG12	2	0.03	0.04
(1,2023)	1:B:67:LEU:HA	1:B:86:VAL:HG13	2	0.03	0.04
(1,1996)	1:B:63:LYS:HE2	1:B:70:ALA:HB1	2	0.02	0.02
(1,1996)	1:B:63:LYS:HE2	1:B:70:ALA:HB2	2	0.02	0.02
(1,1996)	1:B:63:LYS:HE2	1:B:70:ALA:HB3	2	0.02	0.02
(1,1996)	1:B:63:LYS:HE3	1:B:70:ALA:HB1	2	0.02	0.02
(1,1996)	1:B:63:LYS:HE3	1:B:70:ALA:HB2	2	0.02	0.02
(1,1996)	1:B:63:LYS:HE3	1:B:70:ALA:HB3	2	0.02	0.02
(1,1956)	1:B:60:GLN:HG2	1:B:61:ALA:HA	2	0.03	0.03
(1,1956)	1:B:60:GLN:HG3	1:B:61:ALA:HA	2	0.03	0.03
(1,1948)	1:B:60:GLN:HA	1:B:60:GLN:HE21	2	0.17	0.29
(1,1942)	1:B:59:LEU:HD21	1:B:79:TYR:HE1	2	0.06	0.06
(1,1942)	1:B:59:LEU:HD22	1:B:79:TYR:HE1	2	0.06	0.06
(1,1942)	1:B:59:LEU:HD23	1:B:79:TYR:HE1	2	0.06	0.06
(1,1898)	1:B:55:ALA:HB1	1:B:58:ASN:HB2	2	0.58	0.69
(1,1898)	1:B:55:ALA:HB2	1:B:58:ASN:HB2	2	0.58	0.69
(1,1898)	1:B:55:ALA:HB3	1:B:58:ASN:HB2	2	0.58	0.69
(1,1893)	1:B:55:ALA:HA	1:B:58:ASN:HB2	2	0.41	0.53
(1,1879)	1:B:53:THR:HB	1:B:54:THR:H	2	0.04	0.08
(1,1835)	1:B:50:MET:HB2	1:B:54:THR:HG21	2	0.17	0.23
(1,1835)	1:B:50:MET:HB2	1:B:54:THR:HG22	2	0.17	0.23
(1,1835)	1:B:50:MET:HB2	1:B:54:THR:HG23	2	0.17	0.23
(1,1750)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	2	0.06	0.07
(1,1750)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	2	0.06	0.07
(1,1750)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	2	0.06	0.07
(1,172)	1:A:11:LEU:HA	1:A:14:GLN:HG2	2	0.04	0.04
(1,1660)	1:B:38:GLU:H	1:B:38:GLU:HG2	2	0.02	0.02
(1,1660)	1:B:38:GLU:H	1:B:38:GLU:HG3	2	0.02	0.02
(1,1647)	1:B:36:GLN:H	1:B:36:GLN:HG2	2	0.13	0.23
(1,1625)	1:B:34:LEU:HD21	1:B:80:ARG:HA	2	0.01	0.02
(1,1625)	1:B:34:LEU:HD22	1:B:80:ARG:HA	2	0.01	0.02
(1,1625)	1:B:34:LEU:HD23	1:B:80:ARG:HA	2	0.01	0.02
(1,1621)	1:B:34:LEU:HD11	1:B:80:ARG:HA	2	0.02	0.03
(1,1621)	1:B:34:LEU:HD12	1:B:80:ARG:HA	2	0.02	0.03
(1,1621)	1:B:34:LEU:HD13	1:B:80:ARG:HA	2	0.02	0.03

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1594)	1:B:33:LEU:HD11	1:B:36:GLN:HB2	2	0.82	1.57
(1,1594)	1:B:33:LEU:HD12	1:B:36:GLN:HB2	2	0.82	1.57
(1,1594)	1:B:33:LEU:HD13	1:B:36:GLN:HB2	2	0.82	1.57
(1,150)	1:A:8:LYS:HB2	1:A:9:ALA:H	2	0.07	0.12
(1,150)	1:A:8:LYS:HB3	1:A:9:ALA:H	2	0.07	0.12
(1,1484)	1:B:29:GLN:HB2	1:B:29:GLN:HE21	2	0.01	0.01
(1,1440)	1:B:23:ALA:H	1:B:24:ASN:H	2	0.16	0.28
(1,1432)	1:B:22:LEU:HD21	1:B:90:PHE:HD1	2	0.01	0.01
(1,1432)	1:B:22:LEU:HD21	1:B:90:PHE:HD2	2	0.01	0.01
(1,1432)	1:B:22:LEU:HD22	1:B:90:PHE:HD1	2	0.01	0.01
(1,1432)	1:B:22:LEU:HD22	1:B:90:PHE:HD2	2	0.01	0.01
(1,1432)	1:B:22:LEU:HD23	1:B:90:PHE:HD1	2	0.01	0.01
(1,1432)	1:B:22:LEU:HD23	1:B:90:PHE:HD2	2	0.01	0.01
(1,1431)	1:B:22:LEU:HD21	1:B:28:LEU:HD21	2	0.03	0.04
(1,1431)	1:B:22:LEU:HD21	1:B:28:LEU:HD22	2	0.03	0.04
(1,1431)	1:B:22:LEU:HD21	1:B:28:LEU:HD23	2	0.03	0.04
(1,1431)	1:B:22:LEU:HD22	1:B:28:LEU:HD21	2	0.03	0.04
(1,1431)	1:B:22:LEU:HD22	1:B:28:LEU:HD22	2	0.03	0.04
(1,1431)	1:B:22:LEU:HD22	1:B:28:LEU:HD23	2	0.03	0.04
(1,1431)	1:B:22:LEU:HD23	1:B:28:LEU:HD21	2	0.03	0.04
(1,1431)	1:B:22:LEU:HD23	1:B:28:LEU:HD22	2	0.03	0.04
(1,1431)	1:B:22:LEU:HD23	1:B:28:LEU:HD23	2	0.03	0.04
(1,1427)	1:B:22:LEU:HD11	1:B:93:VAL:HB	2	0.04	0.05
(1,1427)	1:B:22:LEU:HD12	1:B:93:VAL:HB	2	0.04	0.05
(1,1427)	1:B:22:LEU:HD13	1:B:93:VAL:HB	2	0.04	0.05
(1,1418)	1:B:22:LEU:HA	1:B:28:LEU:HD21	2	0.04	0.05
(1,1418)	1:B:22:LEU:HA	1:B:28:LEU:HD22	2	0.04	0.05
(1,1418)	1:B:22:LEU:HA	1:B:28:LEU:HD23	2	0.04	0.05
(1,1409)	1:B:21:ALA:HB1	1:B:65:GLY:HA2	2	0.03	0.04
(1,1409)	1:B:21:ALA:HB2	1:B:65:GLY:HA2	2	0.03	0.04
(1,1409)	1:B:21:ALA:HB3	1:B:65:GLY:HA2	2	0.03	0.04
(1,1395)	1:B:20:LYS:HB2	1:B:20:LYS:HE2	2	0.04	0.04
(1,1395)	1:B:20:LYS:HB2	1:B:20:LYS:HE3	2	0.04	0.04
(1,1395)	1:B:20:LYS:HB3	1:B:20:LYS:HE2	2	0.04	0.04
(1,1395)	1:B:20:LYS:HB3	1:B:20:LYS:HE3	2	0.04	0.04
(1,1390)	1:B:20:LYS:HA	1:B:20:LYS:HE2	2	0.04	0.04
(1,1390)	1:B:20:LYS:HA	1:B:20:LYS:HE3	2	0.04	0.04
(1,137)	1:A:7:ARG:HA	1:A:7:ARG:HG2	2	0.11	0.17
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB1	2	0.03	0.06
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB2	2	0.03	0.06
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB3	2	0.03	0.06
(1,1269)	1:B:7:ARG:HA	1:B:7:ARG:HG2	2	0.09	0.1

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD11	2	0.03	0.03
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD12	2	0.03	0.03
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD13	2	0.03	0.03
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD11	2	0.03	0.03
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD12	2	0.03	0.03
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD13	2	0.03	0.03
(1,1210)	1:A:95:VAL:HG11	1:A:99:GLU:HB2	2	0.16	0.17
(1,1210)	1:A:95:VAL:HG12	1:A:99:GLU:HB2	2	0.16	0.17
(1,1210)	1:A:95:VAL:HG13	1:A:99:GLU:HB2	2	0.16	0.17
(1,121)	1:B:88:ARG:HB2	1:A:92:LEU:HD21	2	0.03	0.04
(1,121)	1:B:88:ARG:HB2	1:A:92:LEU:HD22	2	0.03	0.04
(1,121)	1:B:88:ARG:HB2	1:A:92:LEU:HD23	2	0.03	0.04
(1,1208)	1:A:95:VAL:HG11	1:A:98:ASP:HB2	2	0.14	0.17
(1,1208)	1:A:95:VAL:HG12	1:A:98:ASP:HB2	2	0.14	0.17
(1,1208)	1:A:95:VAL:HG13	1:A:98:ASP:HB2	2	0.14	0.17
(1,1195)	1:A:94:GLN:HG2	1:A:95:VAL:H	2	0.39	0.4
(1,1186)	1:A:93:VAL:H	1:A:93:VAL:HG11	2	0.08	0.08
(1,1186)	1:A:93:VAL:H	1:A:93:VAL:HG12	2	0.08	0.08
(1,1186)	1:A:93:VAL:H	1:A:93:VAL:HG13	2	0.08	0.08
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB1	2	0.04	0.05
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB2	2	0.04	0.05
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB3	2	0.04	0.05
(1,1153)	1:A:90:PHE:HA	1:A:93:VAL:HG11	2	0.06	0.06
(1,1153)	1:A:90:PHE:HA	1:A:93:VAL:HG12	2	0.06	0.06
(1,1153)	1:A:90:PHE:HA	1:A:93:VAL:HG13	2	0.06	0.06
(1,1144)	1:A:89:LEU:HD21	1:A:93:VAL:HB	2	0.02	0.02
(1,1144)	1:A:89:LEU:HD22	1:A:93:VAL:HB	2	0.02	0.02
(1,1144)	1:A:89:LEU:HD23	1:A:93:VAL:HB	2	0.02	0.02
(1,11)	1:A:12:LEU:HD11	1:B:32:ASP:HB2	2	0.05	0.07
(1,11)	1:A:12:LEU:HD11	1:B:32:ASP:HB3	2	0.05	0.07
(1,11)	1:A:12:LEU:HD12	1:B:32:ASP:HB2	2	0.05	0.07
(1,11)	1:A:12:LEU:HD12	1:B:32:ASP:HB3	2	0.05	0.07
(1,11)	1:A:12:LEU:HD13	1:B:32:ASP:HB2	2	0.05	0.07
(1,11)	1:A:12:LEU:HD13	1:B:32:ASP:HB3	2	0.05	0.07
(1,105)	1:B:16:ALA:HB1	1:A:25:GLY:HA2	2	0.33	0.48
(1,105)	1:B:16:ALA:HB2	1:A:25:GLY:HA2	2	0.33	0.48
(1,105)	1:B:16:ALA:HB3	1:A:25:GLY:HA2	2	0.33	0.48
(1,1046)	1:A:80:ARG:H	1:A:80:ARG:HD2	2	0.03	0.03
(1,1046)	1:A:80:ARG:H	1:A:80:ARG:HD3	2	0.03	0.03
(1,1044)	1:A:80:ARG:HB2	1:A:80:ARG:HE	2	0.14	0.15
(1,1020)	1:A:76:ARG:HD2	1:A:78:TYR:HE1	2	0.15	0.18
(1,1020)	1:A:76:ARG:HD3	1:A:78:TYR:HE1	2	0.15	0.18

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1003)	1:A:74:GLY:HA2	1:A:76:ARG:H	2	0.06	0.1
(1,997)	1:A:73:GLU:HG2	1:A:78:TYR:HE1	1	1.69	1.69
(1,997)	1:A:73:GLU:HG3	1:A:78:TYR:HE1	1	1.69	1.69
(1,990)	1:A:72:ARG:H	1:A:72:ARG:HD2	1	0.09	0.09
(1,990)	1:A:72:ARG:H	1:A:72:ARG:HD3	1	0.09	0.09
(1,980)	1:A:72:ARG:HA	1:A:77:GLN:HA	1	0.01	0.01
(1,98)	1:B:15:VAL:HG11	1:A:28:LEU:HD11	1	0.05	0.05
(1,98)	1:B:15:VAL:HG11	1:A:28:LEU:HD12	1	0.05	0.05
(1,98)	1:B:15:VAL:HG11	1:A:28:LEU:HD13	1	0.05	0.05
(1,98)	1:B:15:VAL:HG12	1:A:28:LEU:HD11	1	0.05	0.05
(1,98)	1:B:15:VAL:HG12	1:A:28:LEU:HD12	1	0.05	0.05
(1,98)	1:B:15:VAL:HG12	1:A:28:LEU:HD13	1	0.05	0.05
(1,98)	1:B:15:VAL:HG13	1:A:28:LEU:HD11	1	0.05	0.05
(1,98)	1:B:15:VAL:HG13	1:A:28:LEU:HD12	1	0.05	0.05
(1,98)	1:B:15:VAL:HG13	1:A:28:LEU:HD13	1	0.05	0.05
(1,976)	1:A:72:ARG:HA	1:A:72:ARG:HD2	1	0.05	0.05
(1,976)	1:A:72:ARG:HA	1:A:72:ARG:HD3	1	0.05	0.05
(1,973)	1:A:71:ARG:H	1:A:71:ARG:HG2	1	0.14	0.14
(1,97)	1:B:15:VAL:HB	1:A:28:LEU:HD11	1	0.01	0.01
(1,97)	1:B:15:VAL:HB	1:A:28:LEU:HD12	1	0.01	0.01
(1,97)	1:B:15:VAL:HB	1:A:28:LEU:HD13	1	0.01	0.01
(1,959)	1:A:70:ALA:HB1	1:A:77:GLN:HE22	1	0.03	0.03
(1,959)	1:A:70:ALA:HB2	1:A:77:GLN:HE22	1	0.03	0.03
(1,959)	1:A:70:ALA:HB3	1:A:77:GLN:HE22	1	0.03	0.03
(1,958)	1:A:70:ALA:HB1	1:A:77:GLN:HE21	1	0.02	0.02
(1,958)	1:A:70:ALA:HB2	1:A:77:GLN:HE21	1	0.02	0.02
(1,958)	1:A:70:ALA:HB3	1:A:77:GLN:HE21	1	0.02	0.02
(1,94)	1:B:14:GLN:HG3	1:A:97:ALA:HB1	1	0.05	0.05
(1,94)	1:B:14:GLN:HG3	1:A:97:ALA:HB2	1	0.05	0.05
(1,94)	1:B:14:GLN:HG3	1:A:97:ALA:HB3	1	0.05	0.05
(1,921)	1:A:68:VAL:HG11	1:A:86:VAL:HG11	1	0.03	0.03
(1,921)	1:A:68:VAL:HG11	1:A:86:VAL:HG12	1	0.03	0.03
(1,921)	1:A:68:VAL:HG11	1:A:86:VAL:HG13	1	0.03	0.03
(1,921)	1:A:68:VAL:HG12	1:A:86:VAL:HG11	1	0.03	0.03
(1,921)	1:A:68:VAL:HG12	1:A:86:VAL:HG12	1	0.03	0.03
(1,921)	1:A:68:VAL:HG12	1:A:86:VAL:HG13	1	0.03	0.03
(1,921)	1:A:68:VAL:HG13	1:A:86:VAL:HG11	1	0.03	0.03
(1,921)	1:A:68:VAL:HG13	1:A:86:VAL:HG12	1	0.03	0.03
(1,921)	1:A:68:VAL:HG13	1:A:86:VAL:HG13	1	0.03	0.03
(1,89)	1:B:14:GLN:HB2	1:A:101:LEU:HD21	1	0.09	0.09
(1,89)	1:B:14:GLN:HB2	1:A:101:LEU:HD22	1	0.09	0.09
(1,89)	1:B:14:GLN:HB2	1:A:101:LEU:HD23	1	0.09	0.09

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,89)	1:B:14:GLN:HB3	1:A:101:LEU:HD21	1	0.09	0.09
(1,89)	1:B:14:GLN:HB3	1:A:101:LEU:HD22	1	0.09	0.09
(1,89)	1:B:14:GLN:HB3	1:A:101:LEU:HD23	1	0.09	0.09
(1,88)	1:B:14:GLN:HB2	1:A:101:LEU:HD11	1	0.02	0.02
(1,88)	1:B:14:GLN:HB2	1:A:101:LEU:HD12	1	0.02	0.02
(1,88)	1:B:14:GLN:HB2	1:A:101:LEU:HD13	1	0.02	0.02
(1,88)	1:B:14:GLN:HB3	1:A:101:LEU:HD11	1	0.02	0.02
(1,88)	1:B:14:GLN:HB3	1:A:101:LEU:HD12	1	0.02	0.02
(1,88)	1:B:14:GLN:HB3	1:A:101:LEU:HD13	1	0.02	0.02
(1,848)	1:A:62:LEU:H	1:A:62:LEU:HG	1	0.17	0.17
(1,842)	1:A:62:LEU:HB3	1:A:68:VAL:HG21	1	0.03	0.03
(1,842)	1:A:62:LEU:HB3	1:A:68:VAL:HG22	1	0.03	0.03
(1,842)	1:A:62:LEU:HB3	1:A:68:VAL:HG23	1	0.03	0.03
(1,840)	1:A:62:LEU:HB2	1:A:68:VAL:HG11	1	0.41	0.41
(1,840)	1:A:62:LEU:HB2	1:A:68:VAL:HG12	1	0.41	0.41
(1,840)	1:A:62:LEU:HB2	1:A:68:VAL:HG13	1	0.41	0.41
(1,805)	1:A:59:LEU:HD11	1:A:79:TYR:HE1	1	0.14	0.14
(1,805)	1:A:59:LEU:HD12	1:A:79:TYR:HE1	1	0.14	0.14
(1,805)	1:A:59:LEU:HD13	1:A:79:TYR:HE1	1	0.14	0.14
(1,796)	1:A:59:LEU:HA	1:A:62:LEU:HD11	1	0.08	0.08
(1,796)	1:A:59:LEU:HA	1:A:62:LEU:HD12	1	0.08	0.08
(1,796)	1:A:59:LEU:HA	1:A:62:LEU:HD13	1	0.08	0.08
(1,775)	1:A:56:SER:HA	1:A:59:LEU:HD11	1	0.01	0.01
(1,775)	1:A:56:SER:HA	1:A:59:LEU:HD12	1	0.01	0.01
(1,775)	1:A:56:SER:HA	1:A:59:LEU:HD13	1	0.01	0.01
(1,766)	1:A:55:ALA:HB1	1:A:58:ASN:HB2	1	0.4	0.4
(1,766)	1:A:55:ALA:HB2	1:A:58:ASN:HB2	1	0.4	0.4
(1,766)	1:A:55:ALA:HB3	1:A:58:ASN:HB2	1	0.4	0.4
(1,761)	1:A:55:ALA:HA	1:A:58:ASN:HB2	1	0.25	0.25
(1,750)	1:A:53:THR:H	1:A:53:THR:HB	1	0.01	0.01
(1,748)	1:A:53:THR:HB	1:A:55:ALA:H	1	0.01	0.01
(1,703)	1:A:50:MET:HB2	1:A:54:THR:HG21	1	0.55	0.55
(1,703)	1:A:50:MET:HB2	1:A:54:THR:HG22	1	0.55	0.55
(1,703)	1:A:50:MET:HB2	1:A:54:THR:HG23	1	0.55	0.55
(1,68)	1:B:12:LEU:HB2	1:A:28:LEU:HB2	1	0.02	0.02
(1,66)	1:B:11:LEU:HD11	1:A:98:ASP:HB2	1	0.02	0.02
(1,66)	1:B:11:LEU:HD12	1:A:98:ASP:HB2	1	0.02	0.02
(1,66)	1:B:11:LEU:HD13	1:A:98:ASP:HB2	1	0.02	0.02
(1,646)	1:A:44:ILE:HD11	1:A:79:TYR:HD1	1	0.06	0.06
(1,646)	1:A:44:ILE:HD12	1:A:79:TYR:HD1	1	0.06	0.06
(1,646)	1:A:44:ILE:HD13	1:A:79:TYR:HD1	1	0.06	0.06
(1,645)	1:A:44:ILE:HD11	1:A:59:LEU:HD21	1	0.02	0.02

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,645)	1:A:44:ILE:HD11	1:A:59:LEU:HD22	1	0.02	0.02
(1,645)	1:A:44:ILE:HD11	1:A:59:LEU:HD23	1	0.02	0.02
(1,645)	1:A:44:ILE:HD12	1:A:59:LEU:HD21	1	0.02	0.02
(1,645)	1:A:44:ILE:HD12	1:A:59:LEU:HD22	1	0.02	0.02
(1,645)	1:A:44:ILE:HD12	1:A:59:LEU:HD23	1	0.02	0.02
(1,645)	1:A:44:ILE:HD13	1:A:59:LEU:HD21	1	0.02	0.02
(1,645)	1:A:44:ILE:HD13	1:A:59:LEU:HD22	1	0.02	0.02
(1,645)	1:A:44:ILE:HD13	1:A:59:LEU:HD23	1	0.02	0.02
(1,617)	1:A:42:GLU:HG3	1:A:52:LEU:HD21	1	0.04	0.04
(1,617)	1:A:42:GLU:HG3	1:A:52:LEU:HD22	1	0.04	0.04
(1,617)	1:A:42:GLU:HG3	1:A:52:LEU:HD23	1	0.04	0.04
(1,60)	1:A:89:LEU:HB2	1:B:92:LEU:HD11	1	0.03	0.03
(1,60)	1:A:89:LEU:HB2	1:B:92:LEU:HD12	1	0.03	0.03
(1,60)	1:A:89:LEU:HB2	1:B:92:LEU:HD13	1	0.03	0.03
(1,60)	1:A:89:LEU:HB3	1:B:92:LEU:HD11	1	0.03	0.03
(1,60)	1:A:89:LEU:HB3	1:B:92:LEU:HD12	1	0.03	0.03
(1,60)	1:A:89:LEU:HB3	1:B:92:LEU:HD13	1	0.03	0.03
(1,596)	1:A:41:VAL:HG21	1:A:79:TYR:HE1	1	2.31	2.31
(1,596)	1:A:41:VAL:HG22	1:A:79:TYR:HE1	1	2.31	2.31
(1,596)	1:A:41:VAL:HG23	1:A:79:TYR:HE1	1	2.31	2.31
(1,595)	1:A:41:VAL:HG21	1:A:79:TYR:HD1	1	2.19	2.19
(1,595)	1:A:41:VAL:HG22	1:A:79:TYR:HD1	1	2.19	2.19
(1,595)	1:A:41:VAL:HG23	1:A:79:TYR:HD1	1	2.19	2.19
(1,587)	1:A:41:VAL:HG11	1:A:79:TYR:HE1	1	2.41	2.41
(1,587)	1:A:41:VAL:HG12	1:A:79:TYR:HE1	1	2.41	2.41
(1,587)	1:A:41:VAL:HG13	1:A:79:TYR:HE1	1	2.41	2.41
(1,537)	1:A:39:ARG:HD2	1:A:43:ALA:HB1	1	0.08	0.08
(1,537)	1:A:39:ARG:HD2	1:A:43:ALA:HB2	1	0.08	0.08
(1,537)	1:A:39:ARG:HD2	1:A:43:ALA:HB3	1	0.08	0.08
(1,534)	1:A:39:ARG:HB2	1:A:39:ARG:HE	1	0.03	0.03
(1,523)	1:A:38:GLU:HB2	1:A:80:ARG:HG2	1	0.36	0.36
(1,523)	1:A:38:GLU:HB3	1:A:80:ARG:HG2	1	0.36	0.36
(1,515)	1:A:36:GLN:H	1:A:36:GLN:HG2	1	0.4	0.4
(1,512)	1:A:36:GLN:HG2	1:A:36:GLN:HE21	1	0.01	0.01
(1,51)	1:A:20:LYS:HB2	1:B:23:ALA:HB1	1	0.04	0.04
(1,51)	1:A:20:LYS:HB2	1:B:23:ALA:HB2	1	0.04	0.04
(1,51)	1:A:20:LYS:HB2	1:B:23:ALA:HB3	1	0.04	0.04
(1,51)	1:A:20:LYS:HB3	1:B:23:ALA:HB1	1	0.04	0.04
(1,51)	1:A:20:LYS:HB3	1:B:23:ALA:HB2	1	0.04	0.04
(1,51)	1:A:20:LYS:HB3	1:B:23:ALA:HB3	1	0.04	0.04
(1,506)	1:A:35:ALA:HB1	1:A:90:PHE:HD1	1	0.03	0.03
(1,506)	1:A:35:ALA:HB1	1:A:90:PHE:HD2	1	0.03	0.03

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,506)	1:A:35:ALA:HB2	1:A:90:PHE:HD1	1	0.03	0.03
(1,506)	1:A:35:ALA:HB2	1:A:90:PHE:HD2	1	0.03	0.03
(1,506)	1:A:35:ALA:HB3	1:A:90:PHE:HD1	1	0.03	0.03
(1,506)	1:A:35:ALA:HB3	1:A:90:PHE:HD2	1	0.03	0.03
(1,500)	1:A:35:ALA:HA	1:A:81:ILE:HD11	1	0.01	0.01
(1,500)	1:A:35:ALA:HA	1:A:81:ILE:HD12	1	0.01	0.01
(1,500)	1:A:35:ALA:HA	1:A:81:ILE:HD13	1	0.01	0.01
(1,50)	1:A:20:LYS:HA	1:B:23:ALA:HB1	1	0.07	0.07
(1,50)	1:A:20:LYS:HA	1:B:23:ALA:HB2	1	0.07	0.07
(1,50)	1:A:20:LYS:HA	1:B:23:ALA:HB3	1	0.07	0.07
(1,490)	1:A:34:LEU:HD21	1:A:37:GLY:H	1	0.01	0.01
(1,490)	1:A:34:LEU:HD22	1:A:37:GLY:H	1	0.01	0.01
(1,490)	1:A:34:LEU:HD23	1:A:37:GLY:H	1	0.01	0.01
(1,468)	1:A:33:LEU:HD11	1:A:39:ARG:HE	1	0.23	0.23
(1,468)	1:A:33:LEU:HD12	1:A:39:ARG:HE	1	0.23	0.23
(1,468)	1:A:33:LEU:HD13	1:A:39:ARG:HE	1	0.23	0.23
(1,461)	1:A:33:LEU:HD11	1:A:34:LEU:H	1	0.07	0.07
(1,461)	1:A:33:LEU:HD12	1:A:34:LEU:H	1	0.07	0.07
(1,461)	1:A:33:LEU:HD13	1:A:34:LEU:H	1	0.07	0.07
(1,446)	1:A:31:LEU:H	1:A:62:LEU:HD11	1	0.01	0.01
(1,446)	1:A:31:LEU:H	1:A:62:LEU:HD12	1	0.01	0.01
(1,446)	1:A:31:LEU:H	1:A:62:LEU:HD13	1	0.01	0.01
(1,438)	1:A:31:LEU:HD21	1:A:86:VAL:HG11	1	0.02	0.02
(1,438)	1:A:31:LEU:HD21	1:A:86:VAL:HG12	1	0.02	0.02
(1,438)	1:A:31:LEU:HD21	1:A:86:VAL:HG13	1	0.02	0.02
(1,438)	1:A:31:LEU:HD22	1:A:86:VAL:HG11	1	0.02	0.02
(1,438)	1:A:31:LEU:HD22	1:A:86:VAL:HG12	1	0.02	0.02
(1,438)	1:A:31:LEU:HD22	1:A:86:VAL:HG13	1	0.02	0.02
(1,438)	1:A:31:LEU:HD23	1:A:86:VAL:HG11	1	0.02	0.02
(1,438)	1:A:31:LEU:HD23	1:A:86:VAL:HG12	1	0.02	0.02
(1,438)	1:A:31:LEU:HD23	1:A:86:VAL:HG13	1	0.02	0.02
(1,435)	1:A:31:LEU:HD21	1:A:81:ILE:HD11	1	0.02	0.02
(1,435)	1:A:31:LEU:HD21	1:A:81:ILE:HD12	1	0.02	0.02
(1,435)	1:A:31:LEU:HD21	1:A:81:ILE:HD13	1	0.02	0.02
(1,435)	1:A:31:LEU:HD22	1:A:81:ILE:HD11	1	0.02	0.02
(1,435)	1:A:31:LEU:HD22	1:A:81:ILE:HD12	1	0.02	0.02
(1,435)	1:A:31:LEU:HD22	1:A:81:ILE:HD13	1	0.02	0.02
(1,435)	1:A:31:LEU:HD23	1:A:81:ILE:HD11	1	0.02	0.02
(1,435)	1:A:31:LEU:HD23	1:A:81:ILE:HD12	1	0.02	0.02
(1,435)	1:A:31:LEU:HD23	1:A:81:ILE:HD13	1	0.02	0.02
(1,434)	1:A:31:LEU:HD21	1:A:81:ILE:HA	1	0.01	0.01
(1,434)	1:A:31:LEU:HD22	1:A:81:ILE:HA	1	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,434)	1:A:31:LEU:HD23	1:A:81:ILE:HA	1	0.01	0.01
(1,429)	1:A:31:LEU:HD21	1:A:67:LEU:HA	1	0.03	0.03
(1,429)	1:A:31:LEU:HD22	1:A:67:LEU:HA	1	0.03	0.03
(1,429)	1:A:31:LEU:HD23	1:A:67:LEU:HA	1	0.03	0.03
(1,422)	1:A:31:LEU:HD11	1:A:86:VAL:HG11	1	0.01	0.01
(1,422)	1:A:31:LEU:HD11	1:A:86:VAL:HG12	1	0.01	0.01
(1,422)	1:A:31:LEU:HD11	1:A:86:VAL:HG13	1	0.01	0.01
(1,422)	1:A:31:LEU:HD12	1:A:86:VAL:HG11	1	0.01	0.01
(1,422)	1:A:31:LEU:HD12	1:A:86:VAL:HG12	1	0.01	0.01
(1,422)	1:A:31:LEU:HD12	1:A:86:VAL:HG13	1	0.01	0.01
(1,422)	1:A:31:LEU:HD13	1:A:86:VAL:HG11	1	0.01	0.01
(1,422)	1:A:31:LEU:HD13	1:A:86:VAL:HG12	1	0.01	0.01
(1,422)	1:A:31:LEU:HD13	1:A:86:VAL:HG13	1	0.01	0.01
(1,421)	1:A:31:LEU:HD11	1:A:67:LEU:HG	1	0.05	0.05
(1,421)	1:A:31:LEU:HD12	1:A:67:LEU:HG	1	0.05	0.05
(1,421)	1:A:31:LEU:HD13	1:A:67:LEU:HG	1	0.05	0.05
(1,419)	1:A:31:LEU:HD11	1:A:62:LEU:HB2	1	0.01	0.01
(1,419)	1:A:31:LEU:HD12	1:A:62:LEU:HB2	1	0.01	0.01
(1,419)	1:A:31:LEU:HD13	1:A:62:LEU:HB2	1	0.01	0.01
(1,412)	1:A:31:LEU:HB2	1:A:62:LEU:HD11	1	0.01	0.01
(1,412)	1:A:31:LEU:HB2	1:A:62:LEU:HD12	1	0.01	0.01
(1,412)	1:A:31:LEU:HB2	1:A:62:LEU:HD13	1	0.01	0.01
(1,389)	1:A:30:ILE:HG21	1:A:33:LEU:HB2	1	0.07	0.07
(1,389)	1:A:30:ILE:HG22	1:A:33:LEU:HB2	1	0.07	0.07
(1,389)	1:A:30:ILE:HG23	1:A:33:LEU:HB2	1	0.07	0.07
(1,381)	1:A:30:ILE:HD11	1:A:59:LEU:HA	1	0.02	0.02
(1,381)	1:A:30:ILE:HD12	1:A:59:LEU:HA	1	0.02	0.02
(1,381)	1:A:30:ILE:HD13	1:A:59:LEU:HA	1	0.02	0.02
(1,375)	1:A:30:ILE:HB	1:A:62:LEU:HD11	1	0.01	0.01
(1,375)	1:A:30:ILE:HB	1:A:62:LEU:HD12	1	0.01	0.01
(1,375)	1:A:30:ILE:HB	1:A:62:LEU:HD13	1	0.01	0.01
(1,342)	1:A:28:LEU:HD21	1:A:90:PHE:HE1	1	0.01	0.01
(1,342)	1:A:28:LEU:HD22	1:A:90:PHE:HE1	1	0.01	0.01
(1,342)	1:A:28:LEU:HD23	1:A:90:PHE:HE1	1	0.01	0.01
(1,338)	1:A:28:LEU:HD11	1:A:90:PHE:HE1	1	0.02	0.02
(1,338)	1:A:28:LEU:HD12	1:A:90:PHE:HE1	1	0.02	0.02
(1,338)	1:A:28:LEU:HD13	1:A:90:PHE:HE1	1	0.02	0.02
(1,319)	1:A:26:ARG:H	1:A:26:ARG:HG2	1	0.11	0.11
(1,319)	1:A:26:ARG:H	1:A:26:ARG:HG3	1	0.11	0.11
(1,313)	1:A:25:GLY:HA2	1:A:28:LEU:HD11	1	0.08	0.08
(1,313)	1:A:25:GLY:HA2	1:A:28:LEU:HD12	1	0.08	0.08
(1,313)	1:A:25:GLY:HA2	1:A:28:LEU:HD13	1	0.08	0.08

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,309)	1:A:24:ASN:H	1:A:24:ASN:HB2	1	0.14	0.14
(1,296)	1:A:22:LEU:HD11	1:A:93:VAL:HG11	1	0.02	0.02
(1,296)	1:A:22:LEU:HD11	1:A:93:VAL:HG12	1	0.02	0.02
(1,296)	1:A:22:LEU:HD11	1:A:93:VAL:HG13	1	0.02	0.02
(1,296)	1:A:22:LEU:HD12	1:A:93:VAL:HG11	1	0.02	0.02
(1,296)	1:A:22:LEU:HD12	1:A:93:VAL:HG12	1	0.02	0.02
(1,296)	1:A:22:LEU:HD12	1:A:93:VAL:HG13	1	0.02	0.02
(1,296)	1:A:22:LEU:HD13	1:A:93:VAL:HG11	1	0.02	0.02
(1,296)	1:A:22:LEU:HD13	1:A:93:VAL:HG12	1	0.02	0.02
(1,296)	1:A:22:LEU:HD13	1:A:93:VAL:HG13	1	0.02	0.02
(1,28)	1:A:14:GLN:HG2	1:B:101:LEU:HD21	1	0.26	0.26
(1,28)	1:A:14:GLN:HG2	1:B:101:LEU:HD22	1	0.26	0.26
(1,28)	1:A:14:GLN:HG2	1:B:101:LEU:HD23	1	0.26	0.26
(1,278)	1:A:21:ALA:HB1	1:A:65:GLY:HA3	1	0.01	0.01
(1,278)	1:A:21:ALA:HB2	1:A:65:GLY:HA3	1	0.01	0.01
(1,278)	1:A:21:ALA:HB3	1:A:65:GLY:HA3	1	0.01	0.01
(1,270)	1:A:20:LYS:H	1:A:20:LYS:HD2	1	0.02	0.02
(1,270)	1:A:20:LYS:H	1:A:20:LYS:HD3	1	0.02	0.02
(1,2617)	1:B:99:GLU:H	1:B:95:VAL:O	1	0.02	0.02
(1,258)	1:A:20:LYS:HA	1:A:20:LYS:HE2	1	0.03	0.03
(1,258)	1:A:20:LYS:HA	1:A:20:LYS:HE3	1	0.03	0.03
(1,2574)	1:B:66:GLY:N	1:B:63:LYS:O	1	0.06	0.06
(1,2567)	1:B:63:LYS:H	1:B:59:LEU:O	1	0.01	0.01
(1,2565)	1:B:62:LEU:H	1:B:58:ASN:O	1	0.01	0.01
(1,2549)	1:B:50:MET:H	1:B:45:ALA:O	1	0.01	0.01
(1,2541)	1:B:46:THR:H	1:B:42:GLU:O	1	0.01	0.01
(1,2534)	1:B:39:ARG:N	1:B:79:TYR:O	1	0.01	0.01
(1,2516)	1:B:18:VAL:N	1:B:14:GLN:O	1	0.02	0.02
(1,2508)	1:B:14:GLN:N	1:B:10:ALA:O	1	0.01	0.01
(1,2501)	1:A:98:ASP:H	1:A:94:GLN:O	1	0.01	0.01
(1,2495)	1:A:95:VAL:H	1:A:91:ALA:O	1	0.03	0.03
(1,2485)	1:A:90:PHE:H	1:A:86:VAL:O	1	0.01	0.01
(1,2471)	1:A:78:TYR:H	1:A:71:ARG:O	1	0.01	0.01
(1,2462)	1:A:67:LEU:N	1:A:62:LEU:O	1	0.01	0.01
(1,2451)	1:A:62:LEU:H	1:A:58:ASN:O	1	0.01	0.01
(1,2435)	1:A:50:MET:H	1:A:45:ALA:O	1	0.01	0.01
(1,2411)	1:A:32:ASP:H	1:A:28:LEU:O	1	0.02	0.02
(1,2405)	1:A:20:LYS:H	1:A:16:ALA:O	1	0.01	0.01
(1,2403)	1:A:19:GLY:H	1:A:15:VAL:O	1	0.02	0.02
(1,2389)	1:B:102:GLU:H	1:B:102:GLU:HG2	1	0.02	0.02
(1,2389)	1:B:102:GLU:H	1:B:102:GLU:HG3	1	0.02	0.02
(1,2388)	1:B:101:LEU:H	1:B:102:GLU:H	1	0.18	0.18

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2379)	1:B:100:HIS:H	1:B:100:HIS:HD2	1	0.01	0.01
(1,2375)	1:B:99:GLU:H	1:B:99:GLU:HB2	1	0.03	0.03
(1,2356)	1:B:96:VAL:HG21	1:B:97:ALA:H	1	0.01	0.01
(1,2356)	1:B:96:VAL:HG22	1:B:97:ALA:H	1	0.01	0.01
(1,2356)	1:B:96:VAL:HG23	1:B:97:ALA:H	1	0.01	0.01
(1,2352)	1:B:96:VAL:HA	1:B:100:HIS:HD2	1	0.14	0.14
(1,2340)	1:B:95:VAL:HG11	1:B:98:ASP:HB2	1	0.37	0.37
(1,2340)	1:B:95:VAL:HG12	1:B:98:ASP:HB2	1	0.37	0.37
(1,2340)	1:B:95:VAL:HG13	1:B:98:ASP:HB2	1	0.37	0.37
(1,2333)	1:B:95:VAL:HA	1:B:98:ASP:HB2	1	0.03	0.03
(1,2327)	1:B:94:GLN:HG2	1:B:95:VAL:H	1	0.39	0.39
(1,230)	1:A:17:ARG:H	1:A:17:ARG:HD2	1	0.03	0.03
(1,230)	1:A:17:ARG:H	1:A:17:ARG:HD3	1	0.03	0.03
(1,2296)	1:B:91:ALA:HA	1:B:94:GLN:HE21	1	0.05	0.05
(1,2291)	1:B:90:PHE:HD1	1:B:93:VAL:HG11	1	0.02	0.02
(1,2291)	1:B:90:PHE:HD1	1:B:93:VAL:HG12	1	0.02	0.02
(1,2291)	1:B:90:PHE:HD1	1:B:93:VAL:HG13	1	0.02	0.02
(1,2291)	1:B:90:PHE:HD2	1:B:93:VAL:HG11	1	0.02	0.02
(1,2291)	1:B:90:PHE:HD2	1:B:93:VAL:HG12	1	0.02	0.02
(1,2291)	1:B:90:PHE:HD2	1:B:93:VAL:HG13	1	0.02	0.02
(1,2277)	1:B:89:LEU:HD21	1:B:93:VAL:HG11	1	0.01	0.01
(1,2277)	1:B:89:LEU:HD21	1:B:93:VAL:HG12	1	0.01	0.01
(1,2277)	1:B:89:LEU:HD21	1:B:93:VAL:HG13	1	0.01	0.01
(1,2277)	1:B:89:LEU:HD22	1:B:93:VAL:HG11	1	0.01	0.01
(1,2277)	1:B:89:LEU:HD22	1:B:93:VAL:HG12	1	0.01	0.01
(1,2277)	1:B:89:LEU:HD22	1:B:93:VAL:HG13	1	0.01	0.01
(1,2277)	1:B:89:LEU:HD23	1:B:93:VAL:HG11	1	0.01	0.01
(1,2277)	1:B:89:LEU:HD23	1:B:93:VAL:HG12	1	0.01	0.01
(1,2277)	1:B:89:LEU:HD23	1:B:93:VAL:HG13	1	0.01	0.01
(1,2213)	1:B:82:ALA:H	1:B:86:VAL:HG21	1	0.03	0.03
(1,2213)	1:B:82:ALA:H	1:B:86:VAL:HG22	1	0.03	0.03
(1,2213)	1:B:82:ALA:H	1:B:86:VAL:HG23	1	0.03	0.03
(1,2201)	1:B:81:ILE:HG21	1:B:87:ALA:HB1	1	0.02	0.02
(1,2201)	1:B:81:ILE:HG21	1:B:87:ALA:HB2	1	0.02	0.02
(1,2201)	1:B:81:ILE:HG21	1:B:87:ALA:HB3	1	0.02	0.02
(1,2201)	1:B:81:ILE:HG22	1:B:87:ALA:HB1	1	0.02	0.02
(1,2201)	1:B:81:ILE:HG22	1:B:87:ALA:HB2	1	0.02	0.02
(1,2201)	1:B:81:ILE:HG22	1:B:87:ALA:HB3	1	0.02	0.02
(1,2201)	1:B:81:ILE:HG23	1:B:87:ALA:HB1	1	0.02	0.02
(1,2201)	1:B:81:ILE:HG23	1:B:87:ALA:HB2	1	0.02	0.02
(1,2201)	1:B:81:ILE:HG23	1:B:87:ALA:HB3	1	0.02	0.02
(1,2192)	1:B:81:ILE:HG12	1:B:87:ALA:HB1	1	0.19	0.19

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,2192)	1:B:81:ILE:HG12	1:B:87:ALA:HB2	1	0.19	0.19
(1,2192)	1:B:81:ILE:HG12	1:B:87:ALA:HB3	1	0.19	0.19
(1,2156)	1:B:76:ARG:H	1:B:76:ARG:HG3	1	0.18	0.18
(1,2115)	1:B:72:ARG:HB2	1:B:73:GLU:H	1	0.01	0.01
(1,2105)	1:B:71:ARG:H	1:B:71:ARG:HG2	1	0.07	0.07
(1,210)	1:A:15:VAL:HA	1:A:18:VAL:HB	1	0.02	0.02
(1,2099)	1:B:71:ARG:HB2	1:B:71:ARG:HE	1	0.02	0.02
(1,2090)	1:B:70:ALA:HB1	1:B:77:GLN:HE21	1	0.01	0.01
(1,2090)	1:B:70:ALA:HB2	1:B:77:GLN:HE21	1	0.01	0.01
(1,2090)	1:B:70:ALA:HB3	1:B:77:GLN:HE21	1	0.01	0.01
(1,2078)	1:B:69:GLU:HG2	1:B:82:ALA:HB1	1	0.02	0.02
(1,2078)	1:B:69:GLU:HG2	1:B:82:ALA:HB2	1	0.02	0.02
(1,2078)	1:B:69:GLU:HG2	1:B:82:ALA:HB3	1	0.02	0.02
(1,2077)	1:B:69:GLU:HG2	1:B:82:ALA:HA	1	0.05	0.05
(1,2075)	1:B:69:GLU:HG3	1:B:82:ALA:HA	1	0.05	0.05
(1,2053)	1:B:68:VAL:HG11	1:B:86:VAL:HG11	1	0.01	0.01
(1,2053)	1:B:68:VAL:HG11	1:B:86:VAL:HG12	1	0.01	0.01
(1,2053)	1:B:68:VAL:HG11	1:B:86:VAL:HG13	1	0.01	0.01
(1,2053)	1:B:68:VAL:HG12	1:B:86:VAL:HG11	1	0.01	0.01
(1,2053)	1:B:68:VAL:HG12	1:B:86:VAL:HG12	1	0.01	0.01
(1,2053)	1:B:68:VAL:HG12	1:B:86:VAL:HG13	1	0.01	0.01
(1,2053)	1:B:68:VAL:HG13	1:B:86:VAL:HG11	1	0.01	0.01
(1,2053)	1:B:68:VAL:HG13	1:B:86:VAL:HG12	1	0.01	0.01
(1,2053)	1:B:68:VAL:HG13	1:B:86:VAL:HG13	1	0.01	0.01
(1,2035)	1:B:67:LEU:H	1:B:67:LEU:HD21	1	0.03	0.03
(1,2035)	1:B:67:LEU:H	1:B:67:LEU:HD22	1	0.03	0.03
(1,2035)	1:B:67:LEU:H	1:B:67:LEU:HD23	1	0.03	0.03
(1,2032)	1:B:67:LEU:HD11	1:B:86:VAL:HG11	1	0.01	0.01
(1,2032)	1:B:67:LEU:HD11	1:B:86:VAL:HG12	1	0.01	0.01
(1,2032)	1:B:67:LEU:HD11	1:B:86:VAL:HG13	1	0.01	0.01
(1,2032)	1:B:67:LEU:HD12	1:B:86:VAL:HG11	1	0.01	0.01
(1,2032)	1:B:67:LEU:HD12	1:B:86:VAL:HG12	1	0.01	0.01
(1,2032)	1:B:67:LEU:HD12	1:B:86:VAL:HG13	1	0.01	0.01
(1,2032)	1:B:67:LEU:HD13	1:B:86:VAL:HG11	1	0.01	0.01
(1,2032)	1:B:67:LEU:HD13	1:B:86:VAL:HG12	1	0.01	0.01
(1,2032)	1:B:67:LEU:HD13	1:B:86:VAL:HG13	1	0.01	0.01
(1,2020)	1:B:67:LEU:HA	1:B:67:LEU:HD11	1	0.09	0.09
(1,2020)	1:B:67:LEU:HA	1:B:67:LEU:HD12	1	0.09	0.09
(1,2020)	1:B:67:LEU:HA	1:B:67:LEU:HD13	1	0.09	0.09
(1,2)	1:A:11:LEU:HD11	1:B:98:ASP:HB3	1	0.1	0.1
(1,2)	1:A:11:LEU:HD12	1:B:98:ASP:HB3	1	0.1	0.1
(1,2)	1:A:11:LEU:HD13	1:B:98:ASP:HB3	1	0.1	0.1

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1997)	1:B:63:LYS:HE2	1:B:70:ALA:H	1	0.02	0.02
(1,1997)	1:B:63:LYS:HE3	1:B:70:ALA:H	1	0.02	0.02
(1,1995)	1:B:63:LYS:HE2	1:B:69:GLU:HA	1	0.01	0.01
(1,1995)	1:B:63:LYS:HE3	1:B:69:GLU:HA	1	0.01	0.01
(1,1972)	1:B:62:LEU:HB2	1:B:68:VAL:HG11	1	0.13	0.13
(1,1972)	1:B:62:LEU:HB2	1:B:68:VAL:HG12	1	0.13	0.13
(1,1972)	1:B:62:LEU:HB2	1:B:68:VAL:HG13	1	0.13	0.13
(1,1927)	1:B:59:LEU:HA	1:B:62:LEU:HB2	1	0.5	0.5
(1,1907)	1:B:56:SER:HA	1:B:59:LEU:HD11	1	0.01	0.01
(1,1907)	1:B:56:SER:HA	1:B:59:LEU:HD12	1	0.01	0.01
(1,1907)	1:B:56:SER:HA	1:B:59:LEU:HD13	1	0.01	0.01
(1,1889)	1:B:54:THR:HG21	1:B:58:ASN:HD22	1	0.03	0.03
(1,1889)	1:B:54:THR:HG22	1:B:58:ASN:HD22	1	0.03	0.03
(1,1889)	1:B:54:THR:HG23	1:B:58:ASN:HD22	1	0.03	0.03
(1,1887)	1:B:54:THR:HG21	1:B:57:ALA:H	1	0.04	0.04
(1,1887)	1:B:54:THR:HG22	1:B:57:ALA:H	1	0.04	0.04
(1,1887)	1:B:54:THR:HG23	1:B:57:ALA:H	1	0.04	0.04
(1,1882)	1:B:53:THR:H	1:B:53:THR:HB	1	0.01	0.01
(1,1877)	1:B:52:LEU:H	1:B:52:LEU:HG	1	0.03	0.03
(1,1751)	1:B:42:GLU:HG2	1:B:52:LEU:HD21	1	0.01	0.01
(1,1751)	1:B:42:GLU:HG2	1:B:52:LEU:HD22	1	0.01	0.01
(1,1751)	1:B:42:GLU:HG2	1:B:52:LEU:HD23	1	0.01	0.01
(1,1749)	1:B:42:GLU:HG3	1:B:52:LEU:HD21	1	0.03	0.03
(1,1749)	1:B:42:GLU:HG3	1:B:52:LEU:HD22	1	0.03	0.03
(1,1749)	1:B:42:GLU:HG3	1:B:52:LEU:HD23	1	0.03	0.03
(1,1728)	1:B:41:VAL:HG21	1:B:79:TYR:HE1	1	0.01	0.01
(1,1728)	1:B:41:VAL:HG22	1:B:79:TYR:HE1	1	0.01	0.01
(1,1728)	1:B:41:VAL:HG23	1:B:79:TYR:HE1	1	0.01	0.01
(1,1727)	1:B:41:VAL:HG21	1:B:79:TYR:HD1	1	0.01	0.01
(1,1727)	1:B:41:VAL:HG22	1:B:79:TYR:HD1	1	0.01	0.01
(1,1727)	1:B:41:VAL:HG23	1:B:79:TYR:HD1	1	0.01	0.01
(1,1688)	1:B:40:ALA:HB1	1:B:76:ARG:HD2	1	0.12	0.12
(1,1688)	1:B:40:ALA:HB1	1:B:76:ARG:HD3	1	0.12	0.12
(1,1688)	1:B:40:ALA:HB2	1:B:76:ARG:HD2	1	0.12	0.12
(1,1688)	1:B:40:ALA:HB2	1:B:76:ARG:HD3	1	0.12	0.12
(1,1688)	1:B:40:ALA:HB3	1:B:76:ARG:HD2	1	0.12	0.12
(1,1688)	1:B:40:ALA:HB3	1:B:76:ARG:HD3	1	0.12	0.12
(1,1656)	1:B:38:GLU:HG2	1:B:39:ARG:H	1	0.18	0.18
(1,1656)	1:B:38:GLU:HG3	1:B:39:ARG:H	1	0.18	0.18
(1,1654)	1:B:38:GLU:HB2	1:B:80:ARG:HE	1	0.05	0.05
(1,1654)	1:B:38:GLU:HB3	1:B:80:ARG:HE	1	0.05	0.05
(1,1622)	1:B:34:LEU:HD21	1:B:37:GLY:H	1	0.04	0.04

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1622)	1:B:34:LEU:HD22	1:B:37:GLY:H	1	0.04	0.04
(1,1622)	1:B:34:LEU:HD23	1:B:37:GLY:H	1	0.04	0.04
(1,1600)	1:B:33:LEU:HD11	1:B:39:ARG:HE	1	0.29	0.29
(1,1600)	1:B:33:LEU:HD12	1:B:39:ARG:HE	1	0.29	0.29
(1,1600)	1:B:33:LEU:HD13	1:B:39:ARG:HE	1	0.29	0.29
(1,160)	1:A:10:ALA:HA	1:A:13:ASP:HB2	1	0.09	0.09
(1,1597)	1:B:33:LEU:HD11	1:B:36:GLN:H	1	0.35	0.35
(1,1597)	1:B:33:LEU:HD12	1:B:36:GLN:H	1	0.35	0.35
(1,1597)	1:B:33:LEU:HD13	1:B:36:GLN:H	1	0.35	0.35
(1,1593)	1:B:33:LEU:HD11	1:B:34:LEU:H	1	0.25	0.25
(1,1593)	1:B:33:LEU:HD12	1:B:34:LEU:H	1	0.25	0.25
(1,1593)	1:B:33:LEU:HD13	1:B:34:LEU:H	1	0.25	0.25
(1,1591)	1:B:33:LEU:HA	1:B:36:GLN:HE21	1	0.49	0.49
(1,1570)	1:B:31:LEU:HD21	1:B:86:VAL:HG11	1	0.06	0.06
(1,1570)	1:B:31:LEU:HD21	1:B:86:VAL:HG12	1	0.06	0.06
(1,1570)	1:B:31:LEU:HD21	1:B:86:VAL:HG13	1	0.06	0.06
(1,1570)	1:B:31:LEU:HD22	1:B:86:VAL:HG11	1	0.06	0.06
(1,1570)	1:B:31:LEU:HD22	1:B:86:VAL:HG12	1	0.06	0.06
(1,1570)	1:B:31:LEU:HD22	1:B:86:VAL:HG13	1	0.06	0.06
(1,1570)	1:B:31:LEU:HD23	1:B:86:VAL:HG11	1	0.06	0.06
(1,1570)	1:B:31:LEU:HD23	1:B:86:VAL:HG12	1	0.06	0.06
(1,1570)	1:B:31:LEU:HD23	1:B:86:VAL:HG13	1	0.06	0.06
(1,1563)	1:B:31:LEU:HD21	1:B:67:LEU:HD11	1	0.08	0.08
(1,1563)	1:B:31:LEU:HD21	1:B:67:LEU:HD12	1	0.08	0.08
(1,1563)	1:B:31:LEU:HD21	1:B:67:LEU:HD13	1	0.08	0.08
(1,1563)	1:B:31:LEU:HD22	1:B:67:LEU:HD11	1	0.08	0.08
(1,1563)	1:B:31:LEU:HD22	1:B:67:LEU:HD12	1	0.08	0.08
(1,1563)	1:B:31:LEU:HD22	1:B:67:LEU:HD13	1	0.08	0.08
(1,1563)	1:B:31:LEU:HD23	1:B:67:LEU:HD11	1	0.08	0.08
(1,1563)	1:B:31:LEU:HD23	1:B:67:LEU:HD12	1	0.08	0.08
(1,1563)	1:B:31:LEU:HD23	1:B:67:LEU:HD13	1	0.08	0.08
(1,1561)	1:B:31:LEU:HD21	1:B:67:LEU:HA	1	0.05	0.05
(1,1561)	1:B:31:LEU:HD22	1:B:67:LEU:HA	1	0.05	0.05
(1,1561)	1:B:31:LEU:HD23	1:B:67:LEU:HA	1	0.05	0.05
(1,1553)	1:B:31:LEU:HD11	1:B:67:LEU:HG	1	0.01	0.01
(1,1553)	1:B:31:LEU:HD12	1:B:67:LEU:HG	1	0.01	0.01
(1,1553)	1:B:31:LEU:HD13	1:B:67:LEU:HG	1	0.01	0.01
(1,1552)	1:B:31:LEU:HD11	1:B:67:LEU:HB2	1	0.02	0.02
(1,1552)	1:B:31:LEU:HD11	1:B:67:LEU:HB3	1	0.02	0.02
(1,1552)	1:B:31:LEU:HD12	1:B:67:LEU:HB2	1	0.02	0.02
(1,1552)	1:B:31:LEU:HD12	1:B:67:LEU:HB3	1	0.02	0.02
(1,1552)	1:B:31:LEU:HD13	1:B:67:LEU:HB2	1	0.02	0.02

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1552)	1:B:31:LEU:HD13	1:B:67:LEU:HB3	1	0.02	0.02
(1,1541)	1:B:31:LEU:HA	1:B:81:ILE:HD11	1	0.02	0.02
(1,1541)	1:B:31:LEU:HA	1:B:81:ILE:HD12	1	0.02	0.02
(1,1541)	1:B:31:LEU:HA	1:B:81:ILE:HD13	1	0.02	0.02
(1,1537)	1:B:31:LEU:HA	1:B:34:LEU:HD11	1	0.03	0.03
(1,1537)	1:B:31:LEU:HA	1:B:34:LEU:HD12	1	0.03	0.03
(1,1537)	1:B:31:LEU:HA	1:B:34:LEU:HD13	1	0.03	0.03
(1,1512)	1:B:30:ILE:HD11	1:B:58:ASN:H	1	0.02	0.02
(1,1512)	1:B:30:ILE:HD12	1:B:58:ASN:H	1	0.02	0.02
(1,1512)	1:B:30:ILE:HD13	1:B:58:ASN:H	1	0.02	0.02
(1,1510)	1:B:30:ILE:HD11	1:B:58:ASN:HB2	1	0.16	0.16
(1,1510)	1:B:30:ILE:HD12	1:B:58:ASN:HB2	1	0.16	0.16
(1,1510)	1:B:30:ILE:HD13	1:B:58:ASN:HB2	1	0.16	0.16
(1,1448)	1:B:25:GLY:HA2	1:B:28:LEU:H	1	0.01	0.01
(1,1446)	1:B:25:GLY:HA3	1:B:28:LEU:HD11	1	0.08	0.08
(1,1446)	1:B:25:GLY:HA3	1:B:28:LEU:HD12	1	0.08	0.08
(1,1446)	1:B:25:GLY:HA3	1:B:28:LEU:HD13	1	0.08	0.08
(1,1428)	1:B:22:LEU:HD11	1:B:93:VAL:HG11	1	0.02	0.02
(1,1428)	1:B:22:LEU:HD11	1:B:93:VAL:HG12	1	0.02	0.02
(1,1428)	1:B:22:LEU:HD11	1:B:93:VAL:HG13	1	0.02	0.02
(1,1428)	1:B:22:LEU:HD12	1:B:93:VAL:HG11	1	0.02	0.02
(1,1428)	1:B:22:LEU:HD12	1:B:93:VAL:HG12	1	0.02	0.02
(1,1428)	1:B:22:LEU:HD12	1:B:93:VAL:HG13	1	0.02	0.02
(1,1428)	1:B:22:LEU:HD13	1:B:93:VAL:HG11	1	0.02	0.02
(1,1428)	1:B:22:LEU:HD13	1:B:93:VAL:HG12	1	0.02	0.02
(1,1428)	1:B:22:LEU:HD13	1:B:93:VAL:HG13	1	0.02	0.02
(1,1410)	1:B:21:ALA:HB1	1:B:65:GLY:HA3	1	0.05	0.05
(1,1410)	1:B:21:ALA:HB2	1:B:65:GLY:HA3	1	0.05	0.05
(1,1410)	1:B:21:ALA:HB3	1:B:65:GLY:HA3	1	0.05	0.05
(1,1402)	1:B:20:LYS:H	1:B:20:LYS:HD2	1	0.05	0.05
(1,1402)	1:B:20:LYS:H	1:B:20:LYS:HD3	1	0.05	0.05
(1,14)	1:A:12:LEU:HD21	1:B:28:LEU:H	1	0.02	0.02
(1,14)	1:A:12:LEU:HD22	1:B:28:LEU:H	1	0.02	0.02
(1,14)	1:A:12:LEU:HD23	1:B:28:LEU:H	1	0.02	0.02
(1,1362)	1:B:17:ARG:H	1:B:17:ARG:HD2	1	0.02	0.02
(1,1362)	1:B:17:ARG:H	1:B:17:ARG:HD3	1	0.02	0.02
(1,13)	1:A:12:LEU:HD21	1:B:28:LEU:HB2	1	0.16	0.16
(1,13)	1:A:12:LEU:HD22	1:B:28:LEU:HB2	1	0.16	0.16
(1,13)	1:A:12:LEU:HD23	1:B:28:LEU:HB2	1	0.16	0.16
(1,1292)	1:B:10:ALA:HA	1:B:13:ASP:HB2	1	0.13	0.13
(1,1287)	1:B:8:LYS:H	1:B:8:LYS:HG2	1	0.01	0.01
(1,1287)	1:B:8:LYS:H	1:B:8:LYS:HG3	1	0.01	0.01

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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,1264)	1:B:6:ASP:HA	1:B:9:ALA:HB1	1	0.04	0.04
(1,1264)	1:B:6:ASP:HA	1:B:9:ALA:HB2	1	0.04	0.04
(1,1264)	1:B:6:ASP:HA	1:B:9:ALA:HB3	1	0.04	0.04
(1,1257)	1:A:102:GLU:H	1:A:102:GLU:HG2	1	0.07	0.07
(1,1257)	1:A:102:GLU:H	1:A:102:GLU:HG3	1	0.07	0.07
(1,1248)	1:A:101:LEU:HA	1:A:101:LEU:HD21	1	0.08	0.08
(1,1248)	1:A:101:LEU:HA	1:A:101:LEU:HD22	1	0.08	0.08
(1,1248)	1:A:101:LEU:HA	1:A:101:LEU:HD23	1	0.08	0.08
(1,1243)	1:A:99:GLU:H	1:A:99:GLU:HB2	1	0.01	0.01
(1,1230)	1:A:97:ALA:HA	1:A:101:LEU:HD21	1	0.09	0.09
(1,1230)	1:A:97:ALA:HA	1:A:101:LEU:HD22	1	0.09	0.09
(1,1230)	1:A:97:ALA:HA	1:A:101:LEU:HD23	1	0.09	0.09
(1,1225)	1:A:96:VAL:HG21	1:A:100:HIS:HD2	1	0.1	0.1
(1,1225)	1:A:96:VAL:HG22	1:A:100:HIS:HD2	1	0.1	0.1
(1,1225)	1:A:96:VAL:HG23	1:A:100:HIS:HD2	1	0.1	0.1
(1,1223)	1:A:96:VAL:HG11	1:A:100:HIS:HD2	1	0.01	0.01
(1,1223)	1:A:96:VAL:HG12	1:A:100:HIS:HD2	1	0.01	0.01
(1,1223)	1:A:96:VAL:HG13	1:A:100:HIS:HD2	1	0.01	0.01
(1,1211)	1:A:95:VAL:HG11	1:A:99:GLU:HG2	1	0.53	0.53
(1,1211)	1:A:95:VAL:HG12	1:A:99:GLU:HG2	1	0.53	0.53
(1,1211)	1:A:95:VAL:HG13	1:A:99:GLU:HG2	1	0.53	0.53
(1,1164)	1:A:91:ALA:HA	1:A:94:GLN:HE21	1	0.02	0.02
(1,114)	1:B:20:LYS:HB2	1:A:23:ALA:HB1	1	0.03	0.03
(1,114)	1:B:20:LYS:HB2	1:A:23:ALA:HB2	1	0.03	0.03
(1,114)	1:B:20:LYS:HB2	1:A:23:ALA:HB3	1	0.03	0.03
(1,114)	1:B:20:LYS:HB3	1:A:23:ALA:HB1	1	0.03	0.03
(1,114)	1:B:20:LYS:HB3	1:A:23:ALA:HB2	1	0.03	0.03
(1,114)	1:B:20:LYS:HB3	1:A:23:ALA:HB3	1	0.03	0.03
(1,112)	1:B:19:GLY:HA2	1:A:23:ALA:HB1	1	0.01	0.01
(1,112)	1:B:19:GLY:HA2	1:A:23:ALA:HB2	1	0.01	0.01
(1,112)	1:B:19:GLY:HA2	1:A:23:ALA:HB3	1	0.01	0.01
(1,112)	1:B:19:GLY:HA3	1:A:23:ALA:HB1	1	0.01	0.01
(1,112)	1:B:19:GLY:HA3	1:A:23:ALA:HB2	1	0.01	0.01
(1,112)	1:B:19:GLY:HA3	1:A:23:ALA:HB3	1	0.01	0.01
(1,1092)	1:A:84:GLU:HG2	1:A:86:VAL:H	1	0.04	0.04
(1,1092)	1:A:84:GLU:HG3	1:A:86:VAL:H	1	0.04	0.04
(1,1078)	1:A:82:ALA:HB1	1:A:86:VAL:HB	1	0.04	0.04
(1,1078)	1:A:82:ALA:HB2	1:A:86:VAL:HB	1	0.04	0.04
(1,1078)	1:A:82:ALA:HB3	1:A:86:VAL:HB	1	0.04	0.04
(1,1077)	1:A:82:ALA:HB1	1:A:83:GLY:H	1	0.04	0.04
(1,1077)	1:A:82:ALA:HB2	1:A:83:GLY:H	1	0.04	0.04
(1,1077)	1:A:82:ALA:HB3	1:A:83:GLY:H	1	0.04	0.04

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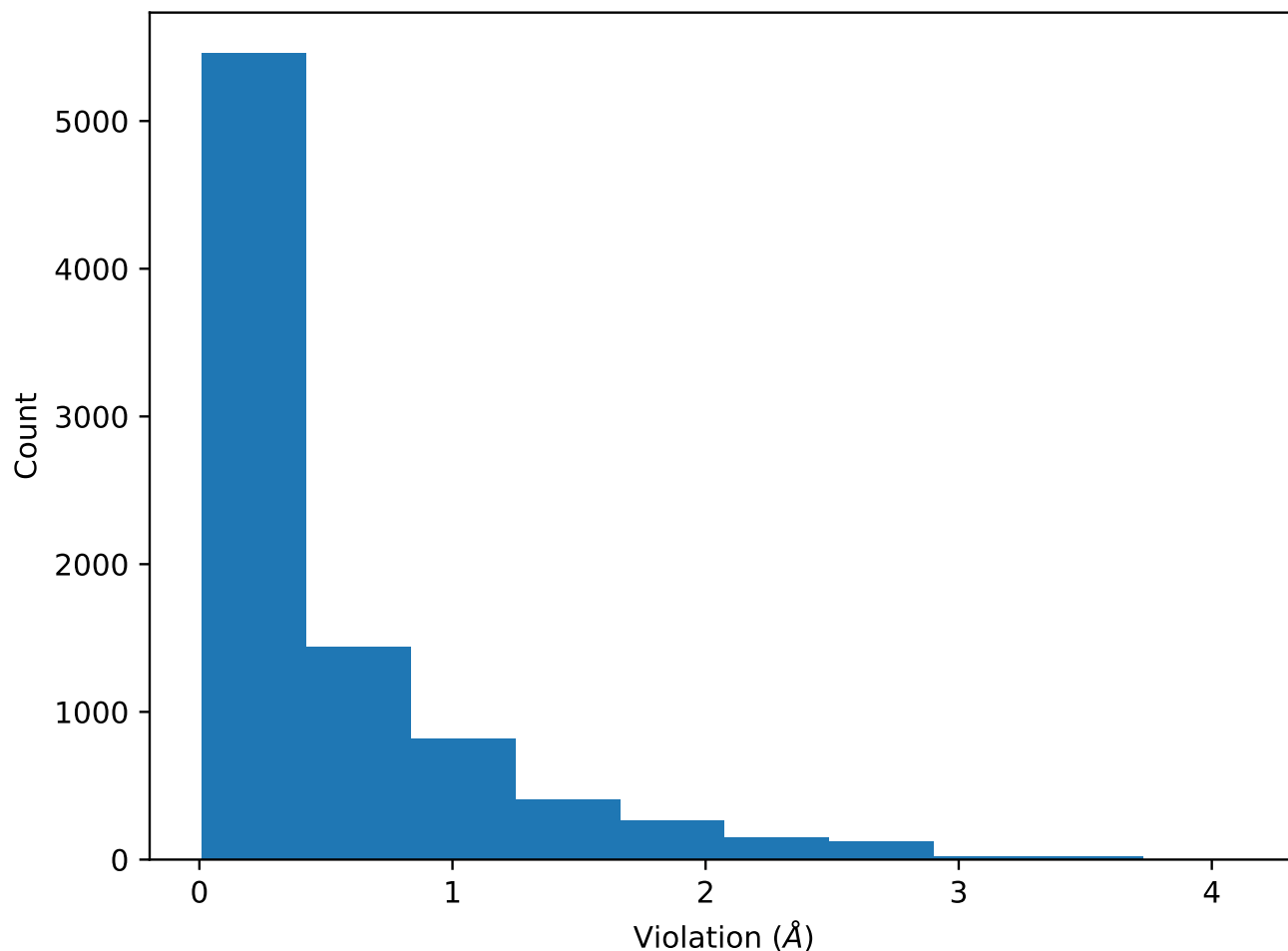
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Key	Atom-1	Atom-2	Models	Mean (Å)	Max (Å)
(1,107)	1:B:16:ALA:H	1:A:28:LEU:HD11	1	0.02	0.02
(1,107)	1:B:16:ALA:H	1:A:28:LEU:HD12	1	0.02	0.02
(1,107)	1:B:16:ALA:H	1:A:28:LEU:HD13	1	0.02	0.02
(1,1042)	1:A:79:TYR:H	1:A:79:TYR:HD1	1	0.35	0.35
(1,1039)	1:A:78:TYR:H	1:A:78:TYR:HD1	1	0.17	0.17
(1,1032)	1:A:77:GLN:HB2	1:A:79:TYR:HE1	1	1.7	1.7
(1,1032)	1:A:77:GLN:HB3	1:A:79:TYR:HE1	1	1.7	1.7
(1,1013)	1:A:76:ARG:HB2	1:A:78:TYR:HD1	1	0.33	0.33
(1,1001)	1:A:73:GLU:H	1:A:78:TYR:HD1	1	1.94	1.94
(1,1)	1:A:11:LEU:HD11	1:B:98:ASP:HA	1	0.31	0.31
(1,1)	1:A:11:LEU:HD12	1:B:98:ASP:HA	1	0.31	0.31
(1,1)	1:A:11:LEU:HD13	1:B:98:ASP:HA	1	0.31	0.31

## 8.8 All distance violations

### 8.8.1 Histogram : Distribution of distance violations

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



### 8.8.2 Table : All distance violations

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

Key	Atom-1	Atom-2	Model	Violation (Å)
(1,574)	1:A:41:VAL:HB	1:A:79:TYR:HE1	11	4.14
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	2	3.81
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	17	3.68
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	18	3.65
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	17	3.59
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	17	3.59
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	10	3.57

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	18	3.47
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	18	3.47
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	7	3.45
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	10	3.44
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	10	3.44
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	10	3.4
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	10	3.4
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	5	3.4
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	4	3.37
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	6	3.35
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	6	3.35
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	2	3.34
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	2	3.34
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	8	3.33
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	8	3.33
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	8	3.33
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	13	3.26
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	2	3.22
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	2	3.22
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	20	3.2
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	2	3.14
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	2	3.14
(1,2127)	1:B:73:GLU:HB2	1:B:78:TYR:HE1	10	3.12
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	17	3.1
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	9	3.1
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	9	3.1
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	4	3.05
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	4	3.05
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	8	3.05
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	8	3.05
(1,2126)	1:B:73:GLU:HB2	1:B:78:TYR:HD1	10	3.01
(1,2125)	1:B:73:GLU:HB2	1:B:76:ARG:HG2	20	3.01
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	4	3.01
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	9	2.99
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	9	2.99
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	12	2.98
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	3	2.96
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	18	2.95
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	20	2.92
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	20	2.92
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	20	2.92
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	10	2.89

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	10	2.89
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	10	2.89
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	3	2.88
(1,2126)	1:B:73:GLU:HB2	1:B:78:TYR:HD1	17	2.88
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	11	2.88
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	16	2.87
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	2	2.87
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	2	2.87
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	2	2.87
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	5	2.87
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	5	2.87
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	14	2.83
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	1	2.8
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	3	2.79
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	3	2.79
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	3	2.79
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	17	2.78
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	17	2.78
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	8	2.78
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	9	2.76
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	7	2.76
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	7	2.76
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	7	2.76
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	7	2.76
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	6	2.76
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	11	2.76
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	11	2.76
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	11	2.76
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	12	2.75
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	12	2.75
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	13	2.75
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	18	2.75
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	18	2.75
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	20	2.74
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	19	2.74
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	16	2.74
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	17	2.73
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	17	2.73
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	18	2.73
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	18	2.73
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	9	2.73
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	5	2.72

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	7	2.72
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	15	2.71
(1,464)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	5	2.7
(1,464)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	5	2.7
(1,464)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	5	2.7
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	20	2.69
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	5	2.69
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	5	2.69
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	9	2.69
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	1	2.68
(1,2127)	1:B:73:GLU:HB2	1:B:78:TYR:HE1	17	2.68
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	11	2.68
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	11	2.68
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	3	2.68
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	3	2.68
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	8	2.68
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	8	2.68
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	8	2.68
(1,2126)	1:B:73:GLU:HB2	1:B:78:TYR:HD1	16	2.67
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	1	2.67
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	1	2.67
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	14	2.67
(1,994)	1:A:73:GLU:HB2	1:A:78:TYR:HD1	18	2.66
(1,2127)	1:B:73:GLU:HB2	1:B:78:TYR:HE1	16	2.66
(1,2126)	1:B:73:GLU:HB2	1:B:78:TYR:HD1	19	2.66
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	13	2.66
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	13	2.66
(1,464)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	17	2.65
(1,464)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	17	2.65
(1,464)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	17	2.65
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	13	2.65
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	13	2.65
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	12	2.64
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	12	2.64
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	12	2.64
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	8	2.63
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	8	2.62
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	8	2.62
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	17	2.62
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	11	2.62
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	3	2.61
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	3	2.61

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	3	2.61
(1,2126)	1:B:73:GLU:HB2	1:B:78:TYR:HD1	3	2.59
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	3	2.58
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	3	2.58
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	4	2.58
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	4	2.58
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	10	2.57
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	1	2.57
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	1	2.57
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	4	2.57
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	4	2.57
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	9	2.57
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	9	2.57
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	9	2.57
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	12	2.57
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	12	2.57
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	12	2.57
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	14	2.57
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	14	2.57
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	14	2.57
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	15	2.56
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	15	2.56
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	11	2.56
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	11	2.56
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	3	2.55
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	3	2.55
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	5	2.54
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	5	2.54
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	2	2.54
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	2	2.54
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	2	2.54
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	20	2.52
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	20	2.52
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	4	2.51
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	16	2.51
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	16	2.51
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	16	2.51
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	16	2.46
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	1	2.45
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	9	2.44
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	7	2.44
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	7	2.44

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,587)	1:A:41:VAL:HG11	1:A:79:TYR:HE1	11	2.41
(1,587)	1:A:41:VAL:HG12	1:A:79:TYR:HE1	11	2.41
(1,587)	1:A:41:VAL:HG13	1:A:79:TYR:HE1	11	2.41
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	17	2.41
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	17	2.41
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	17	2.41
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	8	2.41
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	3	2.41
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	14	2.4
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	14	2.4
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HE21	15	2.4
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HE21	15	2.4
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HE21	15	2.4
(1,1695)	1:B:40:ALA:H	1:B:78:TYR:HE1	5	2.4
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	16	2.39
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	16	2.39
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	3	2.39
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	3	2.39
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	3	2.39
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	12	2.39
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	12	2.39
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	12	2.39
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	1	2.39
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	1	2.39
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	1	2.39
(1,2128)	1:B:73:GLU:HG2	1:B:78:TYR:HD1	17	2.38
(1,2128)	1:B:73:GLU:HG3	1:B:78:TYR:HD1	17	2.38
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	10	2.38
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	10	2.38
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	10	2.38
(1,2125)	1:B:73:GLU:HB2	1:B:76:ARG:HG2	16	2.37
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	14	2.36
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	14	2.36
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	17	2.36
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	9	2.36
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	9	2.36
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	9	2.36
(1,2125)	1:B:73:GLU:HB2	1:B:76:ARG:HG2	10	2.36
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	8	2.35
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	8	2.35
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	1	2.35
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	1	2.35

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	1	2.35
(1,464)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	3	2.33
(1,464)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	3	2.33
(1,464)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	3	2.33
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	2	2.33
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	9	2.33
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	9	2.33
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	18	2.33
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	18	2.33
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	15	2.32
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	15	2.32
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	15	2.32
(1,1695)	1:B:40:ALA:H	1:B:78:TYR:HE1	2	2.32
(1,1695)	1:B:40:ALA:H	1:B:78:TYR:HE1	15	2.32
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	1	2.31
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	1	2.31
(1,596)	1:A:41:VAL:HG21	1:A:79:TYR:HE1	11	2.31
(1,596)	1:A:41:VAL:HG22	1:A:79:TYR:HE1	11	2.31
(1,596)	1:A:41:VAL:HG23	1:A:79:TYR:HE1	11	2.31
(1,1695)	1:B:40:ALA:H	1:B:78:TYR:HE1	8	2.31
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	16	2.3
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	9	2.29
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	9	2.29
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	2	2.29
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	19	2.27
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	19	2.27
(1,464)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	8	2.27
(1,464)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	8	2.27
(1,464)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	8	2.27
(1,1658)	1:B:38:GLU:HG2	1:B:78:TYR:HD1	12	2.27
(1,1658)	1:B:38:GLU:HG3	1:B:78:TYR:HD1	12	2.27
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	17	2.26
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	17	2.26
(1,464)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	15	2.25
(1,464)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	15	2.25
(1,464)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	15	2.25
(1,2125)	1:B:73:GLU:HB2	1:B:76:ARG:HG2	14	2.25
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	15	2.25
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	15	2.25
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	15	2.25
(1,1695)	1:B:40:ALA:H	1:B:78:TYR:HE1	1	2.24
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	17	2.24

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	17	2.24
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	17	2.24
(1,858)	1:A:63:LYS:HB2	1:A:79:TYR:HE1	10	2.23
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	5	2.23
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	5	2.23
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	5	2.23
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	20	2.23
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	20	2.23
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	12	2.23
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	12	2.23
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	6	2.23
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	8	2.22
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	8	2.22
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	12	2.22
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	12	2.22
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	18	2.22
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	18	2.22
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	18	2.22
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	6	2.21
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	16	2.21
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	16	2.21
(1,1658)	1:B:38:GLU:HG2	1:B:78:TYR:HD1	20	2.21
(1,1658)	1:B:38:GLU:HG3	1:B:78:TYR:HD1	20	2.21
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	17	2.2
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	17	2.2
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	12	2.19
(1,595)	1:A:41:VAL:HG21	1:A:79:TYR:HD1	11	2.19
(1,595)	1:A:41:VAL:HG22	1:A:79:TYR:HD1	11	2.19
(1,595)	1:A:41:VAL:HG23	1:A:79:TYR:HD1	11	2.19
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	13	2.18
(1,1695)	1:B:40:ALA:H	1:B:78:TYR:HE1	13	2.17
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	2	2.16
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	2	2.16
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	15	2.16
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	15	2.16
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	15	2.16
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	16	2.15
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	16	2.15
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	16	2.15
(1,2129)	1:B:73:GLU:HG2	1:B:78:TYR:HE1	7	2.14
(1,2129)	1:B:73:GLU:HG3	1:B:78:TYR:HE1	7	2.14
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	19	2.12

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	1	2.12
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	14	2.12
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	14	2.12
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	14	2.12
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	4	2.11
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	15	2.1
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	1	2.1
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	1	2.1
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	5	2.1
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	5	2.1
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	5	2.1
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	5	2.1
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	2	2.09
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	2	2.09
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	2	2.09
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	12	2.08
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	12	2.08
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	12	2.08
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	2	2.08
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	2	2.08
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	2	2.08
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	19	2.07
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	19	2.07
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	10	2.07
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	16	2.07
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	16	2.07
(1,2128)	1:B:73:GLU:HG2	1:B:78:TYR:HD1	16	2.06
(1,2128)	1:B:73:GLU:HG3	1:B:78:TYR:HD1	16	2.06
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	2	2.06
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	2	2.06
(1,1695)	1:B:40:ALA:H	1:B:78:TYR:HE1	9	2.06
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	1	2.06
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	1	2.06
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	1	2.06
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	6	2.05
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	6	2.05
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	10	2.05
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	10	2.05
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	2	2.04
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	7	2.04
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	7	2.04
(1,2126)	1:B:73:GLU:HB2	1:B:78:TYR:HD1	7	2.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	10	2.03
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	10	2.03
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	10	2.03
(1,1695)	1:B:40:ALA:H	1:B:78:TYR:HE1	20	2.03
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	3	2.01
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HE21	5	2.01
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HE21	5	2.01
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HE21	5	2.01
(1,1695)	1:B:40:ALA:H	1:B:78:TYR:HE1	11	2.01
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	9	2.0
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	12	1.99
(1,2125)	1:B:73:GLU:HB2	1:B:76:ARG:HG2	13	1.99
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	8	1.99
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	8	1.98
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	19	1.98
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	19	1.98
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	19	1.98
(1,995)	1:A:73:GLU:HB2	1:A:78:TYR:HE1	18	1.97
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	20	1.97
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	17	1.96
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	17	1.96
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	17	1.96
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	4	1.96
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	4	1.96
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	13	1.96
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	14	1.96
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	14	1.96
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	10	1.95
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	10	1.95
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	10	1.95
(1,1990)	1:B:63:LYS:HB2	1:B:79:TYR:HE1	19	1.95
(1,1695)	1:B:40:ALA:H	1:B:78:TYR:HE1	14	1.95
(1,1694)	1:B:40:ALA:H	1:B:78:TYR:HD1	2	1.95
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	5	1.94
(1,2125)	1:B:73:GLU:HB2	1:B:76:ARG:HG2	17	1.94
(1,1694)	1:B:40:ALA:H	1:B:78:TYR:HD1	5	1.94
(1,1694)	1:B:40:ALA:H	1:B:78:TYR:HD1	15	1.94
(1,1001)	1:A:73:GLU:H	1:A:78:TYR:HD1	18	1.94
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	5	1.93
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	6	1.93
(1,2129)	1:B:73:GLU:HG2	1:B:78:TYR:HE1	17	1.93
(1,2129)	1:B:73:GLU:HG3	1:B:78:TYR:HE1	17	1.93

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	18	1.92
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	18	1.92
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	17	1.91
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	18	1.91
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	18	1.91
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	18	1.91
(1,1658)	1:B:38:GLU:HG2	1:B:78:TYR:HD1	15	1.91
(1,1658)	1:B:38:GLU:HG3	1:B:78:TYR:HD1	15	1.91
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	14	1.91
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	12	1.9
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	12	1.9
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	12	1.9
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	10	1.9
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	10	1.9
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	18	1.9
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	18	1.9
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	18	1.9
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	13	1.9
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	13	1.9
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	13	1.9
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	19	1.9
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	19	1.9
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	19	1.9
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	2	1.9
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	9	1.9
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	18	1.9
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	17	1.89
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	13	1.89
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	13	1.89
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	13	1.89
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	5	1.89
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	5	1.89
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	5	1.89
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	13	1.88
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	13	1.88
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	13	1.88
(1,471)	1:A:33:LEU:HD11	1:A:44:ILE:H	10	1.88
(1,471)	1:A:33:LEU:HD12	1:A:44:ILE:H	10	1.88
(1,471)	1:A:33:LEU:HD13	1:A:44:ILE:H	10	1.88
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	20	1.88
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	13	1.87
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	13	1.87

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	11	1.87
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	11	1.87
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	11	1.87
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	15	1.86
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	15	1.86
(1,1695)	1:B:40:ALA:H	1:B:78:TYR:HE1	12	1.86
(1,471)	1:A:33:LEU:HD11	1:A:44:ILE:H	20	1.85
(1,471)	1:A:33:LEU:HD12	1:A:44:ILE:H	20	1.85
(1,471)	1:A:33:LEU:HD13	1:A:44:ILE:H	20	1.85
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	6	1.85
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	6	1.85
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	6	1.85
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	20	1.85
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	20	1.85
(1,1694)	1:B:40:ALA:H	1:B:78:TYR:HD1	13	1.85
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	7	1.84
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	15	1.84
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG2	19	1.83
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	10	1.83
(1,2127)	1:B:73:GLU:HB2	1:B:78:TYR:HE1	7	1.83
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	13	1.83
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	13	1.83
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	7	1.82
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	7	1.82
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	7	1.82
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	7	1.82
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	7	1.82
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	4	1.81
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	4	1.81
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	4	1.81
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	7	1.81
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	7	1.81
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	7	1.81
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	10	1.81
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	10	1.81
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	4	1.81
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	4	1.81
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	4	1.81
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	12	1.81
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	18	1.8
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	18	1.8
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	18	1.8

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG2	20	1.8
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	2	1.8
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	7	1.8
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	7	1.8
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	7	1.8
(1,471)	1:A:33:LEU:HD11	1:A:44:ILE:H	2	1.79
(1,471)	1:A:33:LEU:HD12	1:A:44:ILE:H	2	1.79
(1,471)	1:A:33:LEU:HD13	1:A:44:ILE:H	2	1.79
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	5	1.79
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	5	1.79
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	5	1.79
(1,1694)	1:B:40:ALA:H	1:B:78:TYR:HD1	12	1.79
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	6	1.79
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	6	1.79
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	6	1.79
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	10	1.79
(1,872)	1:A:63:LYS:HG2	1:A:79:TYR:HE1	20	1.78
(1,872)	1:A:63:LYS:HG3	1:A:79:TYR:HE1	20	1.78
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	8	1.78
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	1	1.78
(1,2128)	1:B:73:GLU:HG2	1:B:78:TYR:HD1	10	1.78
(1,2128)	1:B:73:GLU:HG3	1:B:78:TYR:HD1	10	1.78
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	10	1.78
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	10	1.78
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	8	1.77
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	13	1.77
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	13	1.77
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	13	1.77
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	14	1.77
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	14	1.77
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	14	1.77
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	20	1.77
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	20	1.77
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	20	1.77
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	6	1.77
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	6	1.77
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	5	1.77
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	5	1.77
(1,2127)	1:B:73:GLU:HB2	1:B:78:TYR:HE1	3	1.76
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	6	1.75
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	6	1.75
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	6	1.75

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	20	1.75
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	20	1.75
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	20	1.75
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	13	1.75
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	19	1.75
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	14	1.74
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	14	1.74
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	14	1.74
(1,471)	1:A:33:LEU:HD11	1:A:44:ILE:H	13	1.74
(1,471)	1:A:33:LEU:HD12	1:A:44:ILE:H	13	1.74
(1,471)	1:A:33:LEU:HD13	1:A:44:ILE:H	13	1.74
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	1	1.74
(1,2129)	1:B:73:GLU:HG2	1:B:78:TYR:HE1	16	1.74
(1,2129)	1:B:73:GLU:HG3	1:B:78:TYR:HE1	16	1.74
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	3	1.74
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	3	1.74
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	3	1.74
(1,1694)	1:B:40:ALA:H	1:B:78:TYR:HD1	8	1.74
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	11	1.73
(1,471)	1:A:33:LEU:HD11	1:A:44:ILE:H	1	1.73
(1,471)	1:A:33:LEU:HD12	1:A:44:ILE:H	1	1.73
(1,471)	1:A:33:LEU:HD13	1:A:44:ILE:H	1	1.73
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	15	1.73
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	15	1.73
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	15	1.73
(1,1658)	1:B:38:GLU:HG2	1:B:78:TYR:HD1	13	1.73
(1,1658)	1:B:38:GLU:HG3	1:B:78:TYR:HD1	13	1.73
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	4	1.72
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	4	1.72
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	4	1.72
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	17	1.72
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	17	1.72
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	17	1.72
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	10	1.72
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	5	1.72
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	5	1.72
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	5	1.72
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	7	1.72
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	7	1.72
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	14	1.72
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	14	1.72
(1,1695)	1:B:40:ALA:H	1:B:78:TYR:HE1	6	1.72

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1694)	1:B:40:ALA:H	1:B:78:TYR:HD1	1	1.72
(1,1694)	1:B:40:ALA:H	1:B:78:TYR:HD1	20	1.72
(1,987)	1:A:72:ARG:HD2	1:A:77:GLN:HG2	6	1.71
(1,987)	1:A:72:ARG:HD3	1:A:77:GLN:HG2	6	1.71
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG2	13	1.71
(1,67)	1:B:11:LEU:HD11	1:A:98:ASP:H	10	1.71
(1,67)	1:B:11:LEU:HD12	1:A:98:ASP:H	10	1.71
(1,67)	1:B:11:LEU:HD13	1:A:98:ASP:H	10	1.71
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	3	1.71
(1,987)	1:A:72:ARG:HD2	1:A:77:GLN:HG2	16	1.7
(1,987)	1:A:72:ARG:HD3	1:A:77:GLN:HG2	16	1.7
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	16	1.7
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	16	1.7
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	16	1.7
(1,1694)	1:B:40:ALA:H	1:B:78:TYR:HD1	9	1.7
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	12	1.7
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	12	1.7
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	12	1.7
(1,1032)	1:A:77:GLN:HB2	1:A:79:TYR:HE1	11	1.7
(1,1032)	1:A:77:GLN:HB3	1:A:79:TYR:HE1	11	1.7
(1,997)	1:A:73:GLU:HG2	1:A:78:TYR:HE1	18	1.69
(1,997)	1:A:73:GLU:HG3	1:A:78:TYR:HE1	18	1.69
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	1	1.69
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	14	1.69
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	6	1.69
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	6	1.69
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	3	1.68
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	3	1.68
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	3	1.68
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	19	1.68
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	19	1.68
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	19	1.68
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	19	1.68
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	19	1.68
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	17	1.68
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	17	1.68
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	17	1.68
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	15	1.67
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	5	1.66
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	5	1.66
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	5	1.66
(1,996)	1:A:73:GLU:HG2	1:A:78:TYR:HD1	18	1.65

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,996)	1:A:73:GLU:HG3	1:A:78:TYR:HD1	18	1.65
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	1	1.65
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	1	1.65
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	1	1.65
(1,839)	1:A:62:LEU:HB2	1:A:67:LEU:HD21	15	1.65
(1,839)	1:A:62:LEU:HB2	1:A:67:LEU:HD22	15	1.65
(1,839)	1:A:62:LEU:HB2	1:A:67:LEU:HD23	15	1.65
(1,67)	1:B:11:LEU:HD11	1:A:98:ASP:H	16	1.65
(1,67)	1:B:11:LEU:HD12	1:A:98:ASP:H	16	1.65
(1,67)	1:B:11:LEU:HD13	1:A:98:ASP:H	16	1.65
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	12	1.65
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	13	1.64
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	13	1.64
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	13	1.64
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	4	1.64
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	4	1.64
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD11	18	1.64
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD12	18	1.64
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD13	18	1.64
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	15	1.64
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	4	1.64
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	4	1.64
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	4	1.64
(1,2128)	1:B:73:GLU:HG2	1:B:78:TYR:HD1	7	1.63
(1,2128)	1:B:73:GLU:HG3	1:B:78:TYR:HD1	7	1.63
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	18	1.63
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	18	1.63
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	18	1.63
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	17	1.63
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	17	1.63
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	17	1.63
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	9	1.63
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	9	1.63
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	9	1.63
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	10	1.63
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	10	1.63
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	10	1.63
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	17	1.63
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	9	1.62
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	9	1.62
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	9	1.62
(1,839)	1:A:62:LEU:HB2	1:A:67:LEU:HD21	14	1.62

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,839)	1:A:62:LEU:HB2	1:A:67:LEU:HD22	14	1.62
(1,839)	1:A:62:LEU:HB2	1:A:67:LEU:HD23	14	1.62
(1,467)	1:A:33:LEU:HD11	1:A:39:ARG:HD2	17	1.62
(1,467)	1:A:33:LEU:HD12	1:A:39:ARG:HD2	17	1.62
(1,467)	1:A:33:LEU:HD13	1:A:39:ARG:HD2	17	1.62
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	8	1.61
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	8	1.61
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	8	1.61
(1,2101)	1:B:71:ARG:HB2	1:B:79:TYR:HA	2	1.61
(1,987)	1:A:72:ARG:HD2	1:A:77:GLN:HG2	10	1.6
(1,987)	1:A:72:ARG:HD3	1:A:77:GLN:HG2	10	1.6
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	5	1.6
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	5	1.6
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	5	1.6
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	6	1.6
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	6	1.6
(1,473)	1:A:33:LEU:HD11	1:A:47:ALA:H	13	1.6
(1,473)	1:A:33:LEU:HD12	1:A:47:ALA:H	13	1.6
(1,473)	1:A:33:LEU:HD13	1:A:47:ALA:H	13	1.6
(1,1971)	1:B:62:LEU:HB2	1:B:67:LEU:HD21	3	1.6
(1,1971)	1:B:62:LEU:HB2	1:B:67:LEU:HD22	3	1.6
(1,1971)	1:B:62:LEU:HB2	1:B:67:LEU:HD23	3	1.6
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	1	1.6
(1,987)	1:A:72:ARG:HD2	1:A:77:GLN:HG2	5	1.59
(1,987)	1:A:72:ARG:HD3	1:A:77:GLN:HG2	5	1.59
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	3	1.59
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	3	1.59
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	3	1.59
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	14	1.59
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	14	1.59
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	14	1.59
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	12	1.59
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD11	9	1.59
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD12	9	1.59
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD13	9	1.59
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	15	1.58
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	15	1.58
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	11	1.58
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	6	1.58
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	6	1.58
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	6	1.58
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	16	1.58

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	16	1.58
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	16	1.58
(1,328)	1:A:27:ARG:HD2	1:A:58:ASN:HA	16	1.58
(1,2125)	1:B:73:GLU:HB2	1:B:76:ARG:HG2	5	1.58
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	4	1.58
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	4	1.58
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	4	1.58
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	11	1.58
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	11	1.58
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	11	1.58
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	2	1.57
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	20	1.57
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	20	1.57
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	20	1.57
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	12	1.57
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	12	1.57
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	12	1.57
(1,1594)	1:B:33:LEU:HD11	1:B:36:GLN:HB2	16	1.57
(1,1594)	1:B:33:LEU:HD12	1:B:36:GLN:HB2	16	1.57
(1,1594)	1:B:33:LEU:HD13	1:B:36:GLN:HB2	16	1.57
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	16	1.56
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	16	1.56
(1,1694)	1:B:40:ALA:H	1:B:78:TYR:HD1	11	1.56
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	7	1.55
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	9	1.55
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	15	1.55
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	15	1.55
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	14	1.54
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	8	1.54
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	8	1.54
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	8	1.54
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	18	1.54
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	18	1.54
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	18	1.54
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	10	1.54
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	10	1.54
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	10	1.54
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD11	10	1.54
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD12	10	1.54
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD13	10	1.54
(1,2133)	1:B:73:GLU:H	1:B:78:TYR:HD1	10	1.54
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	1	1.54

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	1	1.54
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	1	1.54
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	11	1.53
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	11	1.53
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	11	1.53
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	16	1.53
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	16	1.53
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	16	1.53
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	1	1.53
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	1	1.53
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	1	1.53
(1,1694)	1:B:40:ALA:H	1:B:78:TYR:HD1	14	1.53
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	5	1.53
(1,67)	1:B:11:LEU:HD11	1:A:98:ASP:H	17	1.52
(1,67)	1:B:11:LEU:HD12	1:A:98:ASP:H	17	1.52
(1,67)	1:B:11:LEU:HD13	1:A:98:ASP:H	17	1.52
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	11	1.52
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	11	1.52
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	15	1.51
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	15	1.51
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	15	1.51
(1,525)	1:A:38:GLU:HG2	1:A:78:TYR:HB2	7	1.51
(1,525)	1:A:38:GLU:HG3	1:A:78:TYR:HB2	7	1.51
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	13	1.51
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	13	1.51
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	13	1.51
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	9	1.51
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	9	1.51
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	9	1.51
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	8	1.51
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	8	1.51
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	8	1.51
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	16	1.5
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	16	1.5
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	16	1.5
(1,507)	1:A:35:ALA:HB1	1:A:90:PHE:HE1	7	1.5
(1,507)	1:A:35:ALA:HB2	1:A:90:PHE:HE1	7	1.5
(1,507)	1:A:35:ALA:HB3	1:A:90:PHE:HE1	7	1.5
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	17	1.5
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	17	1.5
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	17	1.5
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	19	1.5

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	19	1.5
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	19	1.5
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	9	1.5
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	9	1.5
(1,1747)	1:B:42:GLU:HG2	1:B:52:LEU:HG	4	1.5
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	7	1.5
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	7	1.5
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	7	1.5
(1,2133)	1:B:73:GLU:H	1:B:78:TYR:HD1	17	1.49
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	3	1.49
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	3	1.49
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	3	1.49
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	14	1.49
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	6	1.48
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	6	1.48
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	6	1.48
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	9	1.48
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	9	1.48
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	9	1.48
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	20	1.47
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	20	1.47
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	20	1.47
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	20	1.47
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	3	1.47
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	3	1.47
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	11	1.47
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	1	1.47
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	1	1.47
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	1	1.47
(1,2004)	1:B:63:LYS:HG2	1:B:79:TYR:HE1	19	1.47
(1,2004)	1:B:63:LYS:HG3	1:B:79:TYR:HE1	19	1.47
(1,1695)	1:B:40:ALA:H	1:B:78:TYR:HE1	4	1.47
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	4	1.47
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	1	1.46
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	1	1.46
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	7	1.46
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	7	1.46
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	7	1.46
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	8	1.46
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	8	1.46
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG2	17	1.45
(1,473)	1:A:33:LEU:HD11	1:A:47:ALA:H	2	1.45

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,473)	1:A:33:LEU:HD12	1:A:47:ALA:H	2	1.45
(1,473)	1:A:33:LEU:HD13	1:A:47:ALA:H	2	1.45
(1,1658)	1:B:38:GLU:HG2	1:B:78:TYR:HD1	5	1.45
(1,1658)	1:B:38:GLU:HG3	1:B:78:TYR:HD1	5	1.45
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	4	1.44
(1,2133)	1:B:73:GLU:H	1:B:78:TYR:HD1	3	1.44
(1,2119)	1:B:72:ARG:HD2	1:B:77:GLN:HG2	13	1.44
(1,2119)	1:B:72:ARG:HD3	1:B:77:GLN:HG2	13	1.44
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB1	6	1.44
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB2	6	1.44
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB3	6	1.44
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB1	6	1.44
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB2	6	1.44
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB3	6	1.44
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB1	6	1.44
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB2	6	1.44
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB3	6	1.44
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	12	1.43
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	12	1.43
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG2	2	1.43
(1,2104)	1:B:71:ARG:HG2	1:B:78:TYR:HB2	14	1.43
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	4	1.43
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	4	1.43
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	4	1.43
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	4	1.43
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	4	1.43
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	4	1.43
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	15	1.43
(1,467)	1:A:33:LEU:HD11	1:A:39:ARG:HD2	20	1.42
(1,467)	1:A:33:LEU:HD12	1:A:39:ARG:HD2	20	1.42
(1,467)	1:A:33:LEU:HD13	1:A:39:ARG:HD2	20	1.42
(1,4)	1:A:11:LEU:HD11	1:B:98:ASP:H	3	1.42
(1,4)	1:A:11:LEU:HD12	1:B:98:ASP:H	3	1.42
(1,4)	1:A:11:LEU:HD13	1:B:98:ASP:H	3	1.42
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	4	1.42
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	4	1.42
(1,1658)	1:B:38:GLU:HG2	1:B:78:TYR:HD1	2	1.42
(1,1658)	1:B:38:GLU:HG3	1:B:78:TYR:HD1	2	1.42
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	19	1.41
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	19	1.41
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	19	1.41
(1,2119)	1:B:72:ARG:HD2	1:B:77:GLN:HG2	14	1.4

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2119)	1:B:72:ARG:HD3	1:B:77:GLN:HG2	14	1.4
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	14	1.4
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	14	1.4
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	14	1.4
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	14	1.4
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	14	1.4
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	14	1.4
(1,1694)	1:B:40:ALA:H	1:B:78:TYR:HD1	6	1.4
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	13	1.39
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	13	1.39
(1,2133)	1:B:73:GLU:H	1:B:78:TYR:HD1	16	1.39
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	13	1.39
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	1	1.38
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	1	1.38
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	9	1.38
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	9	1.38
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	9	1.38
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	17	1.38
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	17	1.38
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	17	1.38
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD11	3	1.38
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD12	3	1.38
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD13	3	1.38
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	19	1.38
(1,486)	1:A:34:LEU:HB2	1:A:80:ARG:HA	16	1.38
(1,1695)	1:B:40:ALA:H	1:B:78:TYR:HE1	18	1.38
(1,987)	1:A:72:ARG:HD2	1:A:77:GLN:HG2	20	1.37
(1,987)	1:A:72:ARG:HD3	1:A:77:GLN:HG2	20	1.37
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	20	1.37
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	20	1.37
(1,1657)	1:B:38:GLU:HG2	1:B:78:TYR:HB2	20	1.37
(1,1657)	1:B:38:GLU:HG3	1:B:78:TYR:HB2	20	1.37
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	9	1.36
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	9	1.36
(1,1747)	1:B:42:GLU:HG2	1:B:52:LEU:HG	3	1.36
(1,1599)	1:B:33:LEU:HD11	1:B:39:ARG:HD2	16	1.36
(1,1599)	1:B:33:LEU:HD12	1:B:39:ARG:HD2	16	1.36
(1,1599)	1:B:33:LEU:HD13	1:B:39:ARG:HD2	16	1.36
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD11	14	1.36
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD12	14	1.36
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD13	14	1.36
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	7	1.35

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	7	1.35
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	7	1.35
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	10	1.34
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	10	1.34
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	10	1.34
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HE21	12	1.34
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HE21	12	1.34
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HE21	12	1.34
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	1	1.33
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	1	1.33
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	1	1.33
(1,672)	1:A:45:ALA:H	1:A:52:LEU:HD11	14	1.33
(1,672)	1:A:45:ALA:H	1:A:52:LEU:HD12	14	1.33
(1,672)	1:A:45:ALA:H	1:A:52:LEU:HD13	14	1.33
(1,563)	1:A:40:ALA:H	1:A:78:TYR:HE1	14	1.33
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	19	1.33
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	16	1.33
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	16	1.33
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	16	1.33
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	18	1.33
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	18	1.33
(1,1694)	1:B:40:ALA:H	1:B:78:TYR:HD1	4	1.33
(1,1657)	1:B:38:GLU:HG2	1:B:78:TYR:HB2	7	1.33
(1,1657)	1:B:38:GLU:HG3	1:B:78:TYR:HB2	7	1.33
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	18	1.32
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	18	1.32
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	18	1.32
(1,471)	1:A:33:LEU:HD11	1:A:44:ILE:H	9	1.32
(1,471)	1:A:33:LEU:HD12	1:A:44:ILE:H	9	1.32
(1,471)	1:A:33:LEU:HD13	1:A:44:ILE:H	9	1.32
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	6	1.32
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	6	1.32
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	6	1.32
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	12	1.32
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	12	1.32
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	11	1.32
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	3	1.31
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	3	1.31
(1,312)	1:A:25:GLY:HA2	1:A:28:LEU:HB2	6	1.31
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	15	1.31
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	15	1.31
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	15	1.31

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	1	1.31
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	1	1.31
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD11	8	1.31
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD12	8	1.31
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD13	8	1.31
(1,1747)	1:B:42:GLU:HG2	1:B:52:LEU:HG	13	1.31
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	11	1.31
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	11	1.31
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	11	1.31
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD11	17	1.3
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD12	17	1.3
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD13	17	1.3
(1,475)	1:A:33:LEU:HG	1:A:36:GLN:HE21	12	1.3
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	13	1.3
(1,2057)	1:B:68:VAL:HG21	1:B:79:TYR:HD1	8	1.3
(1,2057)	1:B:68:VAL:HG22	1:B:79:TYR:HD1	8	1.3
(1,2057)	1:B:68:VAL:HG23	1:B:79:TYR:HD1	8	1.3
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	15	1.29
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	15	1.29
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	15	1.29
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD11	1	1.29
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD12	1	1.29
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD13	1	1.29
(1,471)	1:A:33:LEU:HD11	1:A:44:ILE:H	19	1.29
(1,471)	1:A:33:LEU:HD12	1:A:44:ILE:H	19	1.29
(1,471)	1:A:33:LEU:HD13	1:A:44:ILE:H	19	1.29
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	5	1.28
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	5	1.28
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	15	1.28
(1,2127)	1:B:73:GLU:HB2	1:B:78:TYR:HE1	19	1.28
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD11	9	1.27
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD12	9	1.27
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD13	9	1.27
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	16	1.27
(1,1747)	1:B:42:GLU:HG2	1:B:52:LEU:HG	2	1.27
(1,1658)	1:B:38:GLU:HG2	1:B:78:TYR:HD1	11	1.27
(1,1658)	1:B:38:GLU:HG3	1:B:78:TYR:HD1	11	1.27
(1,2129)	1:B:73:GLU:HG2	1:B:78:TYR:HE1	10	1.26
(1,2129)	1:B:73:GLU:HG3	1:B:78:TYR:HE1	10	1.26
(1,2104)	1:B:71:ARG:HG2	1:B:78:TYR:HB2	7	1.26
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD11	12	1.26
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD12	12	1.26

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD13	12	1.26
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	14	1.26
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	14	1.26
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	14	1.26
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	3	1.26
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	3	1.26
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	3	1.26
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	19	1.26
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	19	1.26
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	19	1.26
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	14	1.25
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	14	1.25
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	14	1.25
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	5	1.25
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	5	1.25
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	8	1.25
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	8	1.25
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	8	1.25
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	4	1.25
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	4	1.25
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	4	1.25
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD11	4	1.25
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD12	4	1.25
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD13	4	1.25
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	17	1.24
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	17	1.24
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	17	1.24
(1,525)	1:A:38:GLU:HG2	1:A:78:TYR:HB2	10	1.24
(1,525)	1:A:38:GLU:HG3	1:A:78:TYR:HB2	10	1.24
(1,471)	1:A:33:LEU:HD11	1:A:44:ILE:H	14	1.24
(1,471)	1:A:33:LEU:HD12	1:A:44:ILE:H	14	1.24
(1,471)	1:A:33:LEU:HD13	1:A:44:ILE:H	14	1.24
(1,2125)	1:B:73:GLU:HB2	1:B:76:ARG:HG2	1	1.24
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	9	1.24
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	9	1.24
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	9	1.24
(1,1694)	1:B:40:ALA:H	1:B:78:TYR:HD1	18	1.24
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	19	1.24
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	11	1.22
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	11	1.22
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	14	1.22
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	14	1.22

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD21	6	1.22
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD22	6	1.22
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD23	6	1.22
(1,2191)	1:B:81:ILE:HG12	1:B:87:ALA:HA	5	1.22
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	19	1.22
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	19	1.22
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	19	1.22
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	7	1.22
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	7	1.22
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	7	1.22
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	2	1.21
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	2	1.21
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB1	2	1.21
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB2	2	1.21
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB3	2	1.21
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB1	2	1.21
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB2	2	1.21
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB3	2	1.21
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB1	2	1.21
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB2	2	1.21
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB3	2	1.21
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	9	1.21
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	9	1.21
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	9	1.21
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	17	1.21
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	17	1.21
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	17	1.21
(1,1658)	1:B:38:GLU:HG2	1:B:78:TYR:HD1	9	1.21
(1,1658)	1:B:38:GLU:HG3	1:B:78:TYR:HD1	9	1.21
(1,1639)	1:B:35:ALA:HB1	1:B:90:PHE:HE1	20	1.21
(1,1639)	1:B:35:ALA:HB2	1:B:90:PHE:HE1	20	1.21
(1,1639)	1:B:35:ALA:HB3	1:B:90:PHE:HE1	20	1.21
(1,615)	1:A:42:GLU:HG2	1:A:52:LEU:HG	7	1.2
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	13	1.2
(1,2119)	1:B:72:ARG:HD2	1:B:77:GLN:HG2	16	1.2
(1,2119)	1:B:72:ARG:HD3	1:B:77:GLN:HG2	16	1.2
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	18	1.2
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	18	1.2
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	18	1.2
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	12	1.2
(1,615)	1:A:42:GLU:HG2	1:A:52:LEU:HG	14	1.19
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	17	1.19

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2058)	1:B:68:VAL:HG21	1:B:79:TYR:HE1	12	1.19
(1,2058)	1:B:68:VAL:HG22	1:B:79:TYR:HE1	12	1.19
(1,2058)	1:B:68:VAL:HG23	1:B:79:TYR:HE1	12	1.19
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB1	16	1.18
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB2	16	1.18
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB3	16	1.18
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB1	16	1.18
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB2	16	1.18
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB3	16	1.18
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB1	16	1.18
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB2	16	1.18
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB3	16	1.18
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	8	1.18
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	8	1.18
(1,470)	1:A:33:LEU:HD11	1:A:44:ILE:HA	20	1.18
(1,470)	1:A:33:LEU:HD12	1:A:44:ILE:HA	20	1.18
(1,470)	1:A:33:LEU:HD13	1:A:44:ILE:HA	20	1.18
(1,2154)	1:B:76:ARG:HG2	1:B:78:TYR:HE1	10	1.18
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	1	1.18
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	1	1.18
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	1	1.18
(1,470)	1:A:33:LEU:HD11	1:A:44:ILE:HA	13	1.17
(1,470)	1:A:33:LEU:HD12	1:A:44:ILE:HA	13	1.17
(1,470)	1:A:33:LEU:HD13	1:A:44:ILE:HA	13	1.17
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	8	1.17
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	8	1.17
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	8	1.17
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB1	10	1.17
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB2	10	1.17
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB3	10	1.17
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB1	10	1.17
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB2	10	1.17
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB3	10	1.17
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB1	10	1.17
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB2	10	1.17
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB3	10	1.17
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	1	1.17
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	1	1.17
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	1	1.17
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	6	1.16
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	6	1.16
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	6	1.16

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	9	1.16
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	10	1.15
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	10	1.15
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	10	1.15
(1,925)	1:A:68:VAL:HG21	1:A:79:TYR:HD1	2	1.15
(1,925)	1:A:68:VAL:HG22	1:A:79:TYR:HD1	2	1.15
(1,925)	1:A:68:VAL:HG23	1:A:79:TYR:HD1	2	1.15
(1,471)	1:A:33:LEU:HD11	1:A:44:ILE:H	6	1.15
(1,471)	1:A:33:LEU:HD12	1:A:44:ILE:H	6	1.15
(1,471)	1:A:33:LEU:HD13	1:A:44:ILE:H	6	1.15
(1,1971)	1:B:62:LEU:HB2	1:B:67:LEU:HD21	14	1.15
(1,1971)	1:B:62:LEU:HB2	1:B:67:LEU:HD22	14	1.15
(1,1971)	1:B:62:LEU:HB2	1:B:67:LEU:HD23	14	1.15
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	13	1.15
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	13	1.15
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	13	1.15
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	8	1.15
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	8	1.15
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	8	1.15
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	8	1.15
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	8	1.15
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	8	1.15
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	8	1.15
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	8	1.15
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	8	1.15
(1,1607)	1:B:33:LEU:HG	1:B:36:GLN:HE21	10	1.15
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB1	1	1.15
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB2	1	1.15
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB3	1	1.15
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB1	1	1.15
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB2	1	1.15
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB3	1	1.15
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB1	1	1.15
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB2	1	1.15
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB3	1	1.15
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	6	1.15
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD21	14	1.15
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD22	14	1.15
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD23	14	1.15
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB1	7	1.14
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB2	7	1.14
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB3	7	1.14

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB1	7	1.14
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB2	7	1.14
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB3	7	1.14
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB1	7	1.14
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB2	7	1.14
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB3	7	1.14
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	6	1.14
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	6	1.14
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	6	1.14
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	19	1.14
(1,2128)	1:B:73:GLU:HG2	1:B:78:TYR:HD1	19	1.14
(1,2128)	1:B:73:GLU:HG3	1:B:78:TYR:HD1	19	1.14
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB1	13	1.14
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB2	13	1.14
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB3	13	1.14
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB1	13	1.14
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB2	13	1.14
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB3	13	1.14
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB1	13	1.14
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB2	13	1.14
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB3	13	1.14
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD11	19	1.14
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD12	19	1.14
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD13	19	1.14
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	16	1.14
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	16	1.14
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	16	1.14
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	2	1.14
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	2	1.14
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	2	1.14
(1,1595)	1:B:33:LEU:HD11	1:B:36:GLN:HE21	16	1.14
(1,1595)	1:B:33:LEU:HD12	1:B:36:GLN:HE21	16	1.14
(1,1595)	1:B:33:LEU:HD13	1:B:36:GLN:HE21	16	1.14
(1,1002)	1:A:74:GLY:HA2	1:A:75:THR:HB	14	1.14
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD11	2	1.13
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD12	2	1.13
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD13	2	1.13
(1,475)	1:A:33:LEU:HG	1:A:36:GLN:HE21	6	1.13
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB1	10	1.13
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB2	10	1.13
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB3	10	1.13
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB1	10	1.13

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB2	10	1.13
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB3	10	1.13
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB1	10	1.13
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB2	10	1.13
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB3	10	1.13
(1,471)	1:A:33:LEU:HD11	1:A:44:ILE:H	16	1.12
(1,471)	1:A:33:LEU:HD12	1:A:44:ILE:H	16	1.12
(1,471)	1:A:33:LEU:HD13	1:A:44:ILE:H	16	1.12
(1,470)	1:A:33:LEU:HD11	1:A:44:ILE:HA	2	1.12
(1,470)	1:A:33:LEU:HD12	1:A:44:ILE:HA	2	1.12
(1,470)	1:A:33:LEU:HD13	1:A:44:ILE:HA	2	1.12
(1,330)	1:A:27:ARG:HD2	1:A:62:LEU:H	2	1.12
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	9	1.12
(1,2133)	1:B:73:GLU:H	1:B:78:TYR:HD1	19	1.12
(1,2101)	1:B:71:ARG:HB2	1:B:79:TYR:HA	18	1.12
(1,1971)	1:B:62:LEU:HB2	1:B:67:LEU:HD21	13	1.12
(1,1971)	1:B:62:LEU:HB2	1:B:67:LEU:HD22	13	1.12
(1,1971)	1:B:62:LEU:HB2	1:B:67:LEU:HD23	13	1.12
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB2	1	1.12
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB3	1	1.12
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB2	1	1.12
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB3	1	1.12
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB2	1	1.12
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB3	1	1.12
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	8	1.12
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	8	1.12
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	8	1.12
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB1	10	1.12
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB2	10	1.12
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB3	10	1.12
(1,464)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	12	1.11
(1,464)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	12	1.11
(1,464)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	12	1.11
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG21	10	1.11
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG22	10	1.11
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG23	10	1.11
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD11	6	1.11
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD12	6	1.11
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD13	6	1.11
(1,1462)	1:B:27:ARG:HD2	1:B:62:LEU:H	9	1.11
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD21	17	1.11
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD22	17	1.11

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD23	17	1.11
(1,1444)	1:B:25:GLY:HA2	1:B:28:LEU:HB2	11	1.11
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB1	14	1.1
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB2	14	1.1
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB3	14	1.1
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB1	14	1.1
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB2	14	1.1
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB3	14	1.1
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB1	14	1.1
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB2	14	1.1
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB3	14	1.1
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD11	5	1.1
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD12	5	1.1
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD13	5	1.1
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HE21	17	1.1
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HE21	17	1.1
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HE21	17	1.1
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	7	1.1
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB1	6	1.1
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB2	6	1.1
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB3	6	1.1
(1,2154)	1:B:76:ARG:HG2	1:B:78:TYR:HE1	19	1.1
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	9	1.1
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	9	1.1
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	9	1.1
(1,926)	1:A:68:VAL:HG21	1:A:79:TYR:HE1	2	1.09
(1,926)	1:A:68:VAL:HG22	1:A:79:TYR:HE1	2	1.09
(1,926)	1:A:68:VAL:HG23	1:A:79:TYR:HE1	2	1.09
(1,562)	1:A:40:ALA:H	1:A:78:TYR:HD1	14	1.09
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	2	1.09
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	2	1.09
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB1	8	1.09
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB2	8	1.09
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB3	8	1.09
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB1	8	1.09
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB2	8	1.09
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB3	8	1.09
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB1	8	1.09
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB2	8	1.09
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB3	8	1.09
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD11	2	1.09
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD12	2	1.09

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD13	2	1.09
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	13	1.09
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	13	1.09
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	13	1.09
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	20	1.09
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	20	1.09
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	20	1.09
(1,1596)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	18	1.09
(1,1596)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	18	1.09
(1,1596)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	18	1.09
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	4	1.08
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	4	1.08
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	4	1.08
(1,464)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	19	1.08
(1,464)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	19	1.08
(1,464)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	19	1.08
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	18	1.08
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	20	1.08
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	20	1.08
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	20	1.08
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB1	20	1.08
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB2	20	1.08
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB3	20	1.08
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB1	20	1.08
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB2	20	1.08
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB3	20	1.08
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB1	20	1.08
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB2	20	1.08
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB3	20	1.08
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	12	1.08
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	12	1.08
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	12	1.08
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	18	1.08
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	18	1.08
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	18	1.08
(1,1596)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	16	1.08
(1,1596)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	16	1.08
(1,1596)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	16	1.08
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	7	1.07
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	7	1.07
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	7	1.07
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	12	1.07

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	12	1.07
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	12	1.07
(1,471)	1:A:33:LEU:HD11	1:A:44:ILE:H	18	1.07
(1,471)	1:A:33:LEU:HD12	1:A:44:ILE:H	18	1.07
(1,471)	1:A:33:LEU:HD13	1:A:44:ILE:H	18	1.07
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA2	15	1.07
(1,1934)	1:B:59:LEU:HB2	1:B:79:TYR:HE1	2	1.07
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD11	20	1.07
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD12	20	1.07
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD13	20	1.07
(1,1668)	1:B:39:ARG:HD2	1:B:40:ALA:H	13	1.07
(1,1658)	1:B:38:GLU:HG2	1:B:78:TYR:HD1	4	1.07
(1,1658)	1:B:38:GLU:HG3	1:B:78:TYR:HD1	4	1.07
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB1	4	1.07
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB2	4	1.07
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB3	4	1.07
(1,742)	1:A:52:LEU:HD11	1:A:56:SER:H	2	1.06
(1,742)	1:A:52:LEU:HD12	1:A:56:SER:H	2	1.06
(1,742)	1:A:52:LEU:HD13	1:A:56:SER:H	2	1.06
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	18	1.06
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	18	1.06
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	18	1.06
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	10	1.06
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	10	1.06
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	10	1.06
(1,1657)	1:B:38:GLU:HG2	1:B:78:TYR:HB2	12	1.06
(1,1657)	1:B:38:GLU:HG3	1:B:78:TYR:HB2	12	1.06
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	4	1.06
(1,2134)	1:B:74:GLY:HA2	1:B:75:THR:HB	3	1.05
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB1	19	1.05
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB2	19	1.05
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB3	19	1.05
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB1	19	1.05
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB2	19	1.05
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB3	19	1.05
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB1	19	1.05
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB2	19	1.05
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB3	19	1.05
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	6	1.05
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	6	1.05
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	6	1.05
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	11	1.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	11	1.05
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	11	1.05
(1,67)	1:B:11:LEU:HD11	1:A:98:ASP:H	5	1.04
(1,67)	1:B:11:LEU:HD12	1:A:98:ASP:H	5	1.04
(1,67)	1:B:11:LEU:HD13	1:A:98:ASP:H	5	1.04
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	10	1.04
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	7	1.04
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	7	1.04
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	7	1.04
(1,972)	1:A:71:ARG:HG2	1:A:78:TYR:HB2	20	1.03
(1,672)	1:A:45:ALA:H	1:A:52:LEU:HD11	2	1.03
(1,672)	1:A:45:ALA:H	1:A:52:LEU:HD12	2	1.03
(1,672)	1:A:45:ALA:H	1:A:52:LEU:HD13	2	1.03
(1,471)	1:A:33:LEU:HD11	1:A:44:ILE:H	11	1.03
(1,471)	1:A:33:LEU:HD12	1:A:44:ILE:H	11	1.03
(1,471)	1:A:33:LEU:HD13	1:A:44:ILE:H	11	1.03
(1,464)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	7	1.03
(1,464)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	7	1.03
(1,464)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	7	1.03
(1,464)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	10	1.03
(1,464)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	10	1.03
(1,464)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	10	1.03
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HE21	3	1.03
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HE21	3	1.03
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HE21	3	1.03
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	19	1.03
(1,2134)	1:B:74:GLY:HA2	1:B:75:THR:HB	8	1.03
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	3	1.03
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	3	1.03
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD21	12	1.03
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD22	12	1.03
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD23	12	1.03
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD11	18	1.02
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD12	18	1.02
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD13	18	1.02
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD11	18	1.02
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD12	18	1.02
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD13	18	1.02
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD11	18	1.02
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD12	18	1.02
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD13	18	1.02
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	15	1.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	15	1.02
(1,2134)	1:B:74:GLY:HA2	1:B:75:THR:HB	2	1.02
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	9	1.02
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	9	1.02
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	9	1.02
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	9	1.02
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	9	1.02
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	9	1.02
(1,1460)	1:B:27:ARG:HD2	1:B:58:ASN:HA	4	1.02
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	8	1.02
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	18	1.01
(1,2191)	1:B:81:ILE:HG12	1:B:87:ALA:HA	6	1.01
(1,2133)	1:B:73:GLU:H	1:B:78:TYR:HD1	7	1.01
(1,1837)	1:B:50:MET:HB2	1:B:55:ALA:H	19	1.01
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD11	10	1.01
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD12	10	1.01
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD13	10	1.01
(1,1002)	1:A:74:GLY:HA2	1:A:75:THR:HB	10	1.01
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB2	13	1.0
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB3	13	1.0
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB2	13	1.0
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB3	13	1.0
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB2	13	1.0
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB3	13	1.0
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	19	1.0
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	19	1.0
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB1	2	1.0
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB2	2	1.0
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB3	2	1.0
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB1	2	1.0
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB2	2	1.0
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB3	2	1.0
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB1	2	1.0
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB2	2	1.0
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB3	2	1.0
(1,1022)	1:A:76:ARG:HG2	1:A:78:TYR:HE1	18	1.0
(1,972)	1:A:71:ARG:HG2	1:A:78:TYR:HB2	17	0.99
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD11	13	0.99
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD12	13	0.99
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD13	13	0.99
(1,473)	1:A:33:LEU:HD11	1:A:47:ALA:H	1	0.99
(1,473)	1:A:33:LEU:HD12	1:A:47:ALA:H	1	0.99

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,473)	1:A:33:LEU:HD13	1:A:47:ALA:H	1	0.99
(1,2227)	1:B:84:GLU:HG2	1:B:88:ARG:HG2	2	0.99
(1,2227)	1:B:84:GLU:HG3	1:B:88:ARG:HG2	2	0.99
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	14	0.99
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	14	0.99
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	14	0.99
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD21	11	0.99
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD22	11	0.99
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD23	11	0.99
(1,486)	1:A:34:LEU:HB2	1:A:80:ARG:HA	9	0.98
(1,471)	1:A:33:LEU:HD11	1:A:44:ILE:H	7	0.98
(1,471)	1:A:33:LEU:HD12	1:A:44:ILE:H	7	0.98
(1,471)	1:A:33:LEU:HD13	1:A:44:ILE:H	7	0.98
(1,328)	1:A:27:ARG:HD2	1:A:58:ASN:HA	6	0.98
(1,2128)	1:B:73:GLU:HG2	1:B:78:TYR:HD1	3	0.98
(1,2128)	1:B:73:GLU:HG3	1:B:78:TYR:HD1	3	0.98
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	7	0.98
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	7	0.98
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	6	0.98
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	6	0.98
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	6	0.98
(1,1596)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	2	0.98
(1,1596)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	2	0.98
(1,1596)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	2	0.98
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD21	19	0.98
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD22	19	0.98
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD23	19	0.98
(1,995)	1:A:73:GLU:HB2	1:A:78:TYR:HE1	2	0.97
(1,742)	1:A:52:LEU:HD11	1:A:56:SER:H	16	0.97
(1,742)	1:A:52:LEU:HD12	1:A:56:SER:H	16	0.97
(1,742)	1:A:52:LEU:HD13	1:A:56:SER:H	16	0.97
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	11	0.97
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	11	0.97
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	11	0.97
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	13	0.97
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	13	0.97
(1,467)	1:A:33:LEU:HD11	1:A:39:ARG:HD2	3	0.97
(1,467)	1:A:33:LEU:HD12	1:A:39:ARG:HD2	3	0.97
(1,467)	1:A:33:LEU:HD13	1:A:39:ARG:HD2	3	0.97
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	14	0.97
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	14	0.97
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	17	0.97

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	17	0.97
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB1	4	0.97
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB2	4	0.97
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB3	4	0.97
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB1	4	0.97
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB2	4	0.97
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB3	4	0.97
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB1	4	0.97
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB2	4	0.97
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB3	4	0.97
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD21	1	0.97
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD22	1	0.97
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD23	1	0.97
(1,1002)	1:A:74:GLY:HA2	1:A:75:THR:HB	18	0.97
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	19	0.96
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	19	0.96
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	20	0.96
(1,742)	1:A:52:LEU:HD11	1:A:56:SER:H	7	0.96
(1,742)	1:A:52:LEU:HD12	1:A:56:SER:H	7	0.96
(1,742)	1:A:52:LEU:HD13	1:A:56:SER:H	7	0.96
(1,470)	1:A:33:LEU:HD11	1:A:44:ILE:HA	10	0.96
(1,470)	1:A:33:LEU:HD12	1:A:44:ILE:HA	10	0.96
(1,470)	1:A:33:LEU:HD13	1:A:44:ILE:HA	10	0.96
(1,2134)	1:B:74:GLY:HA2	1:B:75:THR:HB	11	0.96
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	13	0.96
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	13	0.96
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	13	0.96
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB2	9	0.96
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB3	9	0.96
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB2	9	0.96
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB3	9	0.96
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB2	9	0.96
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB3	9	0.96
(1,1691)	1:B:40:ALA:HB1	1:B:78:TYR:HE1	1	0.96
(1,1691)	1:B:40:ALA:HB2	1:B:78:TYR:HE1	1	0.96
(1,1691)	1:B:40:ALA:HB3	1:B:78:TYR:HE1	1	0.96
(1,1095)	1:A:84:GLU:HG2	1:A:88:ARG:HG2	7	0.96
(1,1095)	1:A:84:GLU:HG3	1:A:88:ARG:HG2	7	0.96
(1,1059)	1:A:81:ILE:HG12	1:A:87:ALA:HA	5	0.96
(1,1002)	1:A:74:GLY:HA2	1:A:75:THR:HB	1	0.96
(1,449)	1:A:32:ASP:HA	1:A:90:PHE:HE1	6	0.95
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	7	0.95

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	2	0.95
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	2	0.95
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	2	0.95
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB1	10	0.95
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB2	10	0.95
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB3	10	0.95
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB1	10	0.95
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB2	10	0.95
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB3	10	0.95
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB1	10	0.95
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB2	10	0.95
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB3	10	0.95
(1,1596)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	7	0.95
(1,1596)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	7	0.95
(1,1596)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	7	0.95
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG21	8	0.95
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG22	8	0.95
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG23	8	0.95
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG21	10	0.95
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG22	10	0.95
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG23	10	0.95
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD11	19	0.95
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD12	19	0.95
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD13	19	0.95
(1,1450)	1:B:26:ARG:HA	1:B:29:GLN:HG2	8	0.95
(1,1444)	1:B:25:GLY:HA2	1:B:28:LEU:HB2	17	0.95
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD11	3	0.95
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD12	3	0.95
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD13	3	0.95
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	2	0.94
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	2	0.94
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	2	0.94
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	4	0.94
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	4	0.94
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	4	0.94
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD11	13	0.94
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD12	13	0.94
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD13	13	0.94
(1,1002)	1:A:74:GLY:HA2	1:A:75:THR:HB	20	0.94
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	15	0.93
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	15	0.93
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	15	0.93

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,67)	1:B:11:LEU:HD11	1:A:98:ASP:H	12	0.93
(1,67)	1:B:11:LEU:HD12	1:A:98:ASP:H	12	0.93
(1,67)	1:B:11:LEU:HD13	1:A:98:ASP:H	12	0.93
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	9	0.93
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	9	0.93
(1,2134)	1:B:74:GLY:HA2	1:B:75:THR:HB	7	0.93
(1,2134)	1:B:74:GLY:HA2	1:B:75:THR:HB	10	0.93
(1,2125)	1:B:73:GLU:HB2	1:B:76:ARG:HG2	8	0.93
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD21	19	0.93
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD22	19	0.93
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD23	19	0.93
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB1	12	0.93
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB2	12	0.93
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB3	12	0.93
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB1	12	0.93
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB2	12	0.93
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB3	12	0.93
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB1	12	0.93
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB2	12	0.93
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB3	12	0.93
(1,1747)	1:B:42:GLU:HG2	1:B:52:LEU:HG	8	0.93
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	14	0.93
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	14	0.93
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	14	0.93
(1,1596)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	4	0.93
(1,1596)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	4	0.93
(1,1596)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	4	0.93
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD21	7	0.93
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD22	7	0.93
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD23	7	0.93
(1,2134)	1:B:74:GLY:HA2	1:B:75:THR:HB	1	0.92
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	12	0.92
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	12	0.92
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	12	0.92
(1,972)	1:A:71:ARG:HG2	1:A:78:TYR:HB2	16	0.91
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	10	0.91
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	10	0.91
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	10	0.91
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	17	0.91
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	17	0.91
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	17	0.91
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	7	0.91

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,559)	1:A:40:ALA:HB1	1:A:78:TYR:HE1	3	0.91
(1,559)	1:A:40:ALA:HB2	1:A:78:TYR:HE1	3	0.91
(1,559)	1:A:40:ALA:HB3	1:A:78:TYR:HE1	3	0.91
(1,330)	1:A:27:ARG:HD2	1:A:62:LEU:H	6	0.91
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD21	10	0.91
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD22	10	0.91
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD23	10	0.91
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	3	0.91
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	3	0.91
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	3	0.91
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	1	0.91
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	1	0.91
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	1	0.91
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	1	0.91
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	1	0.91
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	1	0.91
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	1	0.91
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	1	0.91
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	1	0.91
(1,1462)	1:B:27:ARG:HD2	1:B:62:LEU:H	19	0.91
(1,1377)	1:B:18:VAL:HG11	1:B:65:GLY:HA2	13	0.91
(1,1377)	1:B:18:VAL:HG12	1:B:65:GLY:HA2	13	0.91
(1,1377)	1:B:18:VAL:HG13	1:B:65:GLY:HA2	13	0.91
(1,1377)	1:B:18:VAL:HG11	1:B:65:GLY:HA2	19	0.91
(1,1377)	1:B:18:VAL:HG12	1:B:65:GLY:HA2	19	0.91
(1,1377)	1:B:18:VAL:HG13	1:B:65:GLY:HA2	19	0.91
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	1	0.9
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	1	0.9
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	1	0.9
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	19	0.9
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	19	0.9
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	19	0.9
(1,839)	1:A:62:LEU:HB2	1:A:67:LEU:HD21	4	0.9
(1,839)	1:A:62:LEU:HB2	1:A:67:LEU:HD22	4	0.9
(1,839)	1:A:62:LEU:HB2	1:A:67:LEU:HD23	4	0.9
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	3	0.9
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	3	0.9
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	3	0.9
(1,672)	1:A:45:ALA:H	1:A:52:LEU:HD11	7	0.9
(1,672)	1:A:45:ALA:H	1:A:52:LEU:HD12	7	0.9
(1,672)	1:A:45:ALA:H	1:A:52:LEU:HD13	7	0.9
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	11	0.9

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	11	0.9
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	11	0.9
(1,470)	1:A:33:LEU:HD11	1:A:44:ILE:HA	1	0.9
(1,470)	1:A:33:LEU:HD12	1:A:44:ILE:HA	1	0.9
(1,470)	1:A:33:LEU:HD13	1:A:44:ILE:HA	1	0.9
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB1	19	0.9
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB2	19	0.9
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB3	19	0.9
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD21	18	0.9
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD22	18	0.9
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD23	18	0.9
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	1	0.9
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	20	0.9
(1,672)	1:A:45:ALA:H	1:A:52:LEU:HD11	16	0.89
(1,672)	1:A:45:ALA:H	1:A:52:LEU:HD12	16	0.89
(1,672)	1:A:45:ALA:H	1:A:52:LEU:HD13	16	0.89
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB1	1	0.89
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB2	1	0.89
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB3	1	0.89
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB1	1	0.89
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB2	1	0.89
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB3	1	0.89
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB1	1	0.89
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB2	1	0.89
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB3	1	0.89
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB1	2	0.89
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB2	2	0.89
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB3	2	0.89
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB1	2	0.89
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB2	2	0.89
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB3	2	0.89
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB1	2	0.89
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB2	2	0.89
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB3	2	0.89
(1,2154)	1:B:76:ARG:HG2	1:B:78:TYR:HE1	17	0.89
(1,1849)	1:B:50:MET:H	1:B:50:MET:HG2	14	0.89
(1,1691)	1:B:40:ALA:HB1	1:B:78:TYR:HE1	15	0.89
(1,1691)	1:B:40:ALA:HB2	1:B:78:TYR:HE1	15	0.89
(1,1691)	1:B:40:ALA:HB3	1:B:78:TYR:HE1	15	0.89
(1,1658)	1:B:38:GLU:HG2	1:B:78:TYR:HD1	1	0.89
(1,1658)	1:B:38:GLU:HG3	1:B:78:TYR:HD1	1	0.89
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD11	19	0.89

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD12	19	0.89
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD13	19	0.89
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	20	0.88
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	20	0.88
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	20	0.88
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	10	0.88
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	10	0.88
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD11	19	0.88
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD12	19	0.88
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD13	19	0.88
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	17	0.88
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	17	0.88
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	17	0.88
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	7	0.88
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	6	0.88
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	7	0.88
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	3	0.87
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	3	0.87
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	3	0.87
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	6	0.87
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	6	0.87
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	4	0.87
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	4	0.87
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	4	0.87
(1,549)	1:A:40:ALA:HB1	1:A:42:GLU:HG2	1	0.87
(1,549)	1:A:40:ALA:HB2	1:A:42:GLU:HG2	1	0.87
(1,549)	1:A:40:ALA:HB3	1:A:42:GLU:HG2	1	0.87
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB1	2	0.87
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB2	2	0.87
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB3	2	0.87
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD21	15	0.87
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD22	15	0.87
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD23	15	0.87
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	12	0.87
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	12	0.87
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	12	0.87
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	5	0.87
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	5	0.87
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	5	0.87
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	13	0.87
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	19	0.87
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	5	0.86

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	5	0.86
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	5	0.86
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD21	16	0.86
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD22	16	0.86
(1,885)	1:A:66:GLY:HA2	1:A:67:LEU:HD23	16	0.86
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD11	17	0.86
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD12	17	0.86
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD13	17	0.86
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD11	3	0.86
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD12	3	0.86
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD13	3	0.86
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD11	3	0.86
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD12	3	0.86
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD13	3	0.86
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD11	3	0.86
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD12	3	0.86
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD13	3	0.86
(1,2113)	1:B:72:ARG:HA	1:B:77:GLN:HG2	10	0.86
(1,1690)	1:B:40:ALA:HB1	1:B:78:TYR:HD1	1	0.86
(1,1690)	1:B:40:ALA:HB2	1:B:78:TYR:HD1	1	0.86
(1,1690)	1:B:40:ALA:HB3	1:B:78:TYR:HD1	1	0.86
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB1	17	0.86
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB2	17	0.86
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB3	17	0.86
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB1	17	0.86
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB2	17	0.86
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB3	17	0.86
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB1	17	0.86
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB2	17	0.86
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB3	17	0.86
(1,1492)	1:B:29:GLN:HG2	1:B:48:THR:HB	18	0.86
(1,1462)	1:B:27:ARG:HD2	1:B:62:LEU:H	10	0.86
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	11	0.85
(1,471)	1:A:33:LEU:HD11	1:A:44:ILE:H	4	0.85
(1,471)	1:A:33:LEU:HD12	1:A:44:ILE:H	4	0.85
(1,471)	1:A:33:LEU:HD13	1:A:44:ILE:H	4	0.85
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	10	0.85
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	10	0.85
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	10	0.85
(1,4)	1:A:11:LEU:HD11	1:B:98:ASP:H	4	0.85
(1,4)	1:A:11:LEU:HD12	1:B:98:ASP:H	4	0.85
(1,4)	1:A:11:LEU:HD13	1:B:98:ASP:H	4	0.85

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,354)	1:A:29:GLN:HB2	1:A:48:THR:HB	10	0.85
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB1	4	0.85
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB2	4	0.85
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB3	4	0.85
(1,1657)	1:B:38:GLU:HG2	1:B:78:TYR:HB2	15	0.85
(1,1657)	1:B:38:GLU:HG3	1:B:78:TYR:HB2	15	0.85
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	4	0.85
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	4	0.85
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	4	0.85
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB1	12	0.85
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB2	12	0.85
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB3	12	0.85
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB1	12	0.85
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB2	12	0.85
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB3	12	0.85
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB1	12	0.85
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB2	12	0.85
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB3	12	0.85
(1,1596)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	14	0.85
(1,1596)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	14	0.85
(1,1596)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	14	0.85
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB1	9	0.85
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB2	9	0.85
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB3	9	0.85
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	16	0.84
(1,9)	1:A:12:LEU:HD11	1:B:29:GLN:HG2	10	0.84
(1,9)	1:A:12:LEU:HD12	1:B:29:GLN:HG2	10	0.84
(1,9)	1:A:12:LEU:HD13	1:B:29:GLN:HG2	10	0.84
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	13	0.84
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	13	0.84
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD21	2	0.84
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD22	2	0.84
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD23	2	0.84
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD21	19	0.84
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD22	19	0.84
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD23	19	0.84
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD21	2	0.84
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD22	2	0.84
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD23	2	0.84
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD21	17	0.84
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD22	17	0.84
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD23	17	0.84

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG21	1	0.84
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG22	1	0.84
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG23	1	0.84
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD11	20	0.84
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD12	20	0.84
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD13	20	0.84
(1,9)	1:A:12:LEU:HD11	1:B:29:GLN:HG2	1	0.83
(1,9)	1:A:12:LEU:HD12	1:B:29:GLN:HG2	1	0.83
(1,9)	1:A:12:LEU:HD13	1:B:29:GLN:HG2	1	0.83
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	18	0.83
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	18	0.83
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	18	0.83
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	15	0.83
(1,1361)	1:B:17:ARG:HA	1:B:65:GLY:HA2	3	0.83
(1,987)	1:A:72:ARG:HD2	1:A:77:GLN:HG2	14	0.82
(1,987)	1:A:72:ARG:HD3	1:A:77:GLN:HG2	14	0.82
(1,473)	1:A:33:LEU:HD11	1:A:47:ALA:H	20	0.82
(1,473)	1:A:33:LEU:HD12	1:A:47:ALA:H	20	0.82
(1,473)	1:A:33:LEU:HD13	1:A:47:ALA:H	20	0.82
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	8	0.82
(1,2095)	1:B:70:ALA:HB1	1:B:79:TYR:HE1	8	0.82
(1,2095)	1:B:70:ALA:HB2	1:B:79:TYR:HE1	8	0.82
(1,2095)	1:B:70:ALA:HB3	1:B:79:TYR:HE1	8	0.82
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD21	7	0.82
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD22	7	0.82
(1,2017)	1:B:66:GLY:HA2	1:B:67:LEU:HD23	7	0.82
(1,1658)	1:B:38:GLU:HG2	1:B:78:TYR:HD1	8	0.82
(1,1658)	1:B:38:GLU:HG3	1:B:78:TYR:HD1	8	0.82
(1,1486)	1:B:29:GLN:HB2	1:B:48:THR:HB	10	0.82
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	16	0.82
(1,1059)	1:A:81:ILE:HG12	1:A:87:ALA:HA	14	0.82
(1,742)	1:A:52:LEU:HD11	1:A:56:SER:H	14	0.81
(1,742)	1:A:52:LEU:HD12	1:A:56:SER:H	14	0.81
(1,742)	1:A:52:LEU:HD13	1:A:56:SER:H	14	0.81
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	2	0.81
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	2	0.81
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	2	0.81
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	11	0.81
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	11	0.81
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	11	0.81
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD11	14	0.81
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD12	14	0.81

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD13	14	0.81
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD11	10	0.81
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD12	10	0.81
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD13	10	0.81
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD11	10	0.81
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD12	10	0.81
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD13	10	0.81
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD11	10	0.81
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD12	10	0.81
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD13	10	0.81
(1,486)	1:A:34:LEU:HB2	1:A:80:ARG:HA	7	0.81
(1,472)	1:A:33:LEU:HD11	1:A:47:ALA:HB1	13	0.81
(1,472)	1:A:33:LEU:HD11	1:A:47:ALA:HB2	13	0.81
(1,472)	1:A:33:LEU:HD11	1:A:47:ALA:HB3	13	0.81
(1,472)	1:A:33:LEU:HD12	1:A:47:ALA:HB1	13	0.81
(1,472)	1:A:33:LEU:HD12	1:A:47:ALA:HB2	13	0.81
(1,472)	1:A:33:LEU:HD12	1:A:47:ALA:HB3	13	0.81
(1,472)	1:A:33:LEU:HD13	1:A:47:ALA:HB1	13	0.81
(1,472)	1:A:33:LEU:HD13	1:A:47:ALA:HB2	13	0.81
(1,472)	1:A:33:LEU:HD13	1:A:47:ALA:HB3	13	0.81
(1,470)	1:A:33:LEU:HD11	1:A:44:ILE:HA	16	0.81
(1,470)	1:A:33:LEU:HD12	1:A:44:ILE:HA	16	0.81
(1,470)	1:A:33:LEU:HD13	1:A:44:ILE:HA	16	0.81
(1,2343)	1:B:95:VAL:HG11	1:B:99:GLU:HG2	9	0.81
(1,2343)	1:B:95:VAL:HG12	1:B:99:GLU:HG2	9	0.81
(1,2343)	1:B:95:VAL:HG13	1:B:99:GLU:HG2	9	0.81
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD11	8	0.81
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD12	8	0.81
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD13	8	0.81
(1,1681)	1:B:40:ALA:HB1	1:B:42:GLU:HG2	1	0.81
(1,1681)	1:B:40:ALA:HB2	1:B:42:GLU:HG2	1	0.81
(1,1681)	1:B:40:ALA:HB3	1:B:42:GLU:HG2	1	0.81
(1,1657)	1:B:38:GLU:HG2	1:B:78:TYR:HB2	13	0.81
(1,1657)	1:B:38:GLU:HG3	1:B:78:TYR:HB2	13	0.81
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	18	0.81
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	18	0.81
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	18	0.81
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	18	0.81
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	18	0.81
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	18	0.81
(1,1596)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	3	0.81
(1,1596)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	3	0.81

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1596)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	3	0.81
(1,9)	1:A:12:LEU:HD11	1:B:29:GLN:HG2	15	0.8
(1,9)	1:A:12:LEU:HD12	1:B:29:GLN:HG2	15	0.8
(1,9)	1:A:12:LEU:HD13	1:B:29:GLN:HG2	15	0.8
(1,862)	1:A:63:LYS:HD2	1:A:79:TYR:HE1	20	0.8
(1,862)	1:A:63:LYS:HD3	1:A:79:TYR:HE1	20	0.8
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG21	20	0.8
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG22	20	0.8
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG23	20	0.8
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD21	11	0.8
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD22	11	0.8
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD23	11	0.8
(1,2191)	1:B:81:ILE:HG12	1:B:87:ALA:HA	7	0.8
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB1	12	0.8
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB2	12	0.8
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB3	12	0.8
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	17	0.8
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	17	0.8
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	17	0.8
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	17	0.8
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	17	0.8
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	17	0.8
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	17	0.8
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	17	0.8
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	17	0.8
(1,1618)	1:B:34:LEU:HB2	1:B:80:ARG:HA	7	0.8
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	8	0.8
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	8	0.8
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	8	0.8
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	9	0.8
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	9	0.8
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	9	0.8
(1,1460)	1:B:27:ARG:HD2	1:B:58:ASN:HA	19	0.8
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD21	8	0.8
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD22	8	0.8
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD23	8	0.8
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	13	0.79
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	14	0.79
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	14	0.79
(1,318)	1:A:26:ARG:HA	1:A:29:GLN:HG2	10	0.79
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD21	7	0.79
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD22	7	0.79

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD23	7	0.79
(1,2351)	1:B:96:VAL:HA	1:B:99:GLU:HB2	18	0.79
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	8	0.79
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	8	0.79
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	8	0.79
(1,1849)	1:B:50:MET:H	1:B:50:MET:HG2	13	0.79
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB1	2	0.79
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB2	2	0.79
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB3	2	0.79
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB1	10	0.79
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB2	10	0.79
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB3	10	0.79
(1,470)	1:A:33:LEU:HD11	1:A:44:ILE:HA	9	0.78
(1,470)	1:A:33:LEU:HD12	1:A:44:ILE:HA	9	0.78
(1,470)	1:A:33:LEU:HD13	1:A:44:ILE:HA	9	0.78
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	5	0.78
(1,2095)	1:B:70:ALA:HB1	1:B:79:TYR:HE1	1	0.78
(1,2095)	1:B:70:ALA:HB2	1:B:79:TYR:HE1	1	0.78
(1,2095)	1:B:70:ALA:HB3	1:B:79:TYR:HE1	1	0.78
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	4	0.78
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	4	0.78
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	4	0.78
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD21	10	0.78
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD22	10	0.78
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD23	10	0.78
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	3	0.78
(1,916)	1:A:68:VAL:HG11	1:A:69:GLU:HB2	3	0.77
(1,916)	1:A:68:VAL:HG12	1:A:69:GLU:HB2	3	0.77
(1,916)	1:A:68:VAL:HG13	1:A:69:GLU:HB2	3	0.77
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	14	0.77
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	14	0.77
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	14	0.77
(1,558)	1:A:40:ALA:HB1	1:A:78:TYR:HD1	3	0.77
(1,558)	1:A:40:ALA:HB2	1:A:78:TYR:HD1	3	0.77
(1,558)	1:A:40:ALA:HB3	1:A:78:TYR:HD1	3	0.77
(1,245)	1:A:18:VAL:HG11	1:A:65:GLY:HA2	17	0.77
(1,245)	1:A:18:VAL:HG12	1:A:65:GLY:HA2	17	0.77
(1,245)	1:A:18:VAL:HG13	1:A:65:GLY:HA2	17	0.77
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA2	14	0.77
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	18	0.77
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	18	0.77
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	18	0.77

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2191)	1:B:81:ILE:HG12	1:B:87:ALA:HA	17	0.77
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	10	0.77
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	10	0.77
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	10	0.77
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	9	0.77
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	9	0.77
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	9	0.77
(1,1668)	1:B:39:ARG:HD2	1:B:40:ALA:H	12	0.77
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG21	17	0.77
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG22	17	0.77
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG23	17	0.77
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD11	18	0.76
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD12	18	0.76
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD13	18	0.76
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	12	0.76
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	12	0.76
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	12	0.76
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD11	4	0.76
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD12	4	0.76
(1,1804)	1:B:45:ALA:H	1:B:52:LEU:HD13	4	0.76
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	2	0.76
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	2	0.76
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	2	0.76
(1,1690)	1:B:40:ALA:HB1	1:B:78:TYR:HD1	15	0.76
(1,1690)	1:B:40:ALA:HB2	1:B:78:TYR:HD1	15	0.76
(1,1690)	1:B:40:ALA:HB3	1:B:78:TYR:HD1	15	0.76
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	8	0.76
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	8	0.76
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	8	0.76
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD21	13	0.76
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD22	13	0.76
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD23	13	0.76
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	4	0.76
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	6	0.75
(1,72)	1:B:12:LEU:HD11	1:A:29:GLN:HG2	13	0.75
(1,72)	1:B:12:LEU:HD12	1:A:29:GLN:HG2	13	0.75
(1,72)	1:B:12:LEU:HD13	1:A:29:GLN:HG2	13	0.75
(1,72)	1:B:12:LEU:HD11	1:A:29:GLN:HG2	19	0.75
(1,72)	1:B:12:LEU:HD12	1:A:29:GLN:HG2	19	0.75
(1,72)	1:B:12:LEU:HD13	1:A:29:GLN:HG2	19	0.75
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	8	0.75
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	8	0.75

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	8	0.75
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB1	13	0.75
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB2	13	0.75
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB3	13	0.75
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB1	13	0.75
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB2	13	0.75
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB3	13	0.75
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB1	13	0.75
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB2	13	0.75
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB3	13	0.75
(1,467)	1:A:33:LEU:HD11	1:A:39:ARG:HD2	18	0.75
(1,467)	1:A:33:LEU:HD12	1:A:39:ARG:HD2	18	0.75
(1,467)	1:A:33:LEU:HD13	1:A:39:ARG:HD2	18	0.75
(1,464)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	13	0.75
(1,464)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	13	0.75
(1,464)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	13	0.75
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB1	16	0.75
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB2	16	0.75
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB3	16	0.75
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	18	0.75
(1,2129)	1:B:73:GLU:HG2	1:B:78:TYR:HE1	3	0.75
(1,2129)	1:B:73:GLU:HG3	1:B:78:TYR:HE1	3	0.75
(1,1603)	1:B:33:LEU:HD11	1:B:44:ILE:H	15	0.75
(1,1603)	1:B:33:LEU:HD12	1:B:44:ILE:H	15	0.75
(1,1603)	1:B:33:LEU:HD13	1:B:44:ILE:H	15	0.75
(1,1596)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	10	0.75
(1,1596)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	10	0.75
(1,1596)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	10	0.75
(1,72)	1:B:12:LEU:HD11	1:A:29:GLN:HG2	20	0.74
(1,72)	1:B:12:LEU:HD12	1:A:29:GLN:HG2	20	0.74
(1,72)	1:B:12:LEU:HD13	1:A:29:GLN:HG2	20	0.74
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB1	4	0.74
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB2	4	0.74
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB3	4	0.74
(1,2153)	1:B:76:ARG:HG2	1:B:77:GLN:H	9	0.74
(1,1596)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	20	0.74
(1,1596)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	20	0.74
(1,1596)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	20	0.74
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	18	0.74
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	17	0.73
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	17	0.73
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	17	0.73

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,525)	1:A:38:GLU:HG2	1:A:78:TYR:HB2	16	0.73
(1,525)	1:A:38:GLU:HG3	1:A:78:TYR:HB2	16	0.73
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	9	0.73
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	16	0.73
(1,1618)	1:B:34:LEU:HB2	1:B:80:ARG:HA	4	0.73
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	6	0.73
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	6	0.73
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	6	0.73
(1,1596)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	11	0.73
(1,1596)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	11	0.73
(1,1596)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	11	0.73
(1,1492)	1:B:29:GLN:HG2	1:B:48:THR:HB	16	0.73
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	1	0.73
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	1	0.73
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	1	0.73
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	7	0.73
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	7	0.73
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	7	0.73
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	13	0.73
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	13	0.73
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	13	0.73
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	20	0.73
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	20	0.73
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	20	0.73
(1,972)	1:A:71:ARG:HG2	1:A:78:TYR:HB2	15	0.72
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	4	0.72
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	4	0.72
(1,513)	1:A:36:GLN:HG2	1:A:37:GLY:H	2	0.72
(1,475)	1:A:33:LEU:HG	1:A:36:GLN:HE21	18	0.72
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	3	0.72
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	3	0.72
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	3	0.72
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	7	0.72
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	7	0.72
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	7	0.72
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD21	15	0.72
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD22	15	0.72
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD23	15	0.72
(1,2113)	1:B:72:ARG:HA	1:B:77:GLN:HG2	19	0.72
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	13	0.72
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	13	0.72
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB1	11	0.72

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB2	11	0.72
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB3	11	0.72
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB1	15	0.72
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB2	15	0.72
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB3	15	0.72
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB1	8	0.72
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB2	8	0.72
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB3	8	0.72
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB1	8	0.72
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB2	8	0.72
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB3	8	0.72
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB1	8	0.72
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB2	8	0.72
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB3	8	0.72
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	2	0.72
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	2	0.72
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	2	0.72
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	10	0.72
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	10	0.72
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	10	0.72
(1,64)	1:B:11:LEU:HD11	1:A:98:ASP:HA	10	0.71
(1,64)	1:B:11:LEU:HD12	1:A:98:ASP:HA	10	0.71
(1,64)	1:B:11:LEU:HD13	1:A:98:ASP:HA	10	0.71
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD11	11	0.71
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD12	11	0.71
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD13	11	0.71
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB1	20	0.71
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB2	20	0.71
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB3	20	0.71
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB1	20	0.71
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB2	20	0.71
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB3	20	0.71
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB1	20	0.71
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB2	20	0.71
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB3	20	0.71
(1,464)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	1	0.71
(1,464)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	1	0.71
(1,464)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	1	0.71
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	10	0.71
(1,318)	1:A:26:ARG:HA	1:A:29:GLN:HG2	13	0.71
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	2	0.71
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	2	0.71

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	2	0.71
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	4	0.71
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	4	0.71
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	4	0.71
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	19	0.71
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	19	0.71
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	19	0.71
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	8	0.71
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	8	0.71
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	8	0.71
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	7	0.71
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	7	0.71
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	7	0.71
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	7	0.71
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	7	0.71
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	7	0.71
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	7	0.71
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	7	0.71
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	7	0.71
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	3	0.71
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	3	0.71
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	3	0.71
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	10	0.71
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	10	0.71
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	10	0.71
(1,1599)	1:B:33:LEU:HD11	1:B:39:ARG:HD2	20	0.71
(1,1599)	1:B:33:LEU:HD12	1:B:39:ARG:HD2	20	0.71
(1,1599)	1:B:33:LEU:HD13	1:B:39:ARG:HD2	20	0.71
(1,1486)	1:B:29:GLN:HB2	1:B:48:THR:HB	1	0.71
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	19	0.71
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	19	0.71
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	19	0.71
(1,9)	1:A:12:LEU:HD11	1:B:29:GLN:HG2	13	0.7
(1,9)	1:A:12:LEU:HD12	1:B:29:GLN:HG2	13	0.7
(1,9)	1:A:12:LEU:HD13	1:B:29:GLN:HG2	13	0.7
(1,549)	1:A:40:ALA:HB1	1:A:42:GLU:HG2	2	0.7
(1,549)	1:A:40:ALA:HB2	1:A:42:GLU:HG2	2	0.7
(1,549)	1:A:40:ALA:HB3	1:A:42:GLU:HG2	2	0.7
(1,328)	1:A:27:ARG:HD2	1:A:58:ASN:HA	4	0.7
(1,312)	1:A:25:GLY:HA2	1:A:28:LEU:HB2	4	0.7
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	1	0.7
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	1	0.7

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	1	0.7
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	8	0.7
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	8	0.7
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	8	0.7
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB1	20	0.7
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB2	20	0.7
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB3	20	0.7
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	9	0.7
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	9	0.7
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	9	0.7
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	9	0.7
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	9	0.7
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	9	0.7
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	9	0.7
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	9	0.7
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	9	0.7
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	12	0.7
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	12	0.7
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	12	0.7
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	12	0.7
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	12	0.7
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	12	0.7
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	12	0.7
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	12	0.7
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	12	0.7
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	20	0.7
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	20	0.7
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	20	0.7
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	20	0.7
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	20	0.7
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	20	0.7
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	20	0.7
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	20	0.7
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	20	0.7
(1,1460)	1:B:27:ARG:HD2	1:B:58:ASN:HA	6	0.7
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	14	0.7
(1,1219)	1:A:96:VAL:HA	1:A:99:GLU:HB2	12	0.7
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	11	0.7
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	11	0.7
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	11	0.7
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD21	17	0.7
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD22	17	0.7

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD23	17	0.7
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	16	0.69
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	16	0.69
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG2	4	0.69
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD11	2	0.69
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD12	2	0.69
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD13	2	0.69
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD11	2	0.69
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD12	2	0.69
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD13	2	0.69
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD11	2	0.69
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD12	2	0.69
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD13	2	0.69
(1,549)	1:A:40:ALA:HB1	1:A:42:GLU:HG2	3	0.69
(1,549)	1:A:40:ALA:HB2	1:A:42:GLU:HG2	3	0.69
(1,549)	1:A:40:ALA:HB3	1:A:42:GLU:HG2	3	0.69
(1,470)	1:A:33:LEU:HD11	1:A:44:ILE:HA	19	0.69
(1,470)	1:A:33:LEU:HD12	1:A:44:ILE:HA	19	0.69
(1,470)	1:A:33:LEU:HD13	1:A:44:ILE:HA	19	0.69
(1,4)	1:A:11:LEU:HD11	1:B:98:ASP:H	11	0.69
(1,4)	1:A:11:LEU:HD12	1:B:98:ASP:H	11	0.69
(1,4)	1:A:11:LEU:HD13	1:B:98:ASP:H	11	0.69
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	12	0.69
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	12	0.69
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	12	0.69
(1,2113)	1:B:72:ARG:HA	1:B:77:GLN:HG2	6	0.69
(1,1898)	1:B:55:ALA:HB1	1:B:58:ASN:HB2	10	0.69
(1,1898)	1:B:55:ALA:HB2	1:B:58:ASN:HB2	10	0.69
(1,1898)	1:B:55:ALA:HB3	1:B:58:ASN:HB2	10	0.69
(1,1595)	1:B:33:LEU:HD11	1:B:36:GLN:HE21	10	0.69
(1,1595)	1:B:33:LEU:HD12	1:B:36:GLN:HE21	10	0.69
(1,1595)	1:B:33:LEU:HD13	1:B:36:GLN:HE21	10	0.69
(1,1450)	1:B:26:ARG:HA	1:B:29:GLN:HG2	13	0.69
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	5	0.69
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	5	0.69
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	5	0.69
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	12	0.69
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	12	0.69
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	12	0.69
(1,866)	1:A:63:LYS:HE2	1:A:79:TYR:HE1	8	0.68
(1,866)	1:A:63:LYS:HE3	1:A:79:TYR:HE1	8	0.68
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD11	11	0.68

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD12	11	0.68
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD13	11	0.68
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	14	0.68
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	14	0.68
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	14	0.68
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	17	0.68
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	17	0.68
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	17	0.68
(1,1618)	1:B:34:LEU:HB2	1:B:80:ARG:HA	8	0.68
(1,1581)	1:B:32:ASP:HA	1:B:90:PHE:HE1	20	0.68
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	6	0.68
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	6	0.68
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	6	0.68
(1,1041)	1:A:79:TYR:HA	1:A:80:ARG:HG2	11	0.68
(1,9)	1:A:12:LEU:HD11	1:B:29:GLN:HG2	8	0.67
(1,9)	1:A:12:LEU:HD12	1:B:29:GLN:HG2	8	0.67
(1,9)	1:A:12:LEU:HD13	1:B:29:GLN:HG2	8	0.67
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB2	11	0.67
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB3	11	0.67
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB2	11	0.67
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB3	11	0.67
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB2	11	0.67
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB3	11	0.67
(1,559)	1:A:40:ALA:HB1	1:A:78:TYR:HE1	5	0.67
(1,559)	1:A:40:ALA:HB2	1:A:78:TYR:HE1	5	0.67
(1,559)	1:A:40:ALA:HB3	1:A:78:TYR:HE1	5	0.67
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	12	0.67
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	12	0.67
(1,513)	1:A:36:GLN:HG2	1:A:37:GLY:H	10	0.67
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	11	0.67
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	11	0.67
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	11	0.67
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	16	0.67
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	16	0.67
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	16	0.67
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD21	10	0.67
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD22	10	0.67
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD23	10	0.67
(1,2173)	1:B:79:TYR:HA	1:B:80:ARG:HG2	2	0.67
(1,2169)	1:B:77:GLN:H	1:B:77:GLN:HG2	10	0.67
(1,2125)	1:B:73:GLU:HB2	1:B:76:ARG:HG2	6	0.67
(1,2119)	1:B:72:ARG:HD2	1:B:77:GLN:HG2	19	0.67

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2119)	1:B:72:ARG:HD3	1:B:77:GLN:HG2	19	0.67
(1,1934)	1:B:59:LEU:HB2	1:B:79:TYR:HE1	20	0.67
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	13	0.67
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	13	0.67
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	13	0.67
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	17	0.67
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	17	0.67
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	17	0.67
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	6	0.67
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	6	0.67
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	6	0.67
(1,1460)	1:B:27:ARG:HD2	1:B:58:ASN:HA	10	0.67
(1,1296)	1:B:10:ALA:HB1	1:B:13:ASP:HB2	12	0.67
(1,1296)	1:B:10:ALA:HB2	1:B:13:ASP:HB2	12	0.67
(1,1296)	1:B:10:ALA:HB3	1:B:13:ASP:HB2	12	0.67
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	17	0.67
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	17	0.67
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	17	0.67
(1,1041)	1:A:79:TYR:HA	1:A:80:ARG:HG2	2	0.67
(1,987)	1:A:72:ARG:HD2	1:A:77:GLN:HG2	9	0.66
(1,987)	1:A:72:ARG:HD3	1:A:77:GLN:HG2	9	0.66
(1,965)	1:A:71:ARG:HA	1:A:72:ARG:HB2	12	0.66
(1,916)	1:A:68:VAL:HG11	1:A:69:GLU:HB2	8	0.66
(1,916)	1:A:68:VAL:HG12	1:A:69:GLU:HB2	8	0.66
(1,916)	1:A:68:VAL:HG13	1:A:69:GLU:HB2	8	0.66
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	7	0.66
(1,502)	1:A:35:ALA:HB1	1:A:36:GLN:HE21	9	0.66
(1,502)	1:A:35:ALA:HB2	1:A:36:GLN:HE21	9	0.66
(1,502)	1:A:35:ALA:HB3	1:A:36:GLN:HE21	9	0.66
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	9	0.66
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	9	0.66
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	9	0.66
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	10	0.66
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	10	0.66
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	10	0.66
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	13	0.66
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	13	0.66
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	13	0.66
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB1	17	0.66
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB2	17	0.66
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB3	17	0.66
(1,1657)	1:B:38:GLU:HG2	1:B:78:TYR:HB2	5	0.66

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1657)	1:B:38:GLU:HG3	1:B:78:TYR:HB2	5	0.66
(1,1645)	1:B:36:GLN:HG2	1:B:37:GLY:H	3	0.66
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD11	2	0.66
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD12	2	0.66
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD13	2	0.66
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD11	11	0.66
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD12	11	0.66
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD13	11	0.66
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	15	0.66
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	15	0.66
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	15	0.66
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	15	0.66
(1,1047)	1:A:80:ARG:H	1:A:80:ARG:HG2	2	0.66
(1,615)	1:A:42:GLU:HG2	1:A:52:LEU:HG	11	0.65
(1,559)	1:A:40:ALA:HB1	1:A:78:TYR:HE1	4	0.65
(1,559)	1:A:40:ALA:HB2	1:A:78:TYR:HE1	4	0.65
(1,559)	1:A:40:ALA:HB3	1:A:78:TYR:HE1	4	0.65
(1,536)	1:A:39:ARG:HD2	1:A:40:ALA:H	15	0.65
(1,4)	1:A:11:LEU:HD11	1:B:98:ASP:H	12	0.65
(1,4)	1:A:11:LEU:HD12	1:B:98:ASP:H	12	0.65
(1,4)	1:A:11:LEU:HD13	1:B:98:ASP:H	12	0.65
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	12	0.65
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	12	0.65
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	12	0.65
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	5	0.65
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	5	0.65
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	5	0.65
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD21	6	0.65
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD22	6	0.65
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD23	6	0.65
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	8	0.65
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	8	0.65
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	1	0.65
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	1	0.65
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	1	0.65
(1,1645)	1:B:36:GLN:HG2	1:B:37:GLY:H	11	0.65
(1,1645)	1:B:36:GLN:HG2	1:B:37:GLY:H	18	0.65
(1,164)	1:A:10:ALA:HB1	1:A:13:ASP:HB2	14	0.65
(1,164)	1:A:10:ALA:HB2	1:A:13:ASP:HB2	14	0.65
(1,164)	1:A:10:ALA:HB3	1:A:13:ASP:HB2	14	0.65
(1,1492)	1:B:29:GLN:HG2	1:B:48:THR:HB	11	0.65
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	8	0.65

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	8	0.65
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	8	0.65
(1,70)	1:B:12:LEU:HD11	1:A:29:GLN:HB2	7	0.64
(1,70)	1:B:12:LEU:HD12	1:A:29:GLN:HB2	7	0.64
(1,70)	1:B:12:LEU:HD13	1:A:29:GLN:HB2	7	0.64
(1,475)	1:A:33:LEU:HG	1:A:36:GLN:HE21	14	0.64
(1,473)	1:A:33:LEU:HD11	1:A:47:ALA:H	14	0.64
(1,473)	1:A:33:LEU:HD12	1:A:47:ALA:H	14	0.64
(1,473)	1:A:33:LEU:HD13	1:A:47:ALA:H	14	0.64
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	3	0.64
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	17	0.64
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	9	0.64
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	9	0.64
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	9	0.64
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	2	0.64
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	2	0.64
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	2	0.64
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	2	0.64
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	2	0.64
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	2	0.64
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	2	0.64
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	2	0.64
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	2	0.64
(1,1681)	1:B:40:ALA:HB1	1:B:42:GLU:HG2	8	0.64
(1,1681)	1:B:40:ALA:HB2	1:B:42:GLU:HG2	8	0.64
(1,1681)	1:B:40:ALA:HB3	1:B:42:GLU:HG2	8	0.64
(1,1658)	1:B:38:GLU:HG2	1:B:78:TYR:HD1	6	0.64
(1,1658)	1:B:38:GLU:HG3	1:B:78:TYR:HD1	6	0.64
(1,1645)	1:B:36:GLN:HG2	1:B:37:GLY:H	2	0.64
(1,1645)	1:B:36:GLN:HG2	1:B:37:GLY:H	14	0.64
(1,1618)	1:B:34:LEU:HB2	1:B:80:ARG:HA	13	0.64
(1,1377)	1:B:18:VAL:HG11	1:B:65:GLY:HA2	8	0.64
(1,1377)	1:B:18:VAL:HG12	1:B:65:GLY:HA2	8	0.64
(1,1377)	1:B:18:VAL:HG13	1:B:65:GLY:HA2	8	0.64
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	9	0.64
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	9	0.64
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	9	0.64
(1,1059)	1:A:81:ILE:HG12	1:A:87:ALA:HA	2	0.64
(1,965)	1:A:71:ARG:HA	1:A:72:ARG:HB2	20	0.63
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG2	7	0.63
(1,486)	1:A:34:LEU:HB2	1:A:80:ARG:HA	3	0.63
(1,312)	1:A:25:GLY:HA2	1:A:28:LEU:HB2	11	0.63

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	20	0.63
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	20	0.63
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	20	0.63
(1,2191)	1:B:81:ILE:HG12	1:B:87:ALA:HA	1	0.63
(1,2167)	1:B:77:GLN:HG2	1:B:79:TYR:HE1	7	0.63
(1,2167)	1:B:77:GLN:HG2	1:B:79:TYR:HE1	8	0.63
(1,2154)	1:B:76:ARG:HG2	1:B:78:TYR:HE1	16	0.63
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	20	0.63
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	20	0.63
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	19	0.63
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	19	0.63
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	19	0.63
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	19	0.63
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	19	0.63
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG21	18	0.63
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG22	18	0.63
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG23	18	0.63
(1,1377)	1:B:18:VAL:HG11	1:B:65:GLY:HA2	5	0.63
(1,1377)	1:B:18:VAL:HG12	1:B:65:GLY:HA2	5	0.63
(1,1377)	1:B:18:VAL:HG13	1:B:65:GLY:HA2	5	0.63
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB2	18	0.62
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB3	18	0.62
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB2	18	0.62
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB3	18	0.62
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB2	18	0.62
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB3	18	0.62
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	6	0.62
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	6	0.62
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	6	0.62
(1,513)	1:A:36:GLN:HG2	1:A:37:GLY:H	7	0.62
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	16	0.62
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	18	0.62
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	3	0.62
(1,2191)	1:B:81:ILE:HG12	1:B:87:ALA:HA	4	0.62
(1,2154)	1:B:76:ARG:HG2	1:B:78:TYR:HE1	3	0.62
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	14	0.62
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	14	0.62
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB1	6	0.62
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB2	6	0.62
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB3	6	0.62
(1,1681)	1:B:40:ALA:HB1	1:B:42:GLU:HG2	12	0.62
(1,1681)	1:B:40:ALA:HB2	1:B:42:GLU:HG2	12	0.62

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1681)	1:B:40:ALA:HB3	1:B:42:GLU:HG2	12	0.62
(1,1657)	1:B:38:GLU:HG2	1:B:78:TYR:HB2	2	0.62
(1,1657)	1:B:38:GLU:HG3	1:B:78:TYR:HB2	2	0.62
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	2	0.62
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	2	0.62
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	2	0.62
(1,141)	1:A:7:ARG:HB2	1:A:8:LYS:H	15	0.62
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	5	0.61
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	5	0.61
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	5	0.61
(1,594)	1:A:41:VAL:HG21	1:A:77:GLN:HG2	3	0.61
(1,594)	1:A:41:VAL:HG22	1:A:77:GLN:HG2	3	0.61
(1,594)	1:A:41:VAL:HG23	1:A:77:GLN:HG2	3	0.61
(1,558)	1:A:40:ALA:HB1	1:A:78:TYR:HD1	4	0.61
(1,558)	1:A:40:ALA:HB2	1:A:78:TYR:HD1	4	0.61
(1,558)	1:A:40:ALA:HB3	1:A:78:TYR:HD1	4	0.61
(1,513)	1:A:36:GLN:HG2	1:A:37:GLY:H	19	0.61
(1,473)	1:A:33:LEU:HD11	1:A:47:ALA:H	9	0.61
(1,473)	1:A:33:LEU:HD12	1:A:47:ALA:H	9	0.61
(1,473)	1:A:33:LEU:HD13	1:A:47:ALA:H	9	0.61
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	11	0.61
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	11	0.61
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	11	0.61
(1,245)	1:A:18:VAL:HG11	1:A:65:GLY:HA2	9	0.61
(1,245)	1:A:18:VAL:HG12	1:A:65:GLY:HA2	9	0.61
(1,245)	1:A:18:VAL:HG13	1:A:65:GLY:HA2	9	0.61
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	15	0.61
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	15	0.61
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	15	0.61
(1,2173)	1:B:79:TYR:HA	1:B:80:ARG:HG2	19	0.61
(1,2167)	1:B:77:GLN:HG2	1:B:79:TYR:HE1	3	0.61
(1,2129)	1:B:73:GLU:HG2	1:B:78:TYR:HE1	19	0.61
(1,2129)	1:B:73:GLU:HG3	1:B:78:TYR:HE1	19	0.61
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	15	0.61
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	15	0.61
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	15	0.61
(1,1596)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	1	0.61
(1,1596)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	1	0.61
(1,1596)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	1	0.61
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	3	0.61
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	3	0.61
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	3	0.61

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	17	0.61
(1,1041)	1:A:79:TYR:HA	1:A:80:ARG:HG2	1	0.61
(1,1002)	1:A:74:GLY:HA2	1:A:75:THR:HB	15	0.61
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	18	0.6
(1,742)	1:A:52:LEU:HD11	1:A:56:SER:H	10	0.6
(1,742)	1:A:52:LEU:HD12	1:A:56:SER:H	10	0.6
(1,742)	1:A:52:LEU:HD13	1:A:56:SER:H	10	0.6
(1,67)	1:B:11:LEU:HD11	1:A:98:ASP:H	13	0.6
(1,67)	1:B:11:LEU:HD12	1:A:98:ASP:H	13	0.6
(1,67)	1:B:11:LEU:HD13	1:A:98:ASP:H	13	0.6
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD11	14	0.6
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD12	14	0.6
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD13	14	0.6
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD11	1	0.6
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD12	1	0.6
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD13	1	0.6
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD11	1	0.6
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD12	1	0.6
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD13	1	0.6
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD11	1	0.6
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD12	1	0.6
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD13	1	0.6
(1,470)	1:A:33:LEU:HD11	1:A:44:ILE:HA	14	0.6
(1,470)	1:A:33:LEU:HD12	1:A:44:ILE:HA	14	0.6
(1,470)	1:A:33:LEU:HD13	1:A:44:ILE:HA	14	0.6
(1,328)	1:A:27:ARG:HD2	1:A:58:ASN:HA	20	0.6
(1,2173)	1:B:79:TYR:HA	1:B:80:ARG:HG2	10	0.6
(1,2125)	1:B:73:GLU:HB2	1:B:76:ARG:HG2	2	0.6
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	9	0.6
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	9	0.6
(1,1934)	1:B:59:LEU:HB2	1:B:79:TYR:HE1	18	0.6
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD11	2	0.6
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD12	2	0.6
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD13	2	0.6
(1,1657)	1:B:38:GLU:HG2	1:B:78:TYR:HB2	9	0.6
(1,1657)	1:B:38:GLU:HG3	1:B:78:TYR:HB2	9	0.6
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	5	0.6
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	5	0.6
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	5	0.6
(1,965)	1:A:71:ARG:HA	1:A:72:ARG:HB2	6	0.59
(1,9)	1:A:12:LEU:HD11	1:B:29:GLN:HG2	19	0.59
(1,9)	1:A:12:LEU:HD12	1:B:29:GLN:HG2	19	0.59

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,9)	1:A:12:LEU:HD13	1:B:29:GLN:HG2	19	0.59
(1,245)	1:A:18:VAL:HG11	1:A:65:GLY:HA2	12	0.59
(1,245)	1:A:18:VAL:HG12	1:A:65:GLY:HA2	12	0.59
(1,245)	1:A:18:VAL:HG13	1:A:65:GLY:HA2	12	0.59
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB1	6	0.59
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB2	6	0.59
(1,2286)	1:B:90:PHE:HB2	1:B:91:ALA:HB3	6	0.59
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	14	0.59
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	16	0.59
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	16	0.59
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	16	0.59
(1,1373)	1:B:18:VAL:HG11	1:B:19:GLY:HA2	20	0.59
(1,1373)	1:B:18:VAL:HG11	1:B:19:GLY:HA3	20	0.59
(1,1373)	1:B:18:VAL:HG12	1:B:19:GLY:HA2	20	0.59
(1,1373)	1:B:18:VAL:HG12	1:B:19:GLY:HA3	20	0.59
(1,1373)	1:B:18:VAL:HG13	1:B:19:GLY:HA2	20	0.59
(1,1373)	1:B:18:VAL:HG13	1:B:19:GLY:HA3	20	0.59
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	14	0.59
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	14	0.59
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	14	0.59
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	16	0.59
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	16	0.59
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	16	0.59
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	18	0.59
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	18	0.59
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	18	0.59
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD21	6	0.59
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD22	6	0.59
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD23	6	0.59
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	6	0.58
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	6	0.58
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	8	0.58
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	8	0.58
(1,742)	1:A:52:LEU:HD11	1:A:56:SER:H	5	0.58
(1,742)	1:A:52:LEU:HD12	1:A:56:SER:H	5	0.58
(1,742)	1:A:52:LEU:HD13	1:A:56:SER:H	5	0.58
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB2	17	0.58
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB3	17	0.58
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB2	17	0.58
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB3	17	0.58
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB2	17	0.58
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB3	17	0.58

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD11	9	0.58
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD12	9	0.58
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD13	9	0.58
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD11	9	0.58
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD12	9	0.58
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD13	9	0.58
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD11	9	0.58
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD12	9	0.58
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD13	9	0.58
(1,486)	1:A:34:LEU:HB2	1:A:80:ARG:HA	17	0.58
(1,241)	1:A:18:VAL:HG11	1:A:19:GLY:HA2	4	0.58
(1,241)	1:A:18:VAL:HG11	1:A:19:GLY:HA3	4	0.58
(1,241)	1:A:18:VAL:HG12	1:A:19:GLY:HA2	4	0.58
(1,241)	1:A:18:VAL:HG12	1:A:19:GLY:HA3	4	0.58
(1,241)	1:A:18:VAL:HG13	1:A:19:GLY:HA2	4	0.58
(1,241)	1:A:18:VAL:HG13	1:A:19:GLY:HA3	4	0.58
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	5	0.58
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	5	0.58
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	11	0.58
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	11	0.58
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	14	0.58
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	14	0.58
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	14	0.58
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB1	19	0.58
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB2	19	0.58
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB3	19	0.58
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	20	0.58
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	20	0.58
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	20	0.58
(1,1645)	1:B:36:GLN:HG2	1:B:37:GLY:H	19	0.58
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	7	0.58
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	7	0.58
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	7	0.58
(1,1595)	1:B:33:LEU:HD11	1:B:36:GLN:HE21	12	0.58
(1,1595)	1:B:33:LEU:HD12	1:B:36:GLN:HE21	12	0.58
(1,1595)	1:B:33:LEU:HD13	1:B:36:GLN:HE21	12	0.58
(1,1041)	1:A:79:TYR:HA	1:A:80:ARG:HG2	13	0.58
(1,1041)	1:A:79:TYR:HA	1:A:80:ARG:HG2	19	0.58
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	19	0.57
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	19	0.57
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	19	0.57
(1,467)	1:A:33:LEU:HD11	1:A:39:ARG:HD2	19	0.57

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,467)	1:A:33:LEU:HD12	1:A:39:ARG:HD2	19	0.57
(1,467)	1:A:33:LEU:HD13	1:A:39:ARG:HD2	19	0.57
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD21	4	0.57
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD22	4	0.57
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD23	4	0.57
(1,2351)	1:B:96:VAL:HA	1:B:99:GLU:HB2	17	0.57
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	8	0.57
(1,2154)	1:B:76:ARG:HG2	1:B:78:TYR:HE1	20	0.57
(1,1681)	1:B:40:ALA:HB1	1:B:42:GLU:HG2	16	0.57
(1,1681)	1:B:40:ALA:HB2	1:B:42:GLU:HG2	16	0.57
(1,1681)	1:B:40:ALA:HB3	1:B:42:GLU:HG2	16	0.57
(1,1668)	1:B:39:ARG:HD2	1:B:40:ALA:H	19	0.57
(1,1648)	1:B:37:GLY:HA2	1:B:38:GLU:HB2	15	0.57
(1,1648)	1:B:37:GLY:HA2	1:B:38:GLU:HB3	15	0.57
(1,1645)	1:B:36:GLN:HG2	1:B:37:GLY:H	15	0.57
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB1	4	0.57
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB2	4	0.57
(1,1154)	1:A:90:PHE:HB2	1:A:91:ALA:HB3	4	0.57
(1,1059)	1:A:81:ILE:HG12	1:A:87:ALA:HA	11	0.57
(1,1041)	1:A:79:TYR:HA	1:A:80:ARG:HG2	15	0.57
(1,981)	1:A:72:ARG:HA	1:A:77:GLN:HG2	11	0.56
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	4	0.56
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	12	0.56
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	12	0.56
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	12	0.56
(1,549)	1:A:40:ALA:HB1	1:A:42:GLU:HG2	20	0.56
(1,549)	1:A:40:ALA:HB2	1:A:42:GLU:HG2	20	0.56
(1,549)	1:A:40:ALA:HB3	1:A:42:GLU:HG2	20	0.56
(1,525)	1:A:38:GLU:HG2	1:A:78:TYR:HB2	3	0.56
(1,525)	1:A:38:GLU:HG3	1:A:78:TYR:HB2	3	0.56
(1,470)	1:A:33:LEU:HD11	1:A:44:ILE:HA	7	0.56
(1,470)	1:A:33:LEU:HD12	1:A:44:ILE:HA	7	0.56
(1,470)	1:A:33:LEU:HD13	1:A:44:ILE:HA	7	0.56
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	20	0.56
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	20	0.56
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	20	0.56
(1,42)	1:A:16:ALA:HB1	1:B:25:GLY:HA2	11	0.56
(1,42)	1:A:16:ALA:HB2	1:B:25:GLY:HA2	11	0.56
(1,42)	1:A:16:ALA:HB3	1:B:25:GLY:HA2	11	0.56
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	16	0.56
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	16	0.56
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	16	0.56

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,241)	1:A:18:VAL:HG11	1:A:19:GLY:HA2	1	0.56
(1,241)	1:A:18:VAL:HG11	1:A:19:GLY:HA3	1	0.56
(1,241)	1:A:18:VAL:HG12	1:A:19:GLY:HA2	1	0.56
(1,241)	1:A:18:VAL:HG12	1:A:19:GLY:HA3	1	0.56
(1,241)	1:A:18:VAL:HG13	1:A:19:GLY:HA2	1	0.56
(1,241)	1:A:18:VAL:HG13	1:A:19:GLY:HA3	1	0.56
(1,241)	1:A:18:VAL:HG11	1:A:19:GLY:HA2	10	0.56
(1,241)	1:A:18:VAL:HG11	1:A:19:GLY:HA3	10	0.56
(1,241)	1:A:18:VAL:HG12	1:A:19:GLY:HA2	10	0.56
(1,241)	1:A:18:VAL:HG12	1:A:19:GLY:HA3	10	0.56
(1,241)	1:A:18:VAL:HG13	1:A:19:GLY:HA2	10	0.56
(1,241)	1:A:18:VAL:HG13	1:A:19:GLY:HA3	10	0.56
(1,2343)	1:B:95:VAL:HG11	1:B:99:GLU:HG2	3	0.56
(1,2343)	1:B:95:VAL:HG12	1:B:99:GLU:HG2	3	0.56
(1,2343)	1:B:95:VAL:HG13	1:B:99:GLU:HG2	3	0.56
(1,2342)	1:B:95:VAL:HG11	1:B:99:GLU:HB2	12	0.56
(1,2342)	1:B:95:VAL:HG12	1:B:99:GLU:HB2	12	0.56
(1,2342)	1:B:95:VAL:HG13	1:B:99:GLU:HB2	12	0.56
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	6	0.56
(1,2227)	1:B:84:GLU:HG2	1:B:88:ARG:HG2	1	0.56
(1,2227)	1:B:84:GLU:HG3	1:B:88:ARG:HG2	1	0.56
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	4	0.56
(1,2173)	1:B:79:TYR:HA	1:B:80:ARG:HG2	3	0.56
(1,2173)	1:B:79:TYR:HA	1:B:80:ARG:HG2	11	0.56
(1,2173)	1:B:79:TYR:HA	1:B:80:ARG:HG2	16	0.56
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	6	0.56
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	6	0.56
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	6	0.56
(1,1726)	1:B:41:VAL:HG21	1:B:77:GLN:HG2	9	0.56
(1,1726)	1:B:41:VAL:HG22	1:B:77:GLN:HG2	9	0.56
(1,1726)	1:B:41:VAL:HG23	1:B:77:GLN:HG2	9	0.56
(1,1645)	1:B:36:GLN:HG2	1:B:37:GLY:H	7	0.56
(1,1492)	1:B:29:GLN:HG2	1:B:48:THR:HB	9	0.56
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD11	14	0.56
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD12	14	0.56
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD13	14	0.56
(1,8)	1:A:12:LEU:HD11	1:B:29:GLN:HE21	10	0.55
(1,8)	1:A:12:LEU:HD12	1:B:29:GLN:HE21	10	0.55
(1,8)	1:A:12:LEU:HD13	1:B:29:GLN:HE21	10	0.55
(1,742)	1:A:52:LEU:HD11	1:A:56:SER:H	17	0.55
(1,742)	1:A:52:LEU:HD12	1:A:56:SER:H	17	0.55
(1,742)	1:A:52:LEU:HD13	1:A:56:SER:H	17	0.55

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,703)	1:A:50:MET:HB2	1:A:54:THR:HG21	1	0.55
(1,703)	1:A:50:MET:HB2	1:A:54:THR:HG22	1	0.55
(1,703)	1:A:50:MET:HB2	1:A:54:THR:HG23	1	0.55
(1,558)	1:A:40:ALA:HB1	1:A:78:TYR:HD1	20	0.55
(1,558)	1:A:40:ALA:HB2	1:A:78:TYR:HD1	20	0.55
(1,558)	1:A:40:ALA:HB3	1:A:78:TYR:HD1	20	0.55
(1,525)	1:A:38:GLU:HG2	1:A:78:TYR:HB2	11	0.55
(1,525)	1:A:38:GLU:HG3	1:A:78:TYR:HB2	11	0.55
(1,525)	1:A:38:GLU:HG2	1:A:78:TYR:HB2	14	0.55
(1,525)	1:A:38:GLU:HG3	1:A:78:TYR:HB2	14	0.55
(1,473)	1:A:33:LEU:HD11	1:A:47:ALA:H	16	0.55
(1,473)	1:A:33:LEU:HD12	1:A:47:ALA:H	16	0.55
(1,473)	1:A:33:LEU:HD13	1:A:47:ALA:H	16	0.55
(1,472)	1:A:33:LEU:HD11	1:A:47:ALA:HB1	2	0.55
(1,472)	1:A:33:LEU:HD11	1:A:47:ALA:HB2	2	0.55
(1,472)	1:A:33:LEU:HD11	1:A:47:ALA:HB3	2	0.55
(1,472)	1:A:33:LEU:HD12	1:A:47:ALA:HB1	2	0.55
(1,472)	1:A:33:LEU:HD12	1:A:47:ALA:HB2	2	0.55
(1,472)	1:A:33:LEU:HD12	1:A:47:ALA:HB3	2	0.55
(1,472)	1:A:33:LEU:HD13	1:A:47:ALA:HB1	2	0.55
(1,472)	1:A:33:LEU:HD13	1:A:47:ALA:HB2	2	0.55
(1,472)	1:A:33:LEU:HD13	1:A:47:ALA:HB3	2	0.55
(1,470)	1:A:33:LEU:HD11	1:A:44:ILE:HA	4	0.55
(1,470)	1:A:33:LEU:HD12	1:A:44:ILE:HA	4	0.55
(1,470)	1:A:33:LEU:HD13	1:A:44:ILE:HA	4	0.55
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	1	0.55
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	17	0.55
(1,2173)	1:B:79:TYR:HA	1:B:80:ARG:HG2	18	0.55
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD11	19	0.55
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD12	19	0.55
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD13	19	0.55
(1,1645)	1:B:36:GLN:HG2	1:B:37:GLY:H	20	0.55
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	3	0.55
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	3	0.55
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	3	0.55
(1,1460)	1:B:27:ARG:HD2	1:B:58:ASN:HA	13	0.55
(1,1373)	1:B:18:VAL:HG11	1:B:19:GLY:HA2	2	0.55
(1,1373)	1:B:18:VAL:HG11	1:B:19:GLY:HA3	2	0.55
(1,1373)	1:B:18:VAL:HG12	1:B:19:GLY:HA2	2	0.55
(1,1373)	1:B:18:VAL:HG12	1:B:19:GLY:HA3	2	0.55
(1,1373)	1:B:18:VAL:HG13	1:B:19:GLY:HA2	2	0.55
(1,1373)	1:B:18:VAL:HG13	1:B:19:GLY:HA3	2	0.55

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD11	1	0.55
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD12	1	0.55
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD13	1	0.55
(1,1021)	1:A:76:ARG:HG2	1:A:77:GLN:H	7	0.55
(1,1002)	1:A:74:GLY:HA2	1:A:75:THR:HB	19	0.55
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	10	0.54
(1,981)	1:A:72:ARG:HA	1:A:77:GLN:HG2	1	0.54
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB2	7	0.54
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB3	7	0.54
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB2	7	0.54
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB3	7	0.54
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB2	7	0.54
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB3	7	0.54
(1,70)	1:B:12:LEU:HD11	1:A:29:GLN:HB2	18	0.54
(1,70)	1:B:12:LEU:HD12	1:A:29:GLN:HB2	18	0.54
(1,70)	1:B:12:LEU:HD13	1:A:29:GLN:HB2	18	0.54
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	8	0.54
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	8	0.54
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	8	0.54
(1,473)	1:A:33:LEU:HD11	1:A:47:ALA:H	19	0.54
(1,473)	1:A:33:LEU:HD12	1:A:47:ALA:H	19	0.54
(1,473)	1:A:33:LEU:HD13	1:A:47:ALA:H	19	0.54
(1,330)	1:A:27:ARG:HD2	1:A:62:LEU:H	16	0.54
(1,2125)	1:B:73:GLU:HB2	1:B:76:ARG:HG2	19	0.54
(1,1668)	1:B:39:ARG:HD2	1:B:40:ALA:H	1	0.54
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB1	12	0.54
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB2	12	0.54
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB3	12	0.54
(1,1444)	1:B:25:GLY:HA2	1:B:28:LEU:HB2	19	0.54
(1,1373)	1:B:18:VAL:HG11	1:B:19:GLY:HA2	1	0.54
(1,1373)	1:B:18:VAL:HG11	1:B:19:GLY:HA3	1	0.54
(1,1373)	1:B:18:VAL:HG12	1:B:19:GLY:HA2	1	0.54
(1,1373)	1:B:18:VAL:HG12	1:B:19:GLY:HA3	1	0.54
(1,1373)	1:B:18:VAL:HG13	1:B:19:GLY:HA2	1	0.54
(1,1373)	1:B:18:VAL:HG13	1:B:19:GLY:HA3	1	0.54
(1,1041)	1:A:79:TYR:HA	1:A:80:ARG:HG2	10	0.54
(1,1021)	1:A:76:ARG:HG2	1:A:77:GLN:H	8	0.54
(1,742)	1:A:52:LEU:HD11	1:A:56:SER:H	13	0.53
(1,742)	1:A:52:LEU:HD12	1:A:56:SER:H	13	0.53
(1,742)	1:A:52:LEU:HD13	1:A:56:SER:H	13	0.53
(1,742)	1:A:52:LEU:HD11	1:A:56:SER:H	18	0.53
(1,742)	1:A:52:LEU:HD12	1:A:56:SER:H	18	0.53

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,742)	1:A:52:LEU:HD13	1:A:56:SER:H	18	0.53
(1,615)	1:A:42:GLU:HG2	1:A:52:LEU:HG	17	0.53
(1,558)	1:A:40:ALA:HB1	1:A:78:TYR:HD1	5	0.53
(1,558)	1:A:40:ALA:HB2	1:A:78:TYR:HD1	5	0.53
(1,558)	1:A:40:ALA:HB3	1:A:78:TYR:HD1	5	0.53
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD21	3	0.53
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD22	3	0.53
(1,2263)	1:B:88:ARG:HB2	1:B:92:LEU:HD23	3	0.53
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	2	0.53
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	6	0.53
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	18	0.53
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	18	0.53
(1,1998)	1:B:63:LYS:HE2	1:B:79:TYR:HE1	16	0.53
(1,1998)	1:B:63:LYS:HE3	1:B:79:TYR:HE1	16	0.53
(1,1893)	1:B:55:ALA:HA	1:B:58:ASN:HB2	10	0.53
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB2	14	0.53
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB3	14	0.53
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB2	14	0.53
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB3	14	0.53
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB2	14	0.53
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB3	14	0.53
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD11	12	0.53
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD12	12	0.53
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD13	12	0.53
(1,1645)	1:B:36:GLN:HG2	1:B:37:GLY:H	8	0.53
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	19	0.53
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	19	0.53
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	19	0.53
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	20	0.53
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	20	0.53
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	20	0.53
(1,1486)	1:B:29:GLN:HB2	1:B:48:THR:HB	17	0.53
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD11	9	0.53
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD12	9	0.53
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD13	9	0.53
(1,1211)	1:A:95:VAL:HG11	1:A:99:GLU:HG2	17	0.53
(1,1211)	1:A:95:VAL:HG12	1:A:99:GLU:HG2	17	0.53
(1,1211)	1:A:95:VAL:HG13	1:A:99:GLU:HG2	17	0.53
(1,1166)	1:A:91:ALA:HA	1:A:94:GLN:HG2	16	0.53
(1,1041)	1:A:79:TYR:HA	1:A:80:ARG:HG2	4	0.53
(1,1002)	1:A:74:GLY:HA2	1:A:75:THR:HB	11	0.53
(1,742)	1:A:52:LEU:HD11	1:A:56:SER:H	9	0.52

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,742)	1:A:52:LEU:HD12	1:A:56:SER:H	9	0.52
(1,742)	1:A:52:LEU:HD13	1:A:56:SER:H	9	0.52
(1,558)	1:A:40:ALA:HB1	1:A:78:TYR:HD1	13	0.52
(1,558)	1:A:40:ALA:HB2	1:A:78:TYR:HD1	13	0.52
(1,558)	1:A:40:ALA:HB3	1:A:78:TYR:HD1	13	0.52
(1,536)	1:A:39:ARG:HD2	1:A:40:ALA:H	16	0.52
(1,2173)	1:B:79:TYR:HA	1:B:80:ARG:HG2	4	0.52
(1,2134)	1:B:74:GLY:HA2	1:B:75:THR:HB	17	0.52
(1,1681)	1:B:40:ALA:HB1	1:B:42:GLU:HG2	17	0.52
(1,1681)	1:B:40:ALA:HB2	1:B:42:GLU:HG2	17	0.52
(1,1681)	1:B:40:ALA:HB3	1:B:42:GLU:HG2	17	0.52
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG21	16	0.52
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG22	16	0.52
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG23	16	0.52
(1,1450)	1:B:26:ARG:HA	1:B:29:GLN:HG2	10	0.52
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD21	3	0.52
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD22	3	0.52
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD23	3	0.52
(1,1037)	1:A:77:GLN:H	1:A:77:GLN:HG2	20	0.52
(1,64)	1:B:11:LEU:HD11	1:A:98:ASP:HA	16	0.51
(1,64)	1:B:11:LEU:HD12	1:A:98:ASP:HA	16	0.51
(1,64)	1:B:11:LEU:HD13	1:A:98:ASP:HA	16	0.51
(1,559)	1:A:40:ALA:HB1	1:A:78:TYR:HE1	9	0.51
(1,559)	1:A:40:ALA:HB2	1:A:78:TYR:HE1	9	0.51
(1,559)	1:A:40:ALA:HB3	1:A:78:TYR:HE1	9	0.51
(1,559)	1:A:40:ALA:HB1	1:A:78:TYR:HE1	20	0.51
(1,559)	1:A:40:ALA:HB2	1:A:78:TYR:HE1	20	0.51
(1,559)	1:A:40:ALA:HB3	1:A:78:TYR:HE1	20	0.51
(1,558)	1:A:40:ALA:HB1	1:A:78:TYR:HD1	16	0.51
(1,558)	1:A:40:ALA:HB2	1:A:78:TYR:HD1	16	0.51
(1,558)	1:A:40:ALA:HB3	1:A:78:TYR:HD1	16	0.51
(1,470)	1:A:33:LEU:HD11	1:A:44:ILE:HA	11	0.51
(1,470)	1:A:33:LEU:HD12	1:A:44:ILE:HA	11	0.51
(1,470)	1:A:33:LEU:HD13	1:A:44:ILE:HA	11	0.51
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	14	0.51
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	14	0.51
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	14	0.51
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	18	0.51
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	18	0.51
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	18	0.51
(1,245)	1:A:18:VAL:HG11	1:A:65:GLY:HA2	16	0.51
(1,245)	1:A:18:VAL:HG12	1:A:65:GLY:HA2	16	0.51

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,245)	1:A:18:VAL:HG13	1:A:65:GLY:HA2	16	0.51
(1,2134)	1:B:74:GLY:HA2	1:B:75:THR:HB	13	0.51
(1,1934)	1:B:59:LEU:HB2	1:B:79:TYR:HE1	3	0.51
(1,1823)	1:B:48:THR:HB	1:B:50:MET:HG2	19	0.51
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD11	14	0.51
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD12	14	0.51
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD13	14	0.51
(1,1634)	1:B:35:ALA:HB1	1:B:36:GLN:HE21	6	0.51
(1,1634)	1:B:35:ALA:HB2	1:B:36:GLN:HE21	6	0.51
(1,1634)	1:B:35:ALA:HB3	1:B:36:GLN:HE21	6	0.51
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB1	9	0.51
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB2	9	0.51
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB3	9	0.51
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB1	9	0.51
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB2	9	0.51
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB3	9	0.51
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB1	9	0.51
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB2	9	0.51
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB3	9	0.51
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD11	9	0.51
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD12	9	0.51
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD13	9	0.51
(1,1122)	1:A:87:ALA:H	1:A:88:ARG:HG2	5	0.51
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	5	0.5
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	5	0.5
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	5	0.5
(1,558)	1:A:40:ALA:HB1	1:A:78:TYR:HD1	9	0.5
(1,558)	1:A:40:ALA:HB2	1:A:78:TYR:HD1	9	0.5
(1,558)	1:A:40:ALA:HB3	1:A:78:TYR:HD1	9	0.5
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD11	17	0.5
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD12	17	0.5
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD13	17	0.5
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD11	17	0.5
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD12	17	0.5
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD13	17	0.5
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD11	17	0.5
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD12	17	0.5
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD13	17	0.5
(1,473)	1:A:33:LEU:HD11	1:A:47:ALA:H	4	0.5
(1,473)	1:A:33:LEU:HD12	1:A:47:ALA:H	4	0.5
(1,473)	1:A:33:LEU:HD13	1:A:47:ALA:H	4	0.5
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	8	0.5

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	8	0.5
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	8	0.5
(1,1927)	1:B:59:LEU:HA	1:B:62:LEU:HB2	7	0.5
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	5	0.5
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	5	0.5
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	5	0.5
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	7	0.5
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	7	0.5
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	7	0.5
(1,1662)	1:B:39:ARG:HA	1:B:39:ARG:HD2	13	0.5
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG21	9	0.5
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG22	9	0.5
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG23	9	0.5
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD11	18	0.5
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD12	18	0.5
(1,148)	1:A:8:LYS:HA	1:A:11:LEU:HD13	18	0.5
(1,1460)	1:B:27:ARG:HD2	1:B:58:ASN:HA	9	0.5
(1,1273)	1:B:7:ARG:HB2	1:B:8:LYS:H	13	0.5
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	8	0.5
(1,1041)	1:A:79:TYR:HA	1:A:80:ARG:HG2	20	0.5
(1,1037)	1:A:77:GLN:H	1:A:77:GLN:HG2	5	0.5
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	7	0.49
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	7	0.49
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	16	0.49
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	13	0.49
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	13	0.49
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	13	0.49
(1,621)	1:A:42:GLU:H	1:A:42:GLU:HG2	13	0.49
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	12	0.49
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	12	0.49
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	12	0.49
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD11	5	0.49
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD12	5	0.49
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD13	5	0.49
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD11	5	0.49
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD12	5	0.49
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD13	5	0.49
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD11	5	0.49
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD12	5	0.49
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD13	5	0.49
(1,513)	1:A:36:GLN:HG2	1:A:37:GLY:H	1	0.49
(1,2154)	1:B:76:ARG:HG2	1:B:78:TYR:HE1	5	0.49

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2134)	1:B:74:GLY:HA2	1:B:75:THR:HB	4	0.49
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	8	0.49
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	8	0.49
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	8	0.49
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	5	0.49
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	5	0.49
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	5	0.49
(1,1645)	1:B:36:GLN:HG2	1:B:37:GLY:H	10	0.49
(1,1607)	1:B:33:LEU:HG	1:B:36:GLN:HE21	12	0.49
(1,1591)	1:B:33:LEU:HA	1:B:36:GLN:HE21	12	0.49
(1,1486)	1:B:29:GLN:HB2	1:B:48:THR:HB	8	0.49
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB1	6	0.49
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB2	6	0.49
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB3	6	0.49
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	19	0.49
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD11	14	0.49
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD12	14	0.49
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD13	14	0.49
(1,1037)	1:A:77:GLN:H	1:A:77:GLN:HG2	16	0.49
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	9	0.48
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	9	0.48
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	18	0.48
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	18	0.48
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	11	0.48
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	20	0.48
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	5	0.48
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	5	0.48
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	5	0.48
(1,559)	1:A:40:ALA:HB1	1:A:78:TYR:HE1	16	0.48
(1,559)	1:A:40:ALA:HB2	1:A:78:TYR:HE1	16	0.48
(1,559)	1:A:40:ALA:HB3	1:A:78:TYR:HE1	16	0.48
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD11	14	0.48
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD12	14	0.48
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD13	14	0.48
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD11	14	0.48
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD12	14	0.48
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD13	14	0.48
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD11	14	0.48
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD12	14	0.48
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD13	14	0.48
(1,525)	1:A:38:GLU:HG2	1:A:78:TYR:HB2	1	0.48
(1,525)	1:A:38:GLU:HG3	1:A:78:TYR:HB2	1	0.48

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,525)	1:A:38:GLU:HG2	1:A:78:TYR:HB2	8	0.48
(1,525)	1:A:38:GLU:HG3	1:A:78:TYR:HB2	8	0.48
(1,513)	1:A:36:GLN:HG2	1:A:37:GLY:H	5	0.48
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	1	0.48
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	1	0.48
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	1	0.48
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	10	0.48
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	10	0.48
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	10	0.48
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	11	0.48
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	2	0.48
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD11	20	0.48
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD12	20	0.48
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD13	20	0.48
(1,1681)	1:B:40:ALA:HB1	1:B:42:GLU:HG2	20	0.48
(1,1681)	1:B:40:ALA:HB2	1:B:42:GLU:HG2	20	0.48
(1,1681)	1:B:40:ALA:HB3	1:B:42:GLU:HG2	20	0.48
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	6	0.48
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD11	3	0.48
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD12	3	0.48
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD13	3	0.48
(1,105)	1:B:16:ALA:HB1	1:A:25:GLY:HA2	6	0.48
(1,105)	1:B:16:ALA:HB2	1:A:25:GLY:HA2	6	0.48
(1,105)	1:B:16:ALA:HB3	1:A:25:GLY:HA2	6	0.48
(1,1035)	1:A:77:GLN:HG2	1:A:79:TYR:HE1	8	0.48
(1,1002)	1:A:74:GLY:HA2	1:A:75:THR:HB	6	0.48
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	12	0.47
(1,8)	1:A:12:LEU:HD11	1:B:29:GLN:HE21	15	0.47
(1,8)	1:A:12:LEU:HD12	1:B:29:GLN:HE21	15	0.47
(1,8)	1:A:12:LEU:HD13	1:B:29:GLN:HE21	15	0.47
(1,558)	1:A:40:ALA:HB1	1:A:78:TYR:HD1	12	0.47
(1,558)	1:A:40:ALA:HB2	1:A:78:TYR:HD1	12	0.47
(1,558)	1:A:40:ALA:HB3	1:A:78:TYR:HD1	12	0.47
(1,558)	1:A:40:ALA:HB1	1:A:78:TYR:HD1	17	0.47
(1,558)	1:A:40:ALA:HB2	1:A:78:TYR:HD1	17	0.47
(1,558)	1:A:40:ALA:HB3	1:A:78:TYR:HD1	17	0.47
(1,513)	1:A:36:GLN:HG2	1:A:37:GLY:H	17	0.47
(1,473)	1:A:33:LEU:HD11	1:A:47:ALA:H	10	0.47
(1,473)	1:A:33:LEU:HD12	1:A:47:ALA:H	10	0.47
(1,473)	1:A:33:LEU:HD13	1:A:47:ALA:H	10	0.47
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	11	0.47
(1,245)	1:A:18:VAL:HG11	1:A:65:GLY:HA2	13	0.47

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,245)	1:A:18:VAL:HG12	1:A:65:GLY:HA2	13	0.47
(1,245)	1:A:18:VAL:HG13	1:A:65:GLY:HA2	13	0.47
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	5	0.47
(1,2179)	1:B:80:ARG:H	1:B:80:ARG:HG2	19	0.47
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	4	0.47
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	4	0.47
(1,1934)	1:B:59:LEU:HB2	1:B:79:TYR:HE1	5	0.47
(1,1898)	1:B:55:ALA:HB1	1:B:58:ASN:HB2	12	0.47
(1,1898)	1:B:55:ALA:HB2	1:B:58:ASN:HB2	12	0.47
(1,1898)	1:B:55:ALA:HB3	1:B:58:ASN:HB2	12	0.47
(1,1753)	1:B:42:GLU:H	1:B:42:GLU:HG2	4	0.47
(1,141)	1:A:7:ARG:HB2	1:A:8:LYS:H	17	0.47
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	12	0.47
(1,8)	1:A:12:LEU:HD11	1:B:29:GLN:HE21	17	0.46
(1,8)	1:A:12:LEU:HD12	1:B:29:GLN:HE21	17	0.46
(1,8)	1:A:12:LEU:HD13	1:B:29:GLN:HE21	17	0.46
(1,742)	1:A:52:LEU:HD11	1:A:56:SER:H	1	0.46
(1,742)	1:A:52:LEU:HD12	1:A:56:SER:H	1	0.46
(1,742)	1:A:52:LEU:HD13	1:A:56:SER:H	1	0.46
(1,72)	1:B:12:LEU:HD11	1:A:29:GLN:HG2	17	0.46
(1,72)	1:B:12:LEU:HD12	1:A:29:GLN:HG2	17	0.46
(1,72)	1:B:12:LEU:HD13	1:A:29:GLN:HG2	17	0.46
(1,70)	1:B:12:LEU:HD11	1:A:29:GLN:HB2	4	0.46
(1,70)	1:B:12:LEU:HD12	1:A:29:GLN:HB2	4	0.46
(1,70)	1:B:12:LEU:HD13	1:A:29:GLN:HB2	4	0.46
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	6	0.46
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	6	0.46
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	6	0.46
(1,513)	1:A:36:GLN:HG2	1:A:37:GLY:H	15	0.46
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	9	0.46
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	9	0.46
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	9	0.46
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	1	0.46
(1,2227)	1:B:84:GLU:HG2	1:B:88:ARG:HG2	11	0.46
(1,2227)	1:B:84:GLU:HG3	1:B:88:ARG:HG2	11	0.46
(1,1934)	1:B:59:LEU:HB2	1:B:79:TYR:HE1	15	0.46
(1,1934)	1:B:59:LEU:HB2	1:B:79:TYR:HE1	16	0.46
(1,1849)	1:B:50:MET:H	1:B:50:MET:HG2	19	0.46
(1,1681)	1:B:40:ALA:HB1	1:B:42:GLU:HG2	6	0.46
(1,1681)	1:B:40:ALA:HB2	1:B:42:GLU:HG2	6	0.46
(1,1681)	1:B:40:ALA:HB3	1:B:42:GLU:HG2	6	0.46
(1,1645)	1:B:36:GLN:HG2	1:B:37:GLY:H	1	0.46

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	10	0.46
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	10	0.46
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	10	0.46
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	19	0.46
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	19	0.46
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	19	0.46
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	14	0.46
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	14	0.46
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	14	0.46
(1,1596)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	17	0.46
(1,1596)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	17	0.46
(1,1596)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	17	0.46
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG21	11	0.46
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG22	11	0.46
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG23	11	0.46
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	18	0.46
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD11	4	0.46
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD12	4	0.46
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD13	4	0.46
(1,1041)	1:A:79:TYR:HA	1:A:80:ARG:HG2	3	0.46
(1,1002)	1:A:74:GLY:HA2	1:A:75:THR:HB	16	0.46
(1,72)	1:B:12:LEU:HD11	1:A:29:GLN:HG2	2	0.45
(1,72)	1:B:12:LEU:HD12	1:A:29:GLN:HG2	2	0.45
(1,72)	1:B:12:LEU:HD13	1:A:29:GLN:HG2	2	0.45
(1,67)	1:B:11:LEU:HD11	1:A:98:ASP:H	6	0.45
(1,67)	1:B:11:LEU:HD12	1:A:98:ASP:H	6	0.45
(1,67)	1:B:11:LEU:HD13	1:A:98:ASP:H	6	0.45
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	4	0.45
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	4	0.45
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	4	0.45
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	19	0.45
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	19	0.45
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	19	0.45
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD11	16	0.45
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD12	16	0.45
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD13	16	0.45
(1,475)	1:A:33:LEU:HG	1:A:36:GLN:HE21	1	0.45
(1,462)	1:A:33:LEU:HD11	1:A:36:GLN:HB2	5	0.45
(1,462)	1:A:33:LEU:HD12	1:A:36:GLN:HB2	5	0.45
(1,462)	1:A:33:LEU:HD13	1:A:36:GLN:HB2	5	0.45
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB1	20	0.45
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB2	20	0.45

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB3	20	0.45
(1,318)	1:A:26:ARG:HA	1:A:29:GLN:HG2	2	0.45
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	19	0.45
(1,2298)	1:B:91:ALA:HA	1:B:94:GLN:HG2	10	0.45
(1,2191)	1:B:81:ILE:HG12	1:B:87:ALA:HA	18	0.45
(1,2169)	1:B:77:GLN:H	1:B:77:GLN:HG2	20	0.45
(1,2153)	1:B:76:ARG:HG2	1:B:77:GLN:H	3	0.45
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	19	0.45
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	19	0.45
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	19	0.45
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	10	0.45
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	10	0.45
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	10	0.45
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	10	0.45
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	10	0.45
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	10	0.45
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	10	0.45
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	10	0.45
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	10	0.45
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB1	19	0.45
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB2	19	0.45
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB3	19	0.45
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB1	19	0.45
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB2	19	0.45
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB3	19	0.45
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB1	19	0.45
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB2	19	0.45
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB3	19	0.45
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	11	0.45
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	13	0.45
(1,1041)	1:A:79:TYR:HA	1:A:80:ARG:HG2	8	0.45
(1,1037)	1:A:77:GLN:H	1:A:77:GLN:HG2	10	0.45
(1,1002)	1:A:74:GLY:HA2	1:A:75:THR:HB	4	0.45
(1,987)	1:A:72:ARG:HD2	1:A:77:GLN:HG2	1	0.44
(1,987)	1:A:72:ARG:HD3	1:A:77:GLN:HG2	1	0.44
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	13	0.44
(1,71)	1:B:12:LEU:HD11	1:A:29:GLN:HE21	14	0.44
(1,71)	1:B:12:LEU:HD12	1:A:29:GLN:HE21	14	0.44
(1,71)	1:B:12:LEU:HD13	1:A:29:GLN:HE21	14	0.44
(1,245)	1:A:18:VAL:HG11	1:A:65:GLY:HA2	20	0.44
(1,245)	1:A:18:VAL:HG12	1:A:65:GLY:HA2	20	0.44
(1,245)	1:A:18:VAL:HG13	1:A:65:GLY:HA2	20	0.44

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2134)	1:B:74:GLY:HA2	1:B:75:THR:HB	20	0.44
(1,2125)	1:B:73:GLU:HB2	1:B:76:ARG:HG2	11	0.44
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB2	2	0.44
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB3	2	0.44
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB2	2	0.44
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB3	2	0.44
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB2	2	0.44
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB3	2	0.44
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	3	0.44
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	3	0.44
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	3	0.44
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	11	0.44
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	11	0.44
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	11	0.44
(1,1726)	1:B:41:VAL:HG21	1:B:77:GLN:HG2	7	0.44
(1,1726)	1:B:41:VAL:HG22	1:B:77:GLN:HG2	7	0.44
(1,1726)	1:B:41:VAL:HG23	1:B:77:GLN:HG2	7	0.44
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	6	0.44
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	6	0.44
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	6	0.44
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	6	0.44
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	6	0.44
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	6	0.44
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	6	0.44
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	6	0.44
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	6	0.44
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	3	0.44
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	6	0.44
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	10	0.44
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	17	0.44
(1,1095)	1:A:84:GLU:HG2	1:A:88:ARG:HG2	6	0.44
(1,1095)	1:A:84:GLU:HG3	1:A:88:ARG:HG2	6	0.44
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	8	0.43
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	5	0.43
(1,525)	1:A:38:GLU:HG2	1:A:78:TYR:HB2	2	0.43
(1,525)	1:A:38:GLU:HG3	1:A:78:TYR:HB2	2	0.43
(1,525)	1:A:38:GLU:HG2	1:A:78:TYR:HB2	5	0.43
(1,525)	1:A:38:GLU:HG3	1:A:78:TYR:HB2	5	0.43
(1,513)	1:A:36:GLN:HG2	1:A:37:GLY:H	16	0.43
(1,465)	1:A:33:LEU:HD11	1:A:36:GLN:H	5	0.43
(1,465)	1:A:33:LEU:HD12	1:A:36:GLN:H	5	0.43
(1,465)	1:A:33:LEU:HD13	1:A:36:GLN:H	5	0.43

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,312)	1:A:25:GLY:HA2	1:A:28:LEU:HB2	2	0.43
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	3	0.43
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	4	0.43
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	1	0.43
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	20	0.43
(1,2153)	1:B:76:ARG:HG2	1:B:77:GLN:H	7	0.43
(1,2131)	1:B:73:GLU:H	1:B:76:ARG:HG2	20	0.43
(1,1747)	1:B:42:GLU:HG2	1:B:52:LEU:HG	11	0.43
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD11	10	0.43
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD12	10	0.43
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD13	10	0.43
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD11	17	0.43
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD12	17	0.43
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD13	17	0.43
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD11	19	0.43
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD12	19	0.43
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD13	19	0.43
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	16	0.43
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	16	0.43
(1,810)	1:A:59:LEU:HD21	1:A:79:TYR:HE1	20	0.42
(1,810)	1:A:59:LEU:HD22	1:A:79:TYR:HE1	20	0.42
(1,810)	1:A:59:LEU:HD23	1:A:79:TYR:HE1	20	0.42
(1,8)	1:A:12:LEU:HD11	1:B:29:GLN:HE21	8	0.42
(1,8)	1:A:12:LEU:HD12	1:B:29:GLN:HE21	8	0.42
(1,8)	1:A:12:LEU:HD13	1:B:29:GLN:HE21	8	0.42
(1,513)	1:A:36:GLN:HG2	1:A:37:GLY:H	3	0.42
(1,513)	1:A:36:GLN:HG2	1:A:37:GLY:H	8	0.42
(1,470)	1:A:33:LEU:HD11	1:A:44:ILE:HA	6	0.42
(1,470)	1:A:33:LEU:HD12	1:A:44:ILE:HA	6	0.42
(1,470)	1:A:33:LEU:HD13	1:A:44:ILE:HA	6	0.42
(1,470)	1:A:33:LEU:HD11	1:A:44:ILE:HA	18	0.42
(1,470)	1:A:33:LEU:HD12	1:A:44:ILE:HA	18	0.42
(1,470)	1:A:33:LEU:HD13	1:A:44:ILE:HA	18	0.42
(1,245)	1:A:18:VAL:HG11	1:A:65:GLY:HA2	19	0.42
(1,245)	1:A:18:VAL:HG12	1:A:65:GLY:HA2	19	0.42
(1,245)	1:A:18:VAL:HG13	1:A:65:GLY:HA2	19	0.42
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	2	0.42
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	7	0.42
(1,2287)	1:B:90:PHE:HB2	1:B:93:VAL:HG11	3	0.42
(1,2287)	1:B:90:PHE:HB2	1:B:93:VAL:HG12	3	0.42
(1,2287)	1:B:90:PHE:HB2	1:B:93:VAL:HG13	3	0.42
(1,2287)	1:B:90:PHE:HB2	1:B:93:VAL:HG11	8	0.42

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2287)	1:B:90:PHE:HB2	1:B:93:VAL:HG12	8	0.42
(1,2287)	1:B:90:PHE:HB2	1:B:93:VAL:HG13	8	0.42
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	13	0.42
(1,2134)	1:B:74:GLY:HA2	1:B:75:THR:HB	12	0.42
(1,1994)	1:B:63:LYS:HD2	1:B:79:TYR:HE1	15	0.42
(1,1994)	1:B:63:LYS:HD3	1:B:79:TYR:HE1	15	0.42
(1,1854)	1:B:51:ASN:HB2	1:B:53:THR:H	20	0.42
(1,1753)	1:B:42:GLU:H	1:B:42:GLU:HG2	6	0.42
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD11	6	0.42
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD12	6	0.42
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD13	6	0.42
(1,1657)	1:B:38:GLU:HG2	1:B:78:TYR:HB2	3	0.42
(1,1657)	1:B:38:GLU:HG3	1:B:78:TYR:HB2	3	0.42
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	11	0.42
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	11	0.42
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	11	0.42
(1,1460)	1:B:27:ARG:HD2	1:B:58:ASN:HA	18	0.42
(1,1375)	1:B:18:VAL:HG11	1:B:22:LEU:H	1	0.42
(1,1375)	1:B:18:VAL:HG12	1:B:22:LEU:H	1	0.42
(1,1375)	1:B:18:VAL:HG13	1:B:22:LEU:H	1	0.42
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	2	0.42
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	4	0.42
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG11	2	0.42
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG12	2	0.42
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG13	2	0.42
(1,1041)	1:A:79:TYR:HA	1:A:80:ARG:HG2	6	0.42
(1,1021)	1:A:76:ARG:HG2	1:A:77:GLN:H	2	0.42
(1,989)	1:A:72:ARG:H	1:A:72:ARG:HB2	6	0.41
(1,989)	1:A:72:ARG:H	1:A:72:ARG:HB2	20	0.41
(1,972)	1:A:71:ARG:HG2	1:A:78:TYR:HB2	4	0.41
(1,840)	1:A:62:LEU:HB2	1:A:68:VAL:HG11	5	0.41
(1,840)	1:A:62:LEU:HB2	1:A:68:VAL:HG12	5	0.41
(1,840)	1:A:62:LEU:HB2	1:A:68:VAL:HG13	5	0.41
(1,8)	1:A:12:LEU:HD11	1:B:29:GLN:HE21	12	0.41
(1,8)	1:A:12:LEU:HD12	1:B:29:GLN:HE21	12	0.41
(1,8)	1:A:12:LEU:HD13	1:B:29:GLN:HE21	12	0.41
(1,8)	1:A:12:LEU:HD11	1:B:29:GLN:HE21	14	0.41
(1,8)	1:A:12:LEU:HD12	1:B:29:GLN:HE21	14	0.41
(1,8)	1:A:12:LEU:HD13	1:B:29:GLN:HE21	14	0.41
(1,742)	1:A:52:LEU:HD11	1:A:56:SER:H	11	0.41
(1,742)	1:A:52:LEU:HD12	1:A:56:SER:H	11	0.41
(1,742)	1:A:52:LEU:HD13	1:A:56:SER:H	11	0.41

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	1	0.41
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	1	0.41
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	1	0.41
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD11	11	0.41
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD12	11	0.41
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD13	11	0.41
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD11	11	0.41
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD12	11	0.41
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD13	11	0.41
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD11	11	0.41
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD12	11	0.41
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD13	11	0.41
(1,2383)	1:B:101:LEU:HB2	1:B:102:GLU:H	15	0.41
(1,2374)	1:B:99:GLU:HG2	1:B:100:HIS:H	13	0.41
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	9	0.41
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	11	0.41
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	12	0.41
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	16	0.41
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	20	0.41
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	15	0.41
(1,2179)	1:B:80:ARG:H	1:B:80:ARG:HG2	10	0.41
(1,2154)	1:B:76:ARG:HG2	1:B:78:TYR:HE1	1	0.41
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	18	0.41
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	18	0.41
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	18	0.41
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD11	13	0.41
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD12	13	0.41
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD13	13	0.41
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	10	0.41
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	10	0.41
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	10	0.41
(1,1645)	1:B:36:GLN:HG2	1:B:37:GLY:H	17	0.41
(1,1607)	1:B:33:LEU:HG	1:B:36:GLN:HE21	4	0.41
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG21	12	0.41
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG22	12	0.41
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG23	12	0.41
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	2	0.41
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	11	0.41
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	7	0.41
(1,1035)	1:A:77:GLN:HG2	1:A:79:TYR:HE1	3	0.41
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	17	0.4
(1,766)	1:A:55:ALA:HB1	1:A:58:ASN:HB2	1	0.4

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,766)	1:A:55:ALA:HB2	1:A:58:ASN:HB2	1	0.4
(1,766)	1:A:55:ALA:HB3	1:A:58:ASN:HB2	1	0.4
(1,705)	1:A:50:MET:HB2	1:A:55:ALA:H	1	0.4
(1,515)	1:A:36:GLN:H	1:A:36:GLN:HG2	13	0.4
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	14	0.4
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	17	0.4
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	18	0.4
(1,2169)	1:B:77:GLN:H	1:B:77:GLN:HG2	14	0.4
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB2	18	0.4
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB3	18	0.4
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB2	18	0.4
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB3	18	0.4
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB2	18	0.4
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB3	18	0.4
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB1	18	0.4
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB2	18	0.4
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB3	18	0.4
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	5	0.4
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	5	0.4
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	5	0.4
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	16	0.4
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	16	0.4
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	16	0.4
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	16	0.4
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	16	0.4
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	16	0.4
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	16	0.4
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	16	0.4
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	16	0.4
(1,1668)	1:B:39:ARG:HD2	1:B:40:ALA:H	10	0.4
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	14	0.4
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	14	0.4
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	14	0.4
(1,141)	1:A:7:ARG:HB2	1:A:8:LYS:H	11	0.4
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	17	0.4
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD11	7	0.4
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD12	7	0.4
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD13	7	0.4
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	1	0.4
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	20	0.4
(1,1195)	1:A:94:GLN:HG2	1:A:95:VAL:H	15	0.4
(1,1166)	1:A:91:ALA:HA	1:A:94:GLN:HG2	8	0.4

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1037)	1:A:77:GLN:H	1:A:77:GLN:HG2	6	0.4
(1,1022)	1:A:76:ARG:HG2	1:A:78:TYR:HE1	5	0.4
(1,994)	1:A:73:GLU:HB2	1:A:78:TYR:HD1	2	0.39
(1,993)	1:A:73:GLU:HB2	1:A:76:ARG:HG2	3	0.39
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB2	1	0.39
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB3	1	0.39
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB2	1	0.39
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB3	1	0.39
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB2	1	0.39
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB3	1	0.39
(1,621)	1:A:42:GLU:H	1:A:42:GLU:HG2	20	0.39
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	7	0.39
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	7	0.39
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	7	0.39
(1,559)	1:A:40:ALA:HB1	1:A:78:TYR:HE1	17	0.39
(1,559)	1:A:40:ALA:HB2	1:A:78:TYR:HE1	17	0.39
(1,559)	1:A:40:ALA:HB3	1:A:78:TYR:HE1	17	0.39
(1,513)	1:A:36:GLN:HG2	1:A:37:GLY:H	6	0.39
(1,464)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	6	0.39
(1,464)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	6	0.39
(1,464)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	6	0.39
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	7	0.39
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	7	0.39
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	7	0.39
(1,42)	1:A:16:ALA:HB1	1:B:25:GLY:HA2	17	0.39
(1,42)	1:A:16:ALA:HB2	1:B:25:GLY:HA2	17	0.39
(1,42)	1:A:16:ALA:HB3	1:B:25:GLY:HA2	17	0.39
(1,2383)	1:B:101:LEU:HB2	1:B:102:GLU:H	1	0.39
(1,2327)	1:B:94:GLN:HG2	1:B:95:VAL:H	10	0.39
(1,2169)	1:B:77:GLN:H	1:B:77:GLN:HG2	1	0.39
(1,2169)	1:B:77:GLN:H	1:B:77:GLN:HG2	13	0.39
(1,2167)	1:B:77:GLN:HG2	1:B:79:TYR:HE1	18	0.39
(1,2095)	1:B:70:ALA:HB1	1:B:79:TYR:HE1	13	0.39
(1,2095)	1:B:70:ALA:HB2	1:B:79:TYR:HE1	13	0.39
(1,2095)	1:B:70:ALA:HB3	1:B:79:TYR:HE1	13	0.39
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB2	20	0.39
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB3	20	0.39
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB2	20	0.39
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB3	20	0.39
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB2	20	0.39
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB3	20	0.39
(1,1854)	1:B:51:ASN:HB2	1:B:53:THR:H	18	0.39

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1849)	1:B:50:MET:H	1:B:50:MET:HG2	1	0.39
(1,1753)	1:B:42:GLU:H	1:B:42:GLU:HG2	1	0.39
(1,1669)	1:B:39:ARG:HD2	1:B:43:ALA:HB1	16	0.39
(1,1669)	1:B:39:ARG:HD2	1:B:43:ALA:HB2	16	0.39
(1,1669)	1:B:39:ARG:HD2	1:B:43:ALA:HB3	16	0.39
(1,1668)	1:B:39:ARG:HD2	1:B:40:ALA:H	9	0.39
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG21	14	0.39
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG22	14	0.39
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG23	14	0.39
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB1	18	0.39
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB2	18	0.39
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB3	18	0.39
(1,1375)	1:B:18:VAL:HG11	1:B:22:LEU:H	2	0.39
(1,1375)	1:B:18:VAL:HG12	1:B:22:LEU:H	2	0.39
(1,1375)	1:B:18:VAL:HG13	1:B:22:LEU:H	2	0.39
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	14	0.39
(1,1021)	1:A:76:ARG:HG2	1:A:77:GLN:H	4	0.39
(1,999)	1:A:73:GLU:H	1:A:76:ARG:HG2	13	0.38
(1,972)	1:A:71:ARG:HG2	1:A:78:TYR:HB2	13	0.38
(1,9)	1:A:12:LEU:HD11	1:B:29:GLN:HG2	17	0.38
(1,9)	1:A:12:LEU:HD12	1:B:29:GLN:HG2	17	0.38
(1,9)	1:A:12:LEU:HD13	1:B:29:GLN:HG2	17	0.38
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	19	0.38
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	19	0.38
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	13	0.38
(1,742)	1:A:52:LEU:HD11	1:A:56:SER:H	3	0.38
(1,742)	1:A:52:LEU:HD12	1:A:56:SER:H	3	0.38
(1,742)	1:A:52:LEU:HD13	1:A:56:SER:H	3	0.38
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	8	0.38
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	12	0.38
(1,71)	1:B:12:LEU:HD11	1:A:29:GLN:HE21	8	0.38
(1,71)	1:B:12:LEU:HD12	1:A:29:GLN:HE21	8	0.38
(1,71)	1:B:12:LEU:HD13	1:A:29:GLN:HE21	8	0.38
(1,615)	1:A:42:GLU:HG2	1:A:52:LEU:HG	6	0.38
(1,536)	1:A:39:ARG:HD2	1:A:40:ALA:H	1	0.38
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	6	0.38
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	13	0.38
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA2	4	0.38
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	19	0.38
(1,2171)	1:B:78:TYR:H	1:B:78:TYR:HD1	10	0.38
(1,2169)	1:B:77:GLN:H	1:B:77:GLN:HG2	19	0.38
(1,2134)	1:B:74:GLY:HA2	1:B:75:THR:HB	16	0.38

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1934)	1:B:59:LEU:HB2	1:B:79:TYR:HE1	14	0.38
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB1	3	0.38
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB2	3	0.38
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB3	3	0.38
(1,1726)	1:B:41:VAL:HG21	1:B:77:GLN:HG2	8	0.38
(1,1726)	1:B:41:VAL:HG22	1:B:77:GLN:HG2	8	0.38
(1,1726)	1:B:41:VAL:HG23	1:B:77:GLN:HG2	8	0.38
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	18	0.38
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	18	0.38
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	18	0.38
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	18	0.38
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	18	0.38
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	18	0.38
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	18	0.38
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	18	0.38
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	18	0.38
(1,1681)	1:B:40:ALA:HB1	1:B:42:GLU:HG2	4	0.38
(1,1681)	1:B:40:ALA:HB2	1:B:42:GLU:HG2	4	0.38
(1,1681)	1:B:40:ALA:HB3	1:B:42:GLU:HG2	4	0.38
(1,1681)	1:B:40:ALA:HB1	1:B:42:GLU:HG2	7	0.38
(1,1681)	1:B:40:ALA:HB2	1:B:42:GLU:HG2	7	0.38
(1,1681)	1:B:40:ALA:HB3	1:B:42:GLU:HG2	7	0.38
(1,1657)	1:B:38:GLU:HG2	1:B:78:TYR:HB2	4	0.38
(1,1657)	1:B:38:GLU:HG3	1:B:78:TYR:HB2	4	0.38
(1,1634)	1:B:35:ALA:HB1	1:B:36:GLN:HE21	10	0.38
(1,1634)	1:B:35:ALA:HB2	1:B:36:GLN:HE21	10	0.38
(1,1634)	1:B:35:ALA:HB3	1:B:36:GLN:HE21	10	0.38
(1,1618)	1:B:34:LEU:HB2	1:B:80:ARG:HA	20	0.38
(1,1462)	1:B:27:ARG:HD2	1:B:62:LEU:H	18	0.38
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	10	0.38
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG11	10	0.38
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG12	10	0.38
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG13	10	0.38
(1,1035)	1:A:77:GLN:HG2	1:A:79:TYR:HE1	2	0.38
(1,839)	1:A:62:LEU:HB2	1:A:67:LEU:HD21	13	0.37
(1,839)	1:A:62:LEU:HB2	1:A:67:LEU:HD22	13	0.37
(1,839)	1:A:62:LEU:HB2	1:A:67:LEU:HD23	13	0.37
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	2	0.37
(1,621)	1:A:42:GLU:H	1:A:42:GLU:HG2	1	0.37
(1,4)	1:A:11:LEU:HD11	1:B:98:ASP:H	10	0.37
(1,4)	1:A:11:LEU:HD12	1:B:98:ASP:H	10	0.37
(1,4)	1:A:11:LEU:HD13	1:B:98:ASP:H	10	0.37

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2340)	1:B:95:VAL:HG11	1:B:98:ASP:HB2	8	0.37
(1,2340)	1:B:95:VAL:HG12	1:B:98:ASP:HB2	8	0.37
(1,2340)	1:B:95:VAL:HG13	1:B:98:ASP:HB2	8	0.37
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	14	0.37
(1,2328)	1:B:94:GLN:H	1:B:94:GLN:HG2	15	0.37
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	4	0.37
(1,2179)	1:B:80:ARG:H	1:B:80:ARG:HG2	14	0.37
(1,2179)	1:B:80:ARG:H	1:B:80:ARG:HG2	17	0.37
(1,2169)	1:B:77:GLN:H	1:B:77:GLN:HG2	15	0.37
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	1	0.37
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	1	0.37
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	16	0.37
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	16	0.37
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB1	14	0.37
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB2	14	0.37
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB3	14	0.37
(1,1747)	1:B:42:GLU:HG2	1:B:52:LEU:HG	14	0.37
(1,1596)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	15	0.37
(1,1596)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	15	0.37
(1,1596)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	15	0.37
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	12	0.37
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	12	0.37
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	12	0.37
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG21	7	0.37
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG22	7	0.37
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG23	7	0.37
(1,141)	1:A:7:ARG:HB2	1:A:8:LYS:H	20	0.37
(1,1377)	1:B:18:VAL:HG11	1:B:65:GLY:HA2	18	0.37
(1,1377)	1:B:18:VAL:HG12	1:B:65:GLY:HA2	18	0.37
(1,1377)	1:B:18:VAL:HG13	1:B:65:GLY:HA2	18	0.37
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	3	0.37
(1,1304)	1:B:11:LEU:HA	1:B:14:GLN:HG2	19	0.37
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	9	0.37
(1,1195)	1:A:94:GLN:HG2	1:A:95:VAL:H	18	0.37
(1,1059)	1:A:81:ILE:HG12	1:A:87:ALA:HA	12	0.37
(1,1002)	1:A:74:GLY:HA2	1:A:75:THR:HB	13	0.37
(1,989)	1:A:72:ARG:H	1:A:72:ARG:HB2	12	0.36
(1,987)	1:A:72:ARG:HD2	1:A:77:GLN:HG2	19	0.36
(1,987)	1:A:72:ARG:HD3	1:A:77:GLN:HG2	19	0.36
(1,859)	1:A:63:LYS:HB2	1:A:69:GLU:HA	15	0.36
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG2	18	0.36
(1,594)	1:A:41:VAL:HG21	1:A:77:GLN:HG2	2	0.36

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,594)	1:A:41:VAL:HG22	1:A:77:GLN:HG2	2	0.36
(1,594)	1:A:41:VAL:HG23	1:A:77:GLN:HG2	2	0.36
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD11	8	0.36
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD12	8	0.36
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD13	8	0.36
(1,523)	1:A:38:GLU:HB2	1:A:80:ARG:HG2	17	0.36
(1,523)	1:A:38:GLU:HB3	1:A:80:ARG:HG2	17	0.36
(1,513)	1:A:36:GLN:HG2	1:A:37:GLY:H	12	0.36
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	18	0.36
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	18	0.36
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	18	0.36
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	6	0.36
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	6	0.36
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	6	0.36
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	15	0.36
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD11	10	0.36
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD12	10	0.36
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD13	10	0.36
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA2	3	0.36
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	11	0.36
(1,1874)	1:B:52:LEU:HD11	1:B:56:SER:H	17	0.36
(1,1874)	1:B:52:LEU:HD12	1:B:56:SER:H	17	0.36
(1,1874)	1:B:52:LEU:HD13	1:B:56:SER:H	17	0.36
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB1	1	0.36
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB2	1	0.36
(1,1846)	1:B:50:MET:HG2	1:B:55:ALA:HB3	1	0.36
(1,1753)	1:B:42:GLU:H	1:B:42:GLU:HG2	16	0.36
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	19	0.36
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	19	0.36
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	19	0.36
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	19	0.36
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	19	0.36
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	19	0.36
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	19	0.36
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	19	0.36
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	19	0.36
(1,1668)	1:B:39:ARG:HD2	1:B:40:ALA:H	4	0.36
(1,1645)	1:B:36:GLN:HG2	1:B:37:GLY:H	4	0.36
(1,1634)	1:B:35:ALA:HB1	1:B:36:GLN:HE21	12	0.36
(1,1634)	1:B:35:ALA:HB2	1:B:36:GLN:HE21	12	0.36
(1,1634)	1:B:35:ALA:HB3	1:B:36:GLN:HE21	12	0.36
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	18	0.36

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	18	0.36
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	18	0.36
(1,141)	1:A:7:ARG:HB2	1:A:8:LYS:H	12	0.36
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	1	0.36
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	15	0.36
(1,1219)	1:A:96:VAL:HA	1:A:99:GLU:HB2	6	0.36
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	19	0.36
(1,1166)	1:A:91:ALA:HA	1:A:94:GLN:HG2	2	0.36
(1,1166)	1:A:91:ALA:HA	1:A:94:GLN:HG2	10	0.36
(1,1166)	1:A:91:ALA:HA	1:A:94:GLN:HG2	13	0.36
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	14	0.35
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	14	0.35
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	14	0.35
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	14	0.35
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	14	0.35
(1,558)	1:A:40:ALA:HB1	1:A:78:TYR:HD1	8	0.35
(1,558)	1:A:40:ALA:HB2	1:A:78:TYR:HD1	8	0.35
(1,558)	1:A:40:ALA:HB3	1:A:78:TYR:HD1	8	0.35
(1,471)	1:A:33:LEU:HD11	1:A:44:ILE:H	8	0.35
(1,471)	1:A:33:LEU:HD12	1:A:44:ILE:H	8	0.35
(1,471)	1:A:33:LEU:HD13	1:A:44:ILE:H	8	0.35
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	19	0.35
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	19	0.35
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	19	0.35
(1,2298)	1:B:91:ALA:HA	1:B:94:GLN:HG2	7	0.35
(1,2169)	1:B:77:GLN:H	1:B:77:GLN:HG2	16	0.35
(1,2167)	1:B:77:GLN:HG2	1:B:79:TYR:HE1	4	0.35
(1,2134)	1:B:74:GLY:HA2	1:B:75:THR:HB	18	0.35
(1,1934)	1:B:59:LEU:HB2	1:B:79:TYR:HE1	4	0.35
(1,1849)	1:B:50:MET:H	1:B:50:MET:HG2	2	0.35
(1,1726)	1:B:41:VAL:HG21	1:B:77:GLN:HG2	18	0.35
(1,1726)	1:B:41:VAL:HG22	1:B:77:GLN:HG2	18	0.35
(1,1726)	1:B:41:VAL:HG23	1:B:77:GLN:HG2	18	0.35
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	2	0.35
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	2	0.35
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	2	0.35
(1,1597)	1:B:33:LEU:HD11	1:B:36:GLN:H	16	0.35
(1,1597)	1:B:33:LEU:HD12	1:B:36:GLN:H	16	0.35
(1,1597)	1:B:33:LEU:HD13	1:B:36:GLN:H	16	0.35
(1,1492)	1:B:29:GLN:HG2	1:B:48:THR:HB	4	0.35
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	20	0.35
(1,1196)	1:A:94:GLN:H	1:A:94:GLN:HG2	5	0.35

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1042)	1:A:79:TYR:H	1:A:79:TYR:HD1	11	0.35
(1,1037)	1:A:77:GLN:H	1:A:77:GLN:HG2	9	0.35
(1,1022)	1:A:76:ARG:HG2	1:A:78:TYR:HE1	6	0.35
(1,1002)	1:A:74:GLY:HA2	1:A:75:THR:HB	8	0.35
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	2	0.34
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	2	0.34
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	19	0.34
(1,8)	1:A:12:LEU:HD11	1:B:29:GLN:HE21	7	0.34
(1,8)	1:A:12:LEU:HD12	1:B:29:GLN:HE21	7	0.34
(1,8)	1:A:12:LEU:HD13	1:B:29:GLN:HE21	7	0.34
(1,742)	1:A:52:LEU:HD11	1:A:56:SER:H	8	0.34
(1,742)	1:A:52:LEU:HD12	1:A:56:SER:H	8	0.34
(1,742)	1:A:52:LEU:HD13	1:A:56:SER:H	8	0.34
(1,704)	1:A:50:MET:HB2	1:A:55:ALA:HB1	16	0.34
(1,704)	1:A:50:MET:HB2	1:A:55:ALA:HB2	16	0.34
(1,704)	1:A:50:MET:HB2	1:A:55:ALA:HB3	16	0.34
(1,691)	1:A:48:THR:HB	1:A:50:MET:HG2	13	0.34
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	1	0.34
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	1	0.34
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	1	0.34
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	3	0.34
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	3	0.34
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	3	0.34
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG21	13	0.34
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG22	13	0.34
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG23	13	0.34
(1,2298)	1:B:91:ALA:HA	1:B:94:GLN:HG2	5	0.34
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	9	0.34
(1,2227)	1:B:84:GLU:HG2	1:B:88:ARG:HG2	3	0.34
(1,2227)	1:B:84:GLU:HG3	1:B:88:ARG:HG2	3	0.34
(1,2113)	1:B:72:ARG:HA	1:B:77:GLN:HG2	15	0.34
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	12	0.34
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	12	0.34
(1,1849)	1:B:50:MET:H	1:B:50:MET:HG2	3	0.34
(1,1849)	1:B:50:MET:H	1:B:50:MET:HG2	4	0.34
(1,1657)	1:B:38:GLU:HG2	1:B:78:TYR:HB2	11	0.34
(1,1657)	1:B:38:GLU:HG3	1:B:78:TYR:HB2	11	0.34
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG21	5	0.34
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG22	5	0.34
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG23	5	0.34
(1,1361)	1:B:17:ARG:HA	1:B:65:GLY:HA2	8	0.34
(1,1361)	1:B:17:ARG:HA	1:B:65:GLY:HA2	14	0.34

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	8	0.34
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB2	2	0.33
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB3	2	0.33
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB2	2	0.33
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB3	2	0.33
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB2	2	0.33
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB3	2	0.33
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD11	2	0.33
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD12	2	0.33
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD13	2	0.33
(1,594)	1:A:41:VAL:HG21	1:A:77:GLN:HG2	18	0.33
(1,594)	1:A:41:VAL:HG22	1:A:77:GLN:HG2	18	0.33
(1,594)	1:A:41:VAL:HG23	1:A:77:GLN:HG2	18	0.33
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD11	16	0.33
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD12	16	0.33
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD13	16	0.33
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD11	16	0.33
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD12	16	0.33
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD13	16	0.33
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD11	16	0.33
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD12	16	0.33
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD13	16	0.33
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	17	0.33
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	17	0.33
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	17	0.33
(1,4)	1:A:11:LEU:HD11	1:B:98:ASP:H	7	0.33
(1,4)	1:A:11:LEU:HD12	1:B:98:ASP:H	7	0.33
(1,4)	1:A:11:LEU:HD13	1:B:98:ASP:H	7	0.33
(1,330)	1:A:27:ARG:HD2	1:A:62:LEU:H	8	0.33
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD21	2	0.33
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD22	2	0.33
(1,315)	1:A:25:GLY:HA2	1:A:28:LEU:HD23	2	0.33
(1,2383)	1:B:101:LEU:HB2	1:B:102:GLU:H	14	0.33
(1,2254)	1:B:87:ALA:H	1:B:88:ARG:HG2	4	0.33
(1,1691)	1:B:40:ALA:HB1	1:B:78:TYR:HE1	9	0.33
(1,1691)	1:B:40:ALA:HB2	1:B:78:TYR:HE1	9	0.33
(1,1691)	1:B:40:ALA:HB3	1:B:78:TYR:HE1	9	0.33
(1,1691)	1:B:40:ALA:HB1	1:B:78:TYR:HE1	14	0.33
(1,1691)	1:B:40:ALA:HB2	1:B:78:TYR:HE1	14	0.33
(1,1691)	1:B:40:ALA:HB3	1:B:78:TYR:HE1	14	0.33
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD11	2	0.33
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD12	2	0.33

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD13	2	0.33
(1,1602)	1:B:33:LEU:HD11	1:B:44:ILE:HA	13	0.33
(1,1602)	1:B:33:LEU:HD12	1:B:44:ILE:HA	13	0.33
(1,1602)	1:B:33:LEU:HD13	1:B:44:ILE:HA	13	0.33
(1,1596)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	8	0.33
(1,1596)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	8	0.33
(1,1596)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	8	0.33
(1,1441)	1:B:24:ASN:H	1:B:24:ASN:HB2	11	0.33
(1,1296)	1:B:10:ALA:HB1	1:B:13:ASP:HB2	6	0.33
(1,1296)	1:B:10:ALA:HB2	1:B:13:ASP:HB2	6	0.33
(1,1296)	1:B:10:ALA:HB3	1:B:13:ASP:HB2	6	0.33
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD11	1	0.33
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD12	1	0.33
(1,1280)	1:B:8:LYS:HA	1:B:11:LEU:HD13	1	0.33
(1,1273)	1:B:7:ARG:HB2	1:B:8:LYS:H	8	0.33
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD21	4	0.33
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD22	4	0.33
(1,1131)	1:A:88:ARG:HB2	1:A:92:LEU:HD23	4	0.33
(1,1047)	1:A:80:ARG:H	1:A:80:ARG:HG2	11	0.33
(1,1037)	1:A:77:GLN:H	1:A:77:GLN:HG2	1	0.33
(1,1013)	1:A:76:ARG:HB2	1:A:78:TYR:HD1	18	0.33
(1,999)	1:A:73:GLU:H	1:A:76:ARG:HG2	17	0.32
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	10	0.32
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	10	0.32
(1,742)	1:A:52:LEU:HD11	1:A:56:SER:H	19	0.32
(1,742)	1:A:52:LEU:HD12	1:A:56:SER:H	19	0.32
(1,742)	1:A:52:LEU:HD13	1:A:56:SER:H	19	0.32
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB2	3	0.32
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB3	3	0.32
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB2	3	0.32
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB3	3	0.32
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB2	3	0.32
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB3	3	0.32
(1,7)	1:A:12:LEU:HD11	1:B:29:GLN:HB2	4	0.32
(1,7)	1:A:12:LEU:HD12	1:B:29:GLN:HB2	4	0.32
(1,7)	1:A:12:LEU:HD13	1:B:29:GLN:HB2	4	0.32
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD11	7	0.32
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD12	7	0.32
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD13	7	0.32
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD21	10	0.32
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD22	10	0.32
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD23	10	0.32

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	14	0.32
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	14	0.32
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	14	0.32
(1,2343)	1:B:95:VAL:HG11	1:B:99:GLU:HG2	11	0.32
(1,2343)	1:B:95:VAL:HG12	1:B:99:GLU:HG2	11	0.32
(1,2343)	1:B:95:VAL:HG13	1:B:99:GLU:HG2	11	0.32
(1,2298)	1:B:91:ALA:HA	1:B:94:GLN:HG2	9	0.32
(1,2179)	1:B:80:ARG:H	1:B:80:ARG:HG2	2	0.32
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	3	0.32
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	3	0.32
(1,1934)	1:B:59:LEU:HB2	1:B:79:TYR:HE1	12	0.32
(1,1849)	1:B:50:MET:H	1:B:50:MET:HG2	10	0.32
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB1	8	0.32
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB2	8	0.32
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB3	8	0.32
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB1	16	0.32
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB2	16	0.32
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB3	16	0.32
(1,1669)	1:B:39:ARG:HD2	1:B:43:ALA:HB1	12	0.32
(1,1669)	1:B:39:ARG:HD2	1:B:43:ALA:HB2	12	0.32
(1,1669)	1:B:39:ARG:HD2	1:B:43:ALA:HB3	12	0.32
(1,1599)	1:B:33:LEU:HD11	1:B:39:ARG:HD2	7	0.32
(1,1599)	1:B:33:LEU:HD12	1:B:39:ARG:HD2	7	0.32
(1,1599)	1:B:33:LEU:HD13	1:B:39:ARG:HD2	7	0.32
(1,1492)	1:B:29:GLN:HG2	1:B:48:THR:HB	5	0.32
(1,141)	1:A:7:ARG:HB2	1:A:8:LYS:H	8	0.32
(1,1361)	1:B:17:ARG:HA	1:B:65:GLY:HA2	16	0.32
(1,120)	1:B:88:ARG:HB2	1:A:92:LEU:HD11	2	0.32
(1,120)	1:B:88:ARG:HB2	1:A:92:LEU:HD12	2	0.32
(1,120)	1:B:88:ARG:HB2	1:A:92:LEU:HD13	2	0.32
(1,1059)	1:A:81:ILE:HG12	1:A:87:ALA:HA	4	0.32
(1,1047)	1:A:80:ARG:H	1:A:80:ARG:HG2	1	0.32
(1,1047)	1:A:80:ARG:H	1:A:80:ARG:HG2	13	0.32
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD11	19	0.31
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD12	19	0.31
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD13	19	0.31
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD11	19	0.31
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD12	19	0.31
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD13	19	0.31
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD11	19	0.31
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD12	19	0.31
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD13	19	0.31

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,243)	1:A:18:VAL:HG11	1:A:22:LEU:H	10	0.31
(1,243)	1:A:18:VAL:HG12	1:A:22:LEU:H	10	0.31
(1,243)	1:A:18:VAL:HG13	1:A:22:LEU:H	10	0.31
(1,2179)	1:B:80:ARG:H	1:B:80:ARG:HG2	3	0.31
(1,2169)	1:B:77:GLN:H	1:B:77:GLN:HG2	6	0.31
(1,2153)	1:B:76:ARG:HG2	1:B:77:GLN:H	18	0.31
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB2	16	0.31
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB3	16	0.31
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB2	16	0.31
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB3	16	0.31
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB2	16	0.31
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB3	16	0.31
(1,164)	1:A:10:ALA:HB1	1:A:13:ASP:HB2	15	0.31
(1,164)	1:A:10:ALA:HB2	1:A:13:ASP:HB2	15	0.31
(1,164)	1:A:10:ALA:HB3	1:A:13:ASP:HB2	15	0.31
(1,1596)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	9	0.31
(1,1596)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	9	0.31
(1,1596)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	9	0.31
(1,1296)	1:B:10:ALA:HB1	1:B:13:ASP:HB2	9	0.31
(1,1296)	1:B:10:ALA:HB2	1:B:13:ASP:HB2	9	0.31
(1,1296)	1:B:10:ALA:HB3	1:B:13:ASP:HB2	9	0.31
(1,1273)	1:B:7:ARG:HB2	1:B:8:LYS:H	10	0.31
(1,1095)	1:A:84:GLU:HG2	1:A:88:ARG:HG2	14	0.31
(1,1095)	1:A:84:GLU:HG3	1:A:88:ARG:HG2	14	0.31
(1,1)	1:A:11:LEU:HD11	1:B:98:ASP:HA	7	0.31
(1,1)	1:A:11:LEU:HD12	1:B:98:ASP:HA	7	0.31
(1,1)	1:A:11:LEU:HD13	1:B:98:ASP:HA	7	0.31
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD11	14	0.3
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD12	14	0.3
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD13	14	0.3
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	1	0.3
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	1	0.3
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	6	0.3
(1,594)	1:A:41:VAL:HG21	1:A:77:GLN:HG2	7	0.3
(1,594)	1:A:41:VAL:HG22	1:A:77:GLN:HG2	7	0.3
(1,594)	1:A:41:VAL:HG23	1:A:77:GLN:HG2	7	0.3
(1,559)	1:A:40:ALA:HB1	1:A:78:TYR:HE1	1	0.3
(1,559)	1:A:40:ALA:HB2	1:A:78:TYR:HE1	1	0.3
(1,559)	1:A:40:ALA:HB3	1:A:78:TYR:HE1	1	0.3
(1,473)	1:A:33:LEU:HD11	1:A:47:ALA:H	12	0.3
(1,473)	1:A:33:LEU:HD12	1:A:47:ALA:H	12	0.3
(1,473)	1:A:33:LEU:HD13	1:A:47:ALA:H	12	0.3

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB1	14	0.3
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB2	14	0.3
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB3	14	0.3
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB1	14	0.3
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB2	14	0.3
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB3	14	0.3
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB1	14	0.3
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB2	14	0.3
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB3	14	0.3
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB1	19	0.3
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB2	19	0.3
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB3	19	0.3
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB1	19	0.3
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB2	19	0.3
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB3	19	0.3
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB1	19	0.3
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB2	19	0.3
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB3	19	0.3
(1,36)	1:A:15:VAL:HG11	1:B:97:ALA:HB1	16	0.3
(1,36)	1:A:15:VAL:HG11	1:B:97:ALA:HB2	16	0.3
(1,36)	1:A:15:VAL:HG11	1:B:97:ALA:HB3	16	0.3
(1,36)	1:A:15:VAL:HG12	1:B:97:ALA:HB1	16	0.3
(1,36)	1:A:15:VAL:HG12	1:B:97:ALA:HB2	16	0.3
(1,36)	1:A:15:VAL:HG12	1:B:97:ALA:HB3	16	0.3
(1,36)	1:A:15:VAL:HG13	1:B:97:ALA:HB1	16	0.3
(1,36)	1:A:15:VAL:HG13	1:B:97:ALA:HB2	16	0.3
(1,36)	1:A:15:VAL:HG13	1:B:97:ALA:HB3	16	0.3
(1,2383)	1:B:101:LEU:HB2	1:B:102:GLU:H	12	0.3
(1,2173)	1:B:79:TYR:HA	1:B:80:ARG:HG2	1	0.3
(1,2171)	1:B:78:TYR:H	1:B:78:TYR:HD1	16	0.3
(1,2139)	1:B:75:THR:H	1:B:76:ARG:HG2	12	0.3
(1,2095)	1:B:70:ALA:HB1	1:B:79:TYR:HE1	11	0.3
(1,2095)	1:B:70:ALA:HB2	1:B:79:TYR:HE1	11	0.3
(1,2095)	1:B:70:ALA:HB3	1:B:79:TYR:HE1	11	0.3
(1,1934)	1:B:59:LEU:HB2	1:B:79:TYR:HE1	7	0.3
(1,1691)	1:B:40:ALA:HB1	1:B:78:TYR:HE1	5	0.3
(1,1691)	1:B:40:ALA:HB2	1:B:78:TYR:HE1	5	0.3
(1,1691)	1:B:40:ALA:HB3	1:B:78:TYR:HE1	5	0.3
(1,1690)	1:B:40:ALA:HB1	1:B:78:TYR:HD1	14	0.3
(1,1690)	1:B:40:ALA:HB2	1:B:78:TYR:HD1	14	0.3
(1,1690)	1:B:40:ALA:HB3	1:B:78:TYR:HD1	14	0.3
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	14	0.3

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	14	0.3
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	14	0.3
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	14	0.3
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	14	0.3
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	14	0.3
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	14	0.3
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	14	0.3
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	14	0.3
(1,164)	1:A:10:ALA:HB1	1:A:13:ASP:HB2	2	0.3
(1,164)	1:A:10:ALA:HB2	1:A:13:ASP:HB2	2	0.3
(1,164)	1:A:10:ALA:HB3	1:A:13:ASP:HB2	2	0.3
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	15	0.3
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	15	0.3
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	15	0.3
(1,1451)	1:B:26:ARG:H	1:B:26:ARG:HG2	15	0.3
(1,1451)	1:B:26:ARG:H	1:B:26:ARG:HG3	15	0.3
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	7	0.3
(1,1059)	1:A:81:ILE:HG12	1:A:87:ALA:HA	8	0.3
(1,1037)	1:A:77:GLN:H	1:A:77:GLN:HG2	14	0.3
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	15	0.29
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	15	0.29
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	3	0.29
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	14	0.29
(1,549)	1:A:40:ALA:HB1	1:A:42:GLU:HG2	15	0.29
(1,549)	1:A:40:ALA:HB2	1:A:42:GLU:HG2	15	0.29
(1,549)	1:A:40:ALA:HB3	1:A:42:GLU:HG2	15	0.29
(1,525)	1:A:38:GLU:HG2	1:A:78:TYR:HB2	9	0.29
(1,525)	1:A:38:GLU:HG3	1:A:78:TYR:HB2	9	0.29
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	15	0.29
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	15	0.29
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	15	0.29
(1,2298)	1:B:91:ALA:HA	1:B:94:GLN:HG2	3	0.29
(1,2173)	1:B:79:TYR:HA	1:B:80:ARG:HG2	14	0.29
(1,1991)	1:B:63:LYS:HB2	1:B:69:GLU:HA	20	0.29
(1,1948)	1:B:60:GLN:HA	1:B:60:GLN:HE21	20	0.29
(1,1934)	1:B:59:LEU:HB2	1:B:79:TYR:HE1	17	0.29
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB1	5	0.29
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB2	5	0.29
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB3	5	0.29
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	4	0.29
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	4	0.29
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	4	0.29

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1690)	1:B:40:ALA:HB1	1:B:78:TYR:HD1	12	0.29
(1,1690)	1:B:40:ALA:HB2	1:B:78:TYR:HD1	12	0.29
(1,1690)	1:B:40:ALA:HB3	1:B:78:TYR:HD1	12	0.29
(1,1690)	1:B:40:ALA:HB1	1:B:78:TYR:HD1	13	0.29
(1,1690)	1:B:40:ALA:HB2	1:B:78:TYR:HD1	13	0.29
(1,1690)	1:B:40:ALA:HB3	1:B:78:TYR:HD1	13	0.29
(1,1600)	1:B:33:LEU:HD11	1:B:39:ARG:HE	16	0.29
(1,1600)	1:B:33:LEU:HD12	1:B:39:ARG:HE	16	0.29
(1,1600)	1:B:33:LEU:HD13	1:B:39:ARG:HE	16	0.29
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	8	0.29
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	8	0.29
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	8	0.29
(1,1450)	1:B:26:ARG:HA	1:B:29:GLN:HG2	1	0.29
(1,1361)	1:B:17:ARG:HA	1:B:65:GLY:HA2	15	0.29
(1,1047)	1:A:80:ARG:H	1:A:80:ARG:HG2	3	0.29
(1,1047)	1:A:80:ARG:H	1:A:80:ARG:HG2	19	0.29
(1,1002)	1:A:74:GLY:HA2	1:A:75:THR:HB	17	0.29
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	3	0.28
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	3	0.28
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB1	10	0.28
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB2	10	0.28
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB3	10	0.28
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB1	10	0.28
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB2	10	0.28
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB3	10	0.28
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB1	10	0.28
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB2	10	0.28
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB3	10	0.28
(1,594)	1:A:41:VAL:HG21	1:A:77:GLN:HG2	19	0.28
(1,594)	1:A:41:VAL:HG22	1:A:77:GLN:HG2	19	0.28
(1,594)	1:A:41:VAL:HG23	1:A:77:GLN:HG2	19	0.28
(1,486)	1:A:34:LEU:HB2	1:A:80:ARG:HA	2	0.28
(1,455)	1:A:33:LEU:HA	1:A:33:LEU:HD11	5	0.28
(1,455)	1:A:33:LEU:HA	1:A:33:LEU:HD12	5	0.28
(1,455)	1:A:33:LEU:HA	1:A:33:LEU:HD13	5	0.28
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	3	0.28
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	3	0.28
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	3	0.28
(1,312)	1:A:25:GLY:HA2	1:A:28:LEU:HB2	7	0.28
(1,2383)	1:B:101:LEU:HB2	1:B:102:GLU:H	11	0.28
(1,2298)	1:B:91:ALA:HA	1:B:94:GLN:HG2	20	0.28
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA2	5	0.28

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2191)	1:B:81:ILE:HG12	1:B:87:ALA:HA	3	0.28
(1,2167)	1:B:77:GLN:HG2	1:B:79:TYR:HE1	9	0.28
(1,2094)	1:B:70:ALA:HB1	1:B:79:TYR:HD1	1	0.28
(1,2094)	1:B:70:ALA:HB2	1:B:79:TYR:HD1	1	0.28
(1,2094)	1:B:70:ALA:HB3	1:B:79:TYR:HD1	1	0.28
(1,1893)	1:B:55:ALA:HA	1:B:58:ASN:HB2	12	0.28
(1,1849)	1:B:50:MET:H	1:B:50:MET:HG2	15	0.28
(1,1837)	1:B:50:MET:HB2	1:B:55:ALA:H	10	0.28
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	13	0.28
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	13	0.28
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	13	0.28
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	13	0.28
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	13	0.28
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	13	0.28
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	13	0.28
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	13	0.28
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	13	0.28
(1,1648)	1:B:37:GLY:HA2	1:B:38:GLU:HB2	1	0.28
(1,1648)	1:B:37:GLY:HA2	1:B:38:GLU:HB3	1	0.28
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	15	0.28
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	15	0.28
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	15	0.28
(1,1599)	1:B:33:LEU:HD11	1:B:39:ARG:HD2	6	0.28
(1,1599)	1:B:33:LEU:HD12	1:B:39:ARG:HD2	6	0.28
(1,1599)	1:B:33:LEU:HD13	1:B:39:ARG:HD2	6	0.28
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	3	0.28
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	3	0.28
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	3	0.28
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	9	0.28
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	9	0.28
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	9	0.28
(1,1440)	1:B:23:ALA:H	1:B:24:ASN:H	3	0.28
(1,1166)	1:A:91:ALA:HA	1:A:94:GLN:HG2	1	0.28
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG11	14	0.28
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG12	14	0.28
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG13	14	0.28
(1,1095)	1:A:84:GLU:HG2	1:A:88:ARG:HG2	4	0.28
(1,1095)	1:A:84:GLU:HG3	1:A:88:ARG:HG2	4	0.28
(1,1059)	1:A:81:ILE:HG12	1:A:87:ALA:HA	3	0.28
(1,1047)	1:A:80:ARG:H	1:A:80:ARG:HG2	6	0.28
(1,1037)	1:A:77:GLN:H	1:A:77:GLN:HG2	11	0.28
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB1	9	0.27

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB2	9	0.27
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB3	9	0.27
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB1	9	0.27
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB2	9	0.27
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB3	9	0.27
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB1	9	0.27
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB2	9	0.27
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB3	9	0.27
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	12	0.27
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	12	0.27
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	16	0.27
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	16	0.27
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB2	5	0.27
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB3	5	0.27
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB2	5	0.27
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB3	5	0.27
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB2	5	0.27
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB3	5	0.27
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	17	0.27
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	7	0.27
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	7	0.27
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	7	0.27
(1,7)	1:A:12:LEU:HD11	1:B:29:GLN:HB2	18	0.27
(1,7)	1:A:12:LEU:HD12	1:B:29:GLN:HB2	18	0.27
(1,7)	1:A:12:LEU:HD13	1:B:29:GLN:HB2	18	0.27
(1,691)	1:A:48:THR:HB	1:A:50:MET:HG2	20	0.27
(1,65)	1:B:11:LEU:HD11	1:A:98:ASP:HB3	10	0.27
(1,65)	1:B:11:LEU:HD12	1:A:98:ASP:HB3	10	0.27
(1,65)	1:B:11:LEU:HD13	1:A:98:ASP:HB3	10	0.27
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD11	17	0.27
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD12	17	0.27
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD13	17	0.27
(1,559)	1:A:40:ALA:HB1	1:A:78:TYR:HE1	13	0.27
(1,559)	1:A:40:ALA:HB2	1:A:78:TYR:HE1	13	0.27
(1,559)	1:A:40:ALA:HB3	1:A:78:TYR:HE1	13	0.27
(1,516)	1:A:37:GLY:HA2	1:A:38:GLU:HB2	8	0.27
(1,516)	1:A:37:GLY:HA2	1:A:38:GLU:HB3	8	0.27
(1,475)	1:A:33:LEU:HG	1:A:36:GLN:HE21	4	0.27
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB1	6	0.27
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB2	6	0.27
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB3	6	0.27
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB1	6	0.27

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB2	6	0.27
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB3	6	0.27
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB1	6	0.27
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB2	6	0.27
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB3	6	0.27
(1,467)	1:A:33:LEU:HD11	1:A:39:ARG:HD2	8	0.27
(1,467)	1:A:33:LEU:HD12	1:A:39:ARG:HD2	8	0.27
(1,467)	1:A:33:LEU:HD13	1:A:39:ARG:HD2	8	0.27
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG21	2	0.27
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG22	2	0.27
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG23	2	0.27
(1,328)	1:A:27:ARG:HD2	1:A:58:ASN:HA	7	0.27
(1,2287)	1:B:90:PHE:HB2	1:B:93:VAL:HG11	18	0.27
(1,2287)	1:B:90:PHE:HB2	1:B:93:VAL:HG12	18	0.27
(1,2287)	1:B:90:PHE:HB2	1:B:93:VAL:HG13	18	0.27
(1,2179)	1:B:80:ARG:H	1:B:80:ARG:HG2	11	0.27
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB1	7	0.27
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB2	7	0.27
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB3	7	0.27
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	2	0.27
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	2	0.27
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	2	0.27
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	5	0.27
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	5	0.27
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	5	0.27
(1,1377)	1:B:18:VAL:HG11	1:B:65:GLY:HA2	12	0.27
(1,1377)	1:B:18:VAL:HG12	1:B:65:GLY:HA2	12	0.27
(1,1377)	1:B:18:VAL:HG13	1:B:65:GLY:HA2	12	0.27
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG11	15	0.27
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG12	15	0.27
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG13	15	0.27
(1,1047)	1:A:80:ARG:H	1:A:80:ARG:HG2	15	0.27
(1,1035)	1:A:77:GLN:HG2	1:A:79:TYR:HE1	15	0.27
(1,91)	1:B:14:GLN:HG2	1:A:101:LEU:HD21	7	0.26
(1,91)	1:B:14:GLN:HG2	1:A:101:LEU:HD22	7	0.26
(1,91)	1:B:14:GLN:HG2	1:A:101:LEU:HD23	7	0.26
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD11	7	0.26
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD12	7	0.26
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD13	7	0.26
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	11	0.26
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	11	0.26
(1,516)	1:A:37:GLY:HA2	1:A:38:GLU:HB2	5	0.26

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,516)	1:A:37:GLY:HA2	1:A:38:GLU:HB3	5	0.26
(1,465)	1:A:33:LEU:HD11	1:A:36:GLN:H	15	0.26
(1,465)	1:A:33:LEU:HD12	1:A:36:GLN:H	15	0.26
(1,465)	1:A:33:LEU:HD13	1:A:36:GLN:H	15	0.26
(1,354)	1:A:29:GLN:HB2	1:A:48:THR:HB	20	0.26
(1,318)	1:A:26:ARG:HA	1:A:29:GLN:HG2	17	0.26
(1,28)	1:A:14:GLN:HG2	1:B:101:LEU:HD21	5	0.26
(1,28)	1:A:14:GLN:HG2	1:B:101:LEU:HD22	5	0.26
(1,28)	1:A:14:GLN:HG2	1:B:101:LEU:HD23	5	0.26
(1,2298)	1:B:91:ALA:HA	1:B:94:GLN:HG2	12	0.26
(1,2179)	1:B:80:ARG:H	1:B:80:ARG:HG2	18	0.26
(1,1991)	1:B:63:LYS:HB2	1:B:69:GLU:HA	3	0.26
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB2	7	0.26
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB3	7	0.26
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB2	7	0.26
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB3	7	0.26
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB2	7	0.26
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB3	7	0.26
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB1	9	0.26
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB2	9	0.26
(1,1836)	1:B:50:MET:HB2	1:B:55:ALA:HB3	9	0.26
(1,1690)	1:B:40:ALA:HB1	1:B:78:TYR:HD1	5	0.26
(1,1690)	1:B:40:ALA:HB2	1:B:78:TYR:HD1	5	0.26
(1,1690)	1:B:40:ALA:HB3	1:B:78:TYR:HD1	5	0.26
(1,1648)	1:B:37:GLY:HA2	1:B:38:GLU:HB2	12	0.26
(1,1648)	1:B:37:GLY:HA2	1:B:38:GLU:HB3	12	0.26
(1,1462)	1:B:27:ARG:HD2	1:B:62:LEU:H	4	0.26
(1,1377)	1:B:18:VAL:HG11	1:B:65:GLY:HA2	11	0.26
(1,1377)	1:B:18:VAL:HG12	1:B:65:GLY:HA2	11	0.26
(1,1377)	1:B:18:VAL:HG13	1:B:65:GLY:HA2	11	0.26
(1,1361)	1:B:17:ARG:HA	1:B:65:GLY:HA2	5	0.26
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	9	0.26
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD11	18	0.26
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD12	18	0.26
(1,1299)	1:B:10:ALA:H	1:B:11:LEU:HD13	18	0.26
(1,1296)	1:B:10:ALA:HB1	1:B:13:ASP:HB2	20	0.26
(1,1296)	1:B:10:ALA:HB2	1:B:13:ASP:HB2	20	0.26
(1,1296)	1:B:10:ALA:HB3	1:B:13:ASP:HB2	20	0.26
(1,761)	1:A:55:ALA:HA	1:A:58:ASN:HB2	1	0.25
(1,704)	1:A:50:MET:HB2	1:A:55:ALA:HB1	19	0.25
(1,704)	1:A:50:MET:HB2	1:A:55:ALA:HB2	19	0.25
(1,704)	1:A:50:MET:HB2	1:A:55:ALA:HB3	19	0.25

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,70)	1:B:12:LEU:HD11	1:A:29:GLN:HB2	11	0.25
(1,70)	1:B:12:LEU:HD12	1:A:29:GLN:HB2	11	0.25
(1,70)	1:B:12:LEU:HD13	1:A:29:GLN:HB2	11	0.25
(1,559)	1:A:40:ALA:HB1	1:A:78:TYR:HE1	12	0.25
(1,559)	1:A:40:ALA:HB2	1:A:78:TYR:HE1	12	0.25
(1,559)	1:A:40:ALA:HB3	1:A:78:TYR:HE1	12	0.25
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB1	15	0.25
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB2	15	0.25
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB3	15	0.25
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB1	15	0.25
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB2	15	0.25
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB3	15	0.25
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB1	15	0.25
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB2	15	0.25
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB3	15	0.25
(1,464)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	16	0.25
(1,464)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	16	0.25
(1,464)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	16	0.25
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HE21	6	0.25
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HE21	6	0.25
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HE21	6	0.25
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	12	0.25
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	12	0.25
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	12	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	3	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	3	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	3	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	7	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	7	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	7	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	11	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	11	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	11	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	15	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	15	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	15	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	18	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	18	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	18	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	19	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	19	0.25
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	19	0.25

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2383)	1:B:101:LEU:HB2	1:B:102:GLU:H	8	0.25
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD11	8	0.25
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD12	8	0.25
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD13	8	0.25
(1,1691)	1:B:40:ALA:HB1	1:B:78:TYR:HE1	8	0.25
(1,1691)	1:B:40:ALA:HB2	1:B:78:TYR:HE1	8	0.25
(1,1691)	1:B:40:ALA:HB3	1:B:78:TYR:HE1	8	0.25
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD11	7	0.25
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD12	7	0.25
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD13	7	0.25
(1,1593)	1:B:33:LEU:HD11	1:B:34:LEU:H	16	0.25
(1,1593)	1:B:33:LEU:HD12	1:B:34:LEU:H	16	0.25
(1,1593)	1:B:33:LEU:HD13	1:B:34:LEU:H	16	0.25
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG21	20	0.25
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG22	20	0.25
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG23	20	0.25
(1,1441)	1:B:24:ASN:H	1:B:24:ASN:HB2	19	0.25
(1,141)	1:A:7:ARG:HB2	1:A:8:LYS:H	14	0.25
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG11	3	0.25
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG12	3	0.25
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG13	3	0.25
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG11	6	0.25
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG12	6	0.25
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG13	6	0.25
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG11	8	0.25
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG12	8	0.25
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG13	8	0.25
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG11	9	0.25
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG12	9	0.25
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG13	9	0.25
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG11	10	0.25
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG12	10	0.25
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG13	10	0.25
(1,999)	1:A:73:GLU:H	1:A:76:ARG:HG2	16	0.24
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB2	10	0.24
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB3	10	0.24
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB2	10	0.24
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB3	10	0.24
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB2	10	0.24
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB3	10	0.24
(1,722)	1:A:51:ASN:HB2	1:A:53:THR:H	10	0.24
(1,67)	1:B:11:LEU:HD11	1:A:98:ASP:H	8	0.24

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,67)	1:B:11:LEU:HD12	1:A:98:ASP:H	8	0.24
(1,67)	1:B:11:LEU:HD13	1:A:98:ASP:H	8	0.24
(1,559)	1:A:40:ALA:HB1	1:A:78:TYR:HE1	8	0.24
(1,559)	1:A:40:ALA:HB2	1:A:78:TYR:HE1	8	0.24
(1,559)	1:A:40:ALA:HB3	1:A:78:TYR:HE1	8	0.24
(1,558)	1:A:40:ALA:HB1	1:A:78:TYR:HD1	6	0.24
(1,558)	1:A:40:ALA:HB2	1:A:78:TYR:HD1	6	0.24
(1,558)	1:A:40:ALA:HB3	1:A:78:TYR:HD1	6	0.24
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HE21	14	0.24
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HE21	14	0.24
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HE21	14	0.24
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	6	0.24
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	6	0.24
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	6	0.24
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	15	0.24
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	15	0.24
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	15	0.24
(1,4)	1:A:11:LEU:HD11	1:B:98:ASP:H	6	0.24
(1,4)	1:A:11:LEU:HD12	1:B:98:ASP:H	6	0.24
(1,4)	1:A:11:LEU:HD13	1:B:98:ASP:H	6	0.24
(1,4)	1:A:11:LEU:HD11	1:B:98:ASP:H	16	0.24
(1,4)	1:A:11:LEU:HD12	1:B:98:ASP:H	16	0.24
(1,4)	1:A:11:LEU:HD13	1:B:98:ASP:H	16	0.24
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	12	0.24
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG21	19	0.24
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG22	19	0.24
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG23	19	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	2	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	2	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	2	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	5	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	5	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	5	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	6	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	6	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	6	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	8	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	8	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	8	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	9	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	9	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	9	0.24

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	12	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	12	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	12	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	13	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	13	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	13	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	14	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	14	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	14	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	16	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	16	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	16	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	17	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	17	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	17	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG11	20	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG12	20	0.24
(1,247)	1:A:18:VAL:H	1:A:18:VAL:HG13	20	0.24
(1,2298)	1:B:91:ALA:HA	1:B:94:GLN:HG2	2	0.24
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	19	0.24
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	19	0.24
(1,1854)	1:B:51:ASN:HB2	1:B:53:THR:H	3	0.24
(1,164)	1:A:10:ALA:HB1	1:A:13:ASP:HB2	16	0.24
(1,164)	1:A:10:ALA:HB2	1:A:13:ASP:HB2	16	0.24
(1,164)	1:A:10:ALA:HB3	1:A:13:ASP:HB2	16	0.24
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB1	3	0.24
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB2	3	0.24
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB3	3	0.24
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB1	3	0.24
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB2	3	0.24
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB3	3	0.24
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB1	3	0.24
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB2	3	0.24
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB3	3	0.24
(1,1492)	1:B:29:GLN:HG2	1:B:48:THR:HB	2	0.24
(1,1441)	1:B:24:ASN:H	1:B:24:ASN:HB2	12	0.24
(1,1441)	1:B:24:ASN:H	1:B:24:ASN:HB2	16	0.24
(1,141)	1:A:7:ARG:HB2	1:A:8:LYS:H	6	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG11	4	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG12	4	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG13	4	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG11	7	0.24

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG12	7	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG13	7	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG11	11	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG12	11	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG13	11	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG11	12	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG12	12	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG13	12	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG11	13	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG12	13	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG13	13	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG11	14	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG12	14	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG13	14	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG11	15	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG12	15	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG13	15	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG11	16	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG12	16	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG13	16	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG11	19	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG12	19	0.24
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG13	19	0.24
(1,1358)	1:B:17:ARG:HA	1:B:20:LYS:HG2	5	0.24
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD11	8	0.24
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD12	8	0.24
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD13	8	0.24
(1,130)	1:A:5:SER:HB2	1:A:6:ASP:H	7	0.24
(1,1296)	1:B:10:ALA:HB1	1:B:13:ASP:HB2	5	0.24
(1,1296)	1:B:10:ALA:HB2	1:B:13:ASP:HB2	5	0.24
(1,1296)	1:B:10:ALA:HB3	1:B:13:ASP:HB2	5	0.24
(1,1276)	1:B:7:ARG:H	1:B:7:ARG:HG2	8	0.24
(1,1166)	1:A:91:ALA:HA	1:A:94:GLN:HG2	6	0.24
(1,1047)	1:A:80:ARG:H	1:A:80:ARG:HG2	4	0.24
(1,549)	1:A:40:ALA:HB1	1:A:42:GLU:HG2	18	0.23
(1,549)	1:A:40:ALA:HB2	1:A:42:GLU:HG2	18	0.23
(1,549)	1:A:40:ALA:HB3	1:A:42:GLU:HG2	18	0.23
(1,468)	1:A:33:LEU:HD11	1:A:39:ARG:HE	8	0.23
(1,468)	1:A:33:LEU:HD12	1:A:39:ARG:HE	8	0.23
(1,468)	1:A:33:LEU:HD13	1:A:39:ARG:HE	8	0.23
(1,455)	1:A:33:LEU:HA	1:A:33:LEU:HD11	15	0.23
(1,455)	1:A:33:LEU:HA	1:A:33:LEU:HD12	15	0.23

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,455)	1:A:33:LEU:HA	1:A:33:LEU:HD13	15	0.23
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	5	0.23
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	5	0.23
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	5	0.23
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB1	5	0.23
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB2	5	0.23
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB3	5	0.23
(1,2383)	1:B:101:LEU:HB2	1:B:102:GLU:H	6	0.23
(1,2167)	1:B:77:GLN:HG2	1:B:79:TYR:HE1	2	0.23
(1,2119)	1:B:72:ARG:HD2	1:B:77:GLN:HG2	3	0.23
(1,2119)	1:B:72:ARG:HD3	1:B:77:GLN:HG2	3	0.23
(1,2095)	1:B:70:ALA:HB1	1:B:79:TYR:HE1	9	0.23
(1,2095)	1:B:70:ALA:HB2	1:B:79:TYR:HE1	9	0.23
(1,2095)	1:B:70:ALA:HB3	1:B:79:TYR:HE1	9	0.23
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	7	0.23
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	7	0.23
(1,1835)	1:B:50:MET:HB2	1:B:54:THR:HG21	3	0.23
(1,1835)	1:B:50:MET:HB2	1:B:54:THR:HG22	3	0.23
(1,1835)	1:B:50:MET:HB2	1:B:54:THR:HG23	3	0.23
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD11	4	0.23
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD12	4	0.23
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD13	4	0.23
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD11	10	0.23
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD12	10	0.23
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD13	10	0.23
(1,1662)	1:B:39:ARG:HA	1:B:39:ARG:HD2	12	0.23
(1,1647)	1:B:36:GLN:H	1:B:36:GLN:HG2	9	0.23
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	7	0.23
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	7	0.23
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	7	0.23
(1,1492)	1:B:29:GLN:HG2	1:B:48:THR:HB	12	0.23
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG11	17	0.23
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG12	17	0.23
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG13	17	0.23
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG11	18	0.23
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG12	18	0.23
(1,1379)	1:B:18:VAL:H	1:B:18:VAL:HG13	18	0.23
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD11	10	0.23
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD12	10	0.23
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD13	10	0.23
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD11	13	0.23
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD12	13	0.23

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD13	13	0.23
(1,130)	1:A:5:SER:HB2	1:A:6:ASP:H	13	0.23
(1,1095)	1:A:84:GLU:HG2	1:A:88:ARG:HG2	1	0.23
(1,1095)	1:A:84:GLU:HG3	1:A:88:ARG:HG2	1	0.23
(1,1035)	1:A:77:GLN:HG2	1:A:79:TYR:HE1	18	0.23
(1,999)	1:A:73:GLU:H	1:A:76:ARG:HG2	18	0.22
(1,963)	1:A:70:ALA:HB1	1:A:79:TYR:HE1	16	0.22
(1,963)	1:A:70:ALA:HB2	1:A:79:TYR:HE1	16	0.22
(1,963)	1:A:70:ALA:HB3	1:A:79:TYR:HE1	16	0.22
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD11	8	0.22
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD12	8	0.22
(1,90)	1:B:14:GLN:HG2	1:A:101:LEU:HD13	8	0.22
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE2	19	0.22
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE3	19	0.22
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	15	0.22
(1,8)	1:A:12:LEU:HD11	1:B:29:GLN:HE21	5	0.22
(1,8)	1:A:12:LEU:HD12	1:B:29:GLN:HE21	5	0.22
(1,8)	1:A:12:LEU:HD13	1:B:29:GLN:HE21	5	0.22
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	1	0.22
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	14	0.22
(1,70)	1:B:12:LEU:HD11	1:A:29:GLN:HB2	14	0.22
(1,70)	1:B:12:LEU:HD12	1:A:29:GLN:HB2	14	0.22
(1,70)	1:B:12:LEU:HD13	1:A:29:GLN:HB2	14	0.22
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD11	16	0.22
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD12	16	0.22
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD13	16	0.22
(1,558)	1:A:40:ALA:HB1	1:A:78:TYR:HD1	1	0.22
(1,558)	1:A:40:ALA:HB2	1:A:78:TYR:HD1	1	0.22
(1,558)	1:A:40:ALA:HB3	1:A:78:TYR:HD1	1	0.22
(1,243)	1:A:18:VAL:HG11	1:A:22:LEU:H	1	0.22
(1,243)	1:A:18:VAL:HG12	1:A:22:LEU:H	1	0.22
(1,243)	1:A:18:VAL:HG13	1:A:22:LEU:H	1	0.22
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA2	16	0.22
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB2	5	0.22
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB3	5	0.22
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB2	5	0.22
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB3	5	0.22
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB2	5	0.22
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB3	5	0.22
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB1	9	0.22
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB2	9	0.22
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB3	9	0.22

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB1	9	0.22
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB2	9	0.22
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB3	9	0.22
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB1	9	0.22
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB2	9	0.22
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB3	9	0.22
(1,1849)	1:B:50:MET:H	1:B:50:MET:HG2	17	0.22
(1,1845)	1:B:50:MET:HG2	1:B:54:THR:HG21	3	0.22
(1,1845)	1:B:50:MET:HG2	1:B:54:THR:HG22	3	0.22
(1,1845)	1:B:50:MET:HG2	1:B:54:THR:HG23	3	0.22
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD11	6	0.22
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD12	6	0.22
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD13	6	0.22
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD11	11	0.22
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD12	11	0.22
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD13	11	0.22
(1,1691)	1:B:40:ALA:HB1	1:B:78:TYR:HE1	13	0.22
(1,1691)	1:B:40:ALA:HB2	1:B:78:TYR:HE1	13	0.22
(1,1691)	1:B:40:ALA:HB3	1:B:78:TYR:HE1	13	0.22
(1,1681)	1:B:40:ALA:HB1	1:B:42:GLU:HG2	2	0.22
(1,1681)	1:B:40:ALA:HB2	1:B:42:GLU:HG2	2	0.22
(1,1681)	1:B:40:ALA:HB3	1:B:42:GLU:HG2	2	0.22
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	2	0.22
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	2	0.22
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	2	0.22
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	11	0.22
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	11	0.22
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	11	0.22
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	16	0.22
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	16	0.22
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	16	0.22
(1,1492)	1:B:29:GLN:HG2	1:B:48:THR:HB	7	0.22
(1,1361)	1:B:17:ARG:HA	1:B:65:GLY:HA2	1	0.22
(1,1361)	1:B:17:ARG:HA	1:B:65:GLY:HA2	20	0.22
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD11	15	0.22
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD12	15	0.22
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD13	15	0.22
(1,1258)	1:A:107:HIS:HB2	1:A:108:HIS:H	8	0.22
(1,1022)	1:A:76:ARG:HG2	1:A:78:TYR:HE1	20	0.22
(1,999)	1:A:73:GLU:H	1:A:76:ARG:HG2	14	0.21
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE2	3	0.21
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE3	3	0.21

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE2	12	0.21
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE3	12	0.21
(1,722)	1:A:51:ASN:HB2	1:A:53:THR:H	11	0.21
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	15	0.21
(1,713)	1:A:50:MET:HG2	1:A:54:THR:HG21	1	0.21
(1,713)	1:A:50:MET:HG2	1:A:54:THR:HG22	1	0.21
(1,713)	1:A:50:MET:HG2	1:A:54:THR:HG23	1	0.21
(1,549)	1:A:40:ALA:HB1	1:A:42:GLU:HG2	13	0.21
(1,549)	1:A:40:ALA:HB2	1:A:42:GLU:HG2	13	0.21
(1,549)	1:A:40:ALA:HB3	1:A:42:GLU:HG2	13	0.21
(1,475)	1:A:33:LEU:HG	1:A:36:GLN:HE21	15	0.21
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB1	9	0.21
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB2	9	0.21
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB3	9	0.21
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB1	9	0.21
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB2	9	0.21
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB3	9	0.21
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB1	9	0.21
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB2	9	0.21
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB3	9	0.21
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	5	0.21
(1,289)	1:A:22:LEU:HB2	1:A:23:ALA:H	11	0.21
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD11	15	0.21
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD12	15	0.21
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD13	15	0.21
(1,2384)	1:B:101:LEU:HD21	1:B:102:GLU:H	14	0.21
(1,2384)	1:B:101:LEU:HD22	1:B:102:GLU:H	14	0.21
(1,2384)	1:B:101:LEU:HD23	1:B:102:GLU:H	14	0.21
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	14	0.21
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	14	0.21
(1,2191)	1:B:81:ILE:HG12	1:B:87:ALA:HA	16	0.21
(1,2171)	1:B:78:TYR:H	1:B:78:TYR:HD1	17	0.21
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD11	13	0.21
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD12	13	0.21
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD13	13	0.21
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD11	16	0.21
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD12	16	0.21
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD13	16	0.21
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD11	1	0.21
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD12	1	0.21
(1,167)	1:A:10:ALA:H	1:A:11:LEU:HD13	1	0.21
(1,1441)	1:B:24:ASN:H	1:B:24:ASN:HB2	4	0.21

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1399)	1:B:20:LYS:HG2	1:B:20:LYS:HE2	18	0.21
(1,1399)	1:B:20:LYS:HG2	1:B:20:LYS:HE3	18	0.21
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD11	6	0.21
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD12	6	0.21
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD13	6	0.21
(1,1278)	1:B:8:LYS:HA	1:B:8:LYS:HD2	17	0.21
(1,1278)	1:B:8:LYS:HA	1:B:8:LYS:HD3	17	0.21
(1,1166)	1:A:91:ALA:HA	1:A:94:GLN:HG2	12	0.21
(1,1047)	1:A:80:ARG:H	1:A:80:ARG:HG2	10	0.21
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB1	5	0.2
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB2	5	0.2
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB3	5	0.2
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB1	5	0.2
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB2	5	0.2
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB3	5	0.2
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB1	5	0.2
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB2	5	0.2
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB3	5	0.2
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	5	0.2
(1,64)	1:B:11:LEU:HD11	1:A:98:ASP:HA	6	0.2
(1,64)	1:B:11:LEU:HD12	1:A:98:ASP:HA	6	0.2
(1,64)	1:B:11:LEU:HD13	1:A:98:ASP:HA	6	0.2
(1,621)	1:A:42:GLU:H	1:A:42:GLU:HG2	2	0.2
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	13	0.2
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	13	0.2
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	13	0.2
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD11	8	0.2
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD12	8	0.2
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD13	8	0.2
(1,473)	1:A:33:LEU:HD11	1:A:47:ALA:H	11	0.2
(1,473)	1:A:33:LEU:HD12	1:A:47:ALA:H	11	0.2
(1,473)	1:A:33:LEU:HD13	1:A:47:ALA:H	11	0.2
(1,362)	1:A:29:GLN:H	1:A:29:GLN:HG2	13	0.2
(1,245)	1:A:18:VAL:HG11	1:A:65:GLY:HA2	3	0.2
(1,245)	1:A:18:VAL:HG12	1:A:65:GLY:HA2	3	0.2
(1,245)	1:A:18:VAL:HG13	1:A:65:GLY:HA2	3	0.2
(1,2179)	1:B:80:ARG:H	1:B:80:ARG:HG2	4	0.2
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE2	1	0.2
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE3	1	0.2
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE2	8	0.2
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE3	8	0.2
(1,1823)	1:B:48:THR:HB	1:B:50:MET:HG2	13	0.2

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1747)	1:B:42:GLU:HG2	1:B:52:LEU:HG	6	0.2
(1,1726)	1:B:41:VAL:HG21	1:B:77:GLN:HG2	2	0.2
(1,1726)	1:B:41:VAL:HG22	1:B:77:GLN:HG2	2	0.2
(1,1726)	1:B:41:VAL:HG23	1:B:77:GLN:HG2	2	0.2
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD11	5	0.2
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD12	5	0.2
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD13	5	0.2
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD11	12	0.2
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD12	12	0.2
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD13	12	0.2
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD11	20	0.2
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD12	20	0.2
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD13	20	0.2
(1,1494)	1:B:29:GLN:H	1:B:29:GLN:HG2	13	0.2
(1,1494)	1:B:29:GLN:H	1:B:29:GLN:HG2	15	0.2
(1,1441)	1:B:24:ASN:H	1:B:24:ASN:HB2	15	0.2
(1,1399)	1:B:20:LYS:HG2	1:B:20:LYS:HE2	15	0.2
(1,1399)	1:B:20:LYS:HG2	1:B:20:LYS:HE3	15	0.2
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD11	12	0.2
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD12	12	0.2
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD13	12	0.2
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD11	16	0.2
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD12	16	0.2
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD13	16	0.2
(1,1276)	1:B:7:ARG:H	1:B:7:ARG:HG2	1	0.2
(1,969)	1:A:71:ARG:HB2	1:A:79:TYR:HA	6	0.19
(1,729)	1:A:52:LEU:HA	1:A:52:LEU:HD11	2	0.19
(1,729)	1:A:52:LEU:HA	1:A:52:LEU:HD12	2	0.19
(1,729)	1:A:52:LEU:HA	1:A:52:LEU:HD13	2	0.19
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	11	0.19
(1,65)	1:B:11:LEU:HD11	1:A:98:ASP:HB3	17	0.19
(1,65)	1:B:11:LEU:HD12	1:A:98:ASP:HB3	17	0.19
(1,65)	1:B:11:LEU:HD13	1:A:98:ASP:HB3	17	0.19
(1,615)	1:A:42:GLU:HG2	1:A:52:LEU:HG	4	0.19
(1,514)	1:A:36:GLN:H	1:A:36:GLN:HB2	18	0.19
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	2	0.19
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	2	0.19
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	2	0.19
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD11	1	0.19
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD12	1	0.19
(1,27)	1:A:14:GLN:HG2	1:B:101:LEU:HD13	1	0.19
(1,245)	1:A:18:VAL:HG11	1:A:65:GLY:HA2	18	0.19

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,245)	1:A:18:VAL:HG12	1:A:65:GLY:HA2	18	0.19
(1,245)	1:A:18:VAL:HG13	1:A:65:GLY:HA2	18	0.19
(1,2383)	1:B:101:LEU:HB2	1:B:102:GLU:H	19	0.19
(1,2192)	1:B:81:ILE:HG12	1:B:87:ALA:HB1	5	0.19
(1,2192)	1:B:81:ILE:HG12	1:B:87:ALA:HB2	5	0.19
(1,2192)	1:B:81:ILE:HG12	1:B:87:ALA:HB3	5	0.19
(1,2173)	1:B:79:TYR:HA	1:B:80:ARG:HG2	17	0.19
(1,2154)	1:B:76:ARG:HG2	1:B:78:TYR:HE1	14	0.19
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	17	0.19
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	17	0.19
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE2	17	0.19
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE3	17	0.19
(1,1747)	1:B:42:GLU:HG2	1:B:52:LEU:HG	10	0.19
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD11	15	0.19
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD12	15	0.19
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD13	15	0.19
(1,1691)	1:B:40:ALA:HB1	1:B:78:TYR:HE1	11	0.19
(1,1691)	1:B:40:ALA:HB2	1:B:78:TYR:HE1	11	0.19
(1,1691)	1:B:40:ALA:HB3	1:B:78:TYR:HE1	11	0.19
(1,1646)	1:B:36:GLN:H	1:B:36:GLN:HB2	5	0.19
(1,1646)	1:B:36:GLN:H	1:B:36:GLN:HB2	6	0.19
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB1	1	0.19
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB2	1	0.19
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB3	1	0.19
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB1	1	0.19
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB2	1	0.19
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB3	1	0.19
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB1	1	0.19
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB2	1	0.19
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB3	1	0.19
(1,1521)	1:B:30:ILE:HG21	1:B:33:LEU:HB2	18	0.19
(1,1521)	1:B:30:ILE:HG22	1:B:33:LEU:HB2	18	0.19
(1,1521)	1:B:30:ILE:HG23	1:B:33:LEU:HB2	18	0.19
(1,1494)	1:B:29:GLN:H	1:B:29:GLN:HG2	10	0.19
(1,1494)	1:B:29:GLN:H	1:B:29:GLN:HG2	19	0.19
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB1	7	0.19
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB2	7	0.19
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB3	7	0.19
(1,1460)	1:B:27:ARG:HD2	1:B:58:ASN:HA	12	0.19
(1,1399)	1:B:20:LYS:HG2	1:B:20:LYS:HE2	2	0.19
(1,1399)	1:B:20:LYS:HG2	1:B:20:LYS:HE3	2	0.19
(1,1258)	1:A:107:HIS:HB2	1:A:108:HIS:H	18	0.19

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1059)	1:A:81:ILE:HG12	1:A:87:ALA:HA	15	0.19
(1,105)	1:B:16:ALA:HB1	1:A:25:GLY:HA2	7	0.19
(1,105)	1:B:16:ALA:HB2	1:A:25:GLY:HA2	7	0.19
(1,105)	1:B:16:ALA:HB3	1:A:25:GLY:HA2	7	0.19
(1,1047)	1:A:80:ARG:H	1:A:80:ARG:HG2	20	0.19
(1,810)	1:A:59:LEU:HD21	1:A:79:TYR:HE1	13	0.18
(1,810)	1:A:59:LEU:HD22	1:A:79:TYR:HE1	13	0.18
(1,810)	1:A:59:LEU:HD23	1:A:79:TYR:HE1	13	0.18
(1,729)	1:A:52:LEU:HA	1:A:52:LEU:HD11	14	0.18
(1,729)	1:A:52:LEU:HA	1:A:52:LEU:HD12	14	0.18
(1,729)	1:A:52:LEU:HA	1:A:52:LEU:HD13	14	0.18
(1,722)	1:A:51:ASN:HB2	1:A:53:THR:H	7	0.18
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	6	0.18
(1,7)	1:A:12:LEU:HD11	1:B:29:GLN:HB2	12	0.18
(1,7)	1:A:12:LEU:HD12	1:B:29:GLN:HB2	12	0.18
(1,7)	1:A:12:LEU:HD13	1:B:29:GLN:HB2	12	0.18
(1,514)	1:A:36:GLN:H	1:A:36:GLN:HB2	14	0.18
(1,4)	1:A:11:LEU:HD11	1:B:98:ASP:H	15	0.18
(1,4)	1:A:11:LEU:HD12	1:B:98:ASP:H	15	0.18
(1,4)	1:A:11:LEU:HD13	1:B:98:ASP:H	15	0.18
(1,362)	1:A:29:GLN:H	1:A:29:GLN:HG2	19	0.18
(1,328)	1:A:27:ARG:HD2	1:A:58:ASN:HA	5	0.18
(1,2388)	1:B:101:LEU:H	1:B:102:GLU:H	16	0.18
(1,2298)	1:B:91:ALA:HA	1:B:94:GLN:HG2	19	0.18
(1,2156)	1:B:76:ARG:H	1:B:76:ARG:HG3	12	0.18
(1,2152)	1:B:76:ARG:HD2	1:B:78:TYR:HE1	2	0.18
(1,2152)	1:B:76:ARG:HD3	1:B:78:TYR:HE1	2	0.18
(1,2131)	1:B:73:GLU:H	1:B:76:ARG:HG2	10	0.18
(1,2100)	1:B:71:ARG:HB2	1:B:72:ARG:H	8	0.18
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE2	2	0.18
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE3	2	0.18
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD11	6	0.18
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD12	6	0.18
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD13	6	0.18
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD11	13	0.18
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD12	13	0.18
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD13	13	0.18
(1,1669)	1:B:39:ARG:HD2	1:B:43:ALA:HB1	14	0.18
(1,1669)	1:B:39:ARG:HD2	1:B:43:ALA:HB2	14	0.18
(1,1669)	1:B:39:ARG:HD2	1:B:43:ALA:HB3	14	0.18
(1,1656)	1:B:38:GLU:HG2	1:B:39:ARG:H	1	0.18
(1,1656)	1:B:38:GLU:HG3	1:B:39:ARG:H	1	0.18

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1599)	1:B:33:LEU:HD11	1:B:39:ARG:HD2	18	0.18
(1,1599)	1:B:33:LEU:HD12	1:B:39:ARG:HD2	18	0.18
(1,1599)	1:B:33:LEU:HD13	1:B:39:ARG:HD2	18	0.18
(1,1492)	1:B:29:GLN:HG2	1:B:48:THR:HB	14	0.18
(1,1421)	1:B:22:LEU:HB2	1:B:23:ALA:H	16	0.18
(1,1361)	1:B:17:ARG:HA	1:B:65:GLY:HA2	6	0.18
(1,1361)	1:B:17:ARG:HA	1:B:65:GLY:HA2	10	0.18
(1,1278)	1:B:8:LYS:HA	1:B:8:LYS:HD2	13	0.18
(1,1278)	1:B:8:LYS:HA	1:B:8:LYS:HD3	13	0.18
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG11	5	0.18
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG12	5	0.18
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG13	5	0.18
(1,1022)	1:A:76:ARG:HG2	1:A:78:TYR:HE1	3	0.18
(1,1020)	1:A:76:ARG:HD2	1:A:78:TYR:HE1	6	0.18
(1,1020)	1:A:76:ARG:HD3	1:A:78:TYR:HE1	6	0.18
(1,995)	1:A:73:GLU:HB2	1:A:78:TYR:HE1	17	0.17
(1,987)	1:A:72:ARG:HD2	1:A:77:GLN:HG2	7	0.17
(1,987)	1:A:72:ARG:HD3	1:A:77:GLN:HG2	7	0.17
(1,987)	1:A:72:ARG:HD2	1:A:77:GLN:HG2	8	0.17
(1,987)	1:A:72:ARG:HD3	1:A:77:GLN:HG2	8	0.17
(1,981)	1:A:72:ARG:HA	1:A:77:GLN:HG2	14	0.17
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	13	0.17
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	13	0.17
(1,859)	1:A:63:LYS:HB2	1:A:69:GLU:HA	14	0.17
(1,848)	1:A:62:LEU:H	1:A:62:LEU:HG	5	0.17
(1,816)	1:A:60:GLN:HA	1:A:60:GLN:HE21	6	0.17
(1,8)	1:A:12:LEU:HD11	1:B:29:GLN:HE21	20	0.17
(1,8)	1:A:12:LEU:HD12	1:B:29:GLN:HE21	20	0.17
(1,8)	1:A:12:LEU:HD13	1:B:29:GLN:HE21	20	0.17
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB1	9	0.17
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB2	9	0.17
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB3	9	0.17
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB1	9	0.17
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB2	9	0.17
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB3	9	0.17
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB1	9	0.17
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB2	9	0.17
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB3	9	0.17
(1,729)	1:A:52:LEU:HA	1:A:52:LEU:HD11	16	0.17
(1,729)	1:A:52:LEU:HA	1:A:52:LEU:HD12	16	0.17
(1,729)	1:A:52:LEU:HA	1:A:52:LEU:HD13	16	0.17
(1,559)	1:A:40:ALA:HB1	1:A:78:TYR:HE1	6	0.17

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,559)	1:A:40:ALA:HB2	1:A:78:TYR:HE1	6	0.17
(1,559)	1:A:40:ALA:HB3	1:A:78:TYR:HE1	6	0.17
(1,536)	1:A:39:ARG:HD2	1:A:40:ALA:H	13	0.17
(1,502)	1:A:35:ALA:HB1	1:A:36:GLN:HE21	13	0.17
(1,502)	1:A:35:ALA:HB2	1:A:36:GLN:HE21	13	0.17
(1,502)	1:A:35:ALA:HB3	1:A:36:GLN:HE21	13	0.17
(1,473)	1:A:33:LEU:HD11	1:A:47:ALA:H	7	0.17
(1,473)	1:A:33:LEU:HD12	1:A:47:ALA:H	7	0.17
(1,473)	1:A:33:LEU:HD13	1:A:47:ALA:H	7	0.17
(1,362)	1:A:29:GLN:H	1:A:29:GLN:HG2	20	0.17
(1,289)	1:A:22:LEU:HB2	1:A:23:ALA:H	7	0.17
(1,245)	1:A:18:VAL:HG11	1:A:65:GLY:HA2	6	0.17
(1,245)	1:A:18:VAL:HG12	1:A:65:GLY:HA2	6	0.17
(1,245)	1:A:18:VAL:HG13	1:A:65:GLY:HA2	6	0.17
(1,2191)	1:B:81:ILE:HG12	1:B:87:ALA:HA	2	0.17
(1,2153)	1:B:76:ARG:HG2	1:B:77:GLN:H	15	0.17
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE2	7	0.17
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE3	7	0.17
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB2	4	0.17
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB3	4	0.17
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB2	4	0.17
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB3	4	0.17
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB2	4	0.17
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB3	4	0.17
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD11	2	0.17
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD12	2	0.17
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD13	2	0.17
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD11	8	0.17
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD12	8	0.17
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD13	8	0.17
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD11	10	0.17
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD12	10	0.17
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD13	10	0.17
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	17	0.17
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	17	0.17
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	17	0.17
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	20	0.17
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	20	0.17
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	20	0.17
(1,1690)	1:B:40:ALA:HB1	1:B:78:TYR:HD1	8	0.17
(1,1690)	1:B:40:ALA:HB2	1:B:78:TYR:HD1	8	0.17
(1,1690)	1:B:40:ALA:HB3	1:B:78:TYR:HD1	8	0.17

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1646)	1:B:36:GLN:H	1:B:36:GLN:HB2	16	0.17
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	20	0.17
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	20	0.17
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	20	0.17
(1,1596)	1:B:33:LEU:HD11	1:B:36:GLN:HG2	19	0.17
(1,1596)	1:B:33:LEU:HD12	1:B:36:GLN:HG2	19	0.17
(1,1596)	1:B:33:LEU:HD13	1:B:36:GLN:HG2	19	0.17
(1,1499)	1:B:30:ILE:HA	1:B:33:LEU:HD11	18	0.17
(1,1499)	1:B:30:ILE:HA	1:B:33:LEU:HD12	18	0.17
(1,1499)	1:B:30:ILE:HA	1:B:33:LEU:HD13	18	0.17
(1,1494)	1:B:29:GLN:H	1:B:29:GLN:HG2	17	0.17
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG21	6	0.17
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG22	6	0.17
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG23	6	0.17
(1,137)	1:A:7:ARG:HA	1:A:7:ARG:HG2	15	0.17
(1,1278)	1:B:8:LYS:HA	1:B:8:LYS:HD2	20	0.17
(1,1278)	1:B:8:LYS:HA	1:B:8:LYS:HD3	20	0.17
(1,1273)	1:B:7:ARG:HB2	1:B:8:LYS:H	7	0.17
(1,1273)	1:B:7:ARG:HB2	1:B:8:LYS:H	17	0.17
(1,1262)	1:B:5:SER:HB2	1:B:6:ASP:H	8	0.17
(1,1210)	1:A:95:VAL:HG11	1:A:99:GLU:HB2	2	0.17
(1,1210)	1:A:95:VAL:HG12	1:A:99:GLU:HB2	2	0.17
(1,1210)	1:A:95:VAL:HG13	1:A:99:GLU:HB2	2	0.17
(1,1208)	1:A:95:VAL:HG11	1:A:98:ASP:HB2	18	0.17
(1,1208)	1:A:95:VAL:HG12	1:A:98:ASP:HB2	18	0.17
(1,1208)	1:A:95:VAL:HG13	1:A:98:ASP:HB2	18	0.17
(1,1039)	1:A:78:TYR:H	1:A:78:TYR:HD1	18	0.17
(1,999)	1:A:73:GLU:H	1:A:76:ARG:HG2	5	0.16
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG2	10	0.16
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	8	0.16
(1,615)	1:A:42:GLU:HG2	1:A:52:LEU:HG	9	0.16
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	20	0.16
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	20	0.16
(1,614)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	20	0.16
(1,514)	1:A:36:GLN:H	1:A:36:GLN:HB2	11	0.16
(1,472)	1:A:33:LEU:HD11	1:A:47:ALA:HB1	12	0.16
(1,472)	1:A:33:LEU:HD11	1:A:47:ALA:HB2	12	0.16
(1,472)	1:A:33:LEU:HD11	1:A:47:ALA:HB3	12	0.16
(1,472)	1:A:33:LEU:HD12	1:A:47:ALA:HB1	12	0.16
(1,472)	1:A:33:LEU:HD12	1:A:47:ALA:HB2	12	0.16
(1,472)	1:A:33:LEU:HD12	1:A:47:ALA:HB3	12	0.16
(1,472)	1:A:33:LEU:HD13	1:A:47:ALA:HB1	12	0.16

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,472)	1:A:33:LEU:HD13	1:A:47:ALA:HB2	12	0.16
(1,472)	1:A:33:LEU:HD13	1:A:47:ALA:HB3	12	0.16
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG21	17	0.16
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG22	17	0.16
(1,355)	1:A:29:GLN:HB2	1:A:48:THR:HG23	17	0.16
(1,231)	1:A:17:ARG:H	1:A:17:ARG:HG2	12	0.16
(1,2298)	1:B:91:ALA:HA	1:B:94:GLN:HG2	14	0.16
(1,2191)	1:B:81:ILE:HG12	1:B:87:ALA:HA	11	0.16
(1,2169)	1:B:77:GLN:H	1:B:77:GLN:HG2	2	0.16
(1,2151)	1:B:76:ARG:HD2	1:B:77:GLN:H	2	0.16
(1,2151)	1:B:76:ARG:HD3	1:B:77:GLN:H	2	0.16
(1,2151)	1:B:76:ARG:HD2	1:B:77:GLN:H	11	0.16
(1,2151)	1:B:76:ARG:HD3	1:B:77:GLN:H	11	0.16
(1,2095)	1:B:70:ALA:HB1	1:B:79:TYR:HE1	16	0.16
(1,2095)	1:B:70:ALA:HB2	1:B:79:TYR:HE1	16	0.16
(1,2095)	1:B:70:ALA:HB3	1:B:79:TYR:HE1	16	0.16
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD11	12	0.16
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD12	12	0.16
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD13	12	0.16
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD11	20	0.16
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD12	20	0.16
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD13	20	0.16
(1,1744)	1:B:42:GLU:HG2	1:B:43:ALA:H	8	0.16
(1,1726)	1:B:41:VAL:HG21	1:B:77:GLN:HG2	4	0.16
(1,1726)	1:B:41:VAL:HG22	1:B:77:GLN:HG2	4	0.16
(1,1726)	1:B:41:VAL:HG23	1:B:77:GLN:HG2	4	0.16
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD11	13	0.16
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD12	13	0.16
(1,1704)	1:B:41:VAL:HB	1:B:52:LEU:HD13	13	0.16
(1,1681)	1:B:40:ALA:HB1	1:B:42:GLU:HG2	9	0.16
(1,1681)	1:B:40:ALA:HB2	1:B:42:GLU:HG2	9	0.16
(1,1681)	1:B:40:ALA:HB3	1:B:42:GLU:HG2	9	0.16
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	11	0.16
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	11	0.16
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	11	0.16
(1,1599)	1:B:33:LEU:HD11	1:B:39:ARG:HD2	14	0.16
(1,1599)	1:B:33:LEU:HD12	1:B:39:ARG:HD2	14	0.16
(1,1599)	1:B:33:LEU:HD13	1:B:39:ARG:HD2	14	0.16
(1,1510)	1:B:30:ILE:HD11	1:B:58:ASN:HB2	10	0.16
(1,1510)	1:B:30:ILE:HD12	1:B:58:ASN:HB2	10	0.16
(1,1510)	1:B:30:ILE:HD13	1:B:58:ASN:HB2	10	0.16
(1,1494)	1:B:29:GLN:H	1:B:29:GLN:HG2	1	0.16

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1451)	1:B:26:ARG:H	1:B:26:ARG:HG2	20	0.16
(1,1451)	1:B:26:ARG:H	1:B:26:ARG:HG3	20	0.16
(1,144)	1:A:7:ARG:H	1:A:7:ARG:HG2	14	0.16
(1,1421)	1:B:22:LEU:HB2	1:B:23:ALA:H	17	0.16
(1,141)	1:A:7:ARG:HB2	1:A:8:LYS:H	10	0.16
(1,1363)	1:B:17:ARG:H	1:B:17:ARG:HG2	4	0.16
(1,13)	1:A:12:LEU:HD21	1:B:28:LEU:HB2	19	0.16
(1,13)	1:A:12:LEU:HD22	1:B:28:LEU:HB2	19	0.16
(1,13)	1:A:12:LEU:HD23	1:B:28:LEU:HB2	19	0.16
(1,1296)	1:B:10:ALA:HB1	1:B:13:ASP:HB2	19	0.16
(1,1296)	1:B:10:ALA:HB2	1:B:13:ASP:HB2	19	0.16
(1,1296)	1:B:10:ALA:HB3	1:B:13:ASP:HB2	19	0.16
(1,1276)	1:B:7:ARG:H	1:B:7:ARG:HG2	20	0.16
(1,1273)	1:B:7:ARG:HB2	1:B:8:LYS:H	6	0.16
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG11	13	0.16
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG12	13	0.16
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG13	13	0.16
(1,999)	1:A:73:GLU:H	1:A:76:ARG:HG2	1	0.15
(1,816)	1:A:60:GLN:HA	1:A:60:GLN:HE21	8	0.15
(1,809)	1:A:59:LEU:HD21	1:A:79:TYR:HD1	20	0.15
(1,809)	1:A:59:LEU:HD22	1:A:79:TYR:HD1	20	0.15
(1,809)	1:A:59:LEU:HD23	1:A:79:TYR:HD1	20	0.15
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	9	0.15
(1,65)	1:B:11:LEU:HD11	1:A:98:ASP:HB3	16	0.15
(1,65)	1:B:11:LEU:HD12	1:A:98:ASP:HB3	16	0.15
(1,65)	1:B:11:LEU:HD13	1:A:98:ASP:HB3	16	0.15
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	4	0.15
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	4	0.15
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	4	0.15
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	9	0.15
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	9	0.15
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	9	0.15
(1,362)	1:A:29:GLN:H	1:A:29:GLN:HG2	2	0.15
(1,362)	1:A:29:GLN:H	1:A:29:GLN:HG2	17	0.15
(1,36)	1:A:15:VAL:HG11	1:B:97:ALA:HB1	19	0.15
(1,36)	1:A:15:VAL:HG11	1:B:97:ALA:HB2	19	0.15
(1,36)	1:A:15:VAL:HG11	1:B:97:ALA:HB3	19	0.15
(1,36)	1:A:15:VAL:HG12	1:B:97:ALA:HB1	19	0.15
(1,36)	1:A:15:VAL:HG12	1:B:97:ALA:HB2	19	0.15
(1,36)	1:A:15:VAL:HG12	1:B:97:ALA:HB3	19	0.15
(1,36)	1:A:15:VAL:HG13	1:B:97:ALA:HB1	19	0.15
(1,36)	1:A:15:VAL:HG13	1:B:97:ALA:HB2	19	0.15

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,36)	1:A:15:VAL:HG13	1:B:97:ALA:HB3	19	0.15
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	4	0.15
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	4	0.15
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	4	0.15
(1,231)	1:A:17:ARG:H	1:A:17:ARG:HG2	2	0.15
(1,2171)	1:B:78:TYR:H	1:B:78:TYR:HD1	19	0.15
(1,2157)	1:B:76:ARG:H	1:B:76:ARG:HG2	12	0.15
(1,2152)	1:B:76:ARG:HD2	1:B:78:TYR:HE1	19	0.15
(1,2152)	1:B:76:ARG:HD3	1:B:78:TYR:HE1	19	0.15
(1,2152)	1:B:76:ARG:HD2	1:B:78:TYR:HE1	20	0.15
(1,2152)	1:B:76:ARG:HD3	1:B:78:TYR:HE1	20	0.15
(1,2119)	1:B:72:ARG:HD2	1:B:77:GLN:HG2	20	0.15
(1,2119)	1:B:72:ARG:HD3	1:B:77:GLN:HG2	20	0.15
(1,2095)	1:B:70:ALA:HB1	1:B:79:TYR:HE1	10	0.15
(1,2095)	1:B:70:ALA:HB2	1:B:79:TYR:HE1	10	0.15
(1,2095)	1:B:70:ALA:HB3	1:B:79:TYR:HE1	10	0.15
(1,1934)	1:B:59:LEU:HB2	1:B:79:TYR:HE1	13	0.15
(1,1849)	1:B:50:MET:H	1:B:50:MET:HG2	20	0.15
(1,1837)	1:B:50:MET:HB2	1:B:55:ALA:H	1	0.15
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	7	0.15
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	7	0.15
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	7	0.15
(1,1690)	1:B:40:ALA:HB1	1:B:78:TYR:HD1	2	0.15
(1,1690)	1:B:40:ALA:HB2	1:B:78:TYR:HD1	2	0.15
(1,1690)	1:B:40:ALA:HB3	1:B:78:TYR:HD1	2	0.15
(1,1658)	1:B:38:GLU:HG2	1:B:78:TYR:HD1	18	0.15
(1,1658)	1:B:38:GLU:HG3	1:B:78:TYR:HD1	18	0.15
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB1	13	0.15
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB2	13	0.15
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB3	13	0.15
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB1	13	0.15
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB2	13	0.15
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB3	13	0.15
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB1	13	0.15
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB2	13	0.15
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB3	13	0.15
(1,1492)	1:B:29:GLN:HG2	1:B:48:THR:HB	6	0.15
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB1	13	0.15
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB2	13	0.15
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB3	13	0.15
(1,1411)	1:B:21:ALA:HB1	1:B:65:GLY:H	8	0.15
(1,1411)	1:B:21:ALA:HB2	1:B:65:GLY:H	8	0.15

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1411)	1:B:21:ALA:HB3	1:B:65:GLY:H	8	0.15
(1,1304)	1:B:11:LEU:HA	1:B:14:GLN:HG2	7	0.15
(1,1296)	1:B:10:ALA:HB1	1:B:13:ASP:HB2	10	0.15
(1,1296)	1:B:10:ALA:HB2	1:B:13:ASP:HB2	10	0.15
(1,1296)	1:B:10:ALA:HB3	1:B:13:ASP:HB2	10	0.15
(1,1276)	1:B:7:ARG:H	1:B:7:ARG:HG2	13	0.15
(1,1273)	1:B:7:ARG:HB2	1:B:8:LYS:H	1	0.15
(1,1262)	1:B:5:SER:HB2	1:B:6:ASP:H	3	0.15
(1,1044)	1:A:80:ARG:HB2	1:A:80:ARG:HE	2	0.15
(1,973)	1:A:71:ARG:H	1:A:71:ARG:HG2	15	0.14
(1,805)	1:A:59:LEU:HD11	1:A:79:TYR:HE1	11	0.14
(1,805)	1:A:59:LEU:HD12	1:A:79:TYR:HE1	11	0.14
(1,805)	1:A:59:LEU:HD13	1:A:79:TYR:HE1	11	0.14
(1,71)	1:B:12:LEU:HD11	1:A:29:GLN:HE21	13	0.14
(1,71)	1:B:12:LEU:HD12	1:A:29:GLN:HE21	13	0.14
(1,71)	1:B:12:LEU:HD13	1:A:29:GLN:HE21	13	0.14
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD11	7	0.14
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD12	7	0.14
(1,572)	1:A:41:VAL:HB	1:A:52:LEU:HD13	7	0.14
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD11	9	0.14
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD12	9	0.14
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD13	9	0.14
(1,559)	1:A:40:ALA:HB1	1:A:78:TYR:HE1	7	0.14
(1,559)	1:A:40:ALA:HB2	1:A:78:TYR:HE1	7	0.14
(1,559)	1:A:40:ALA:HB3	1:A:78:TYR:HE1	7	0.14
(1,486)	1:A:34:LEU:HB2	1:A:80:ARG:HA	1	0.14
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB1	18	0.14
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB2	18	0.14
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB3	18	0.14
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB1	18	0.14
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB2	18	0.14
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB3	18	0.14
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB1	18	0.14
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB2	18	0.14
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB3	18	0.14
(1,467)	1:A:33:LEU:HD11	1:A:39:ARG:HD2	14	0.14
(1,467)	1:A:33:LEU:HD12	1:A:39:ARG:HD2	14	0.14
(1,467)	1:A:33:LEU:HD13	1:A:39:ARG:HD2	14	0.14
(1,462)	1:A:33:LEU:HD11	1:A:36:GLN:HB2	14	0.14
(1,462)	1:A:33:LEU:HD12	1:A:36:GLN:HB2	14	0.14
(1,462)	1:A:33:LEU:HD13	1:A:36:GLN:HB2	14	0.14
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	5	0.14

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	5	0.14
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	5	0.14
(1,4)	1:A:11:LEU:HD11	1:B:98:ASP:H	20	0.14
(1,4)	1:A:11:LEU:HD12	1:B:98:ASP:H	20	0.14
(1,4)	1:A:11:LEU:HD13	1:B:98:ASP:H	20	0.14
(1,309)	1:A:24:ASN:H	1:A:24:ASN:HB2	8	0.14
(1,2352)	1:B:96:VAL:HA	1:B:100:HIS:HD2	18	0.14
(1,2298)	1:B:91:ALA:HA	1:B:94:GLN:HG2	1	0.14
(1,2298)	1:B:91:ALA:HA	1:B:94:GLN:HG2	4	0.14
(1,226)	1:A:17:ARG:HA	1:A:20:LYS:HG2	5	0.14
(1,2225)	1:B:84:GLU:HG2	1:B:88:ARG:HD2	2	0.14
(1,2225)	1:B:84:GLU:HG2	1:B:88:ARG:HD3	2	0.14
(1,2225)	1:B:84:GLU:HG3	1:B:88:ARG:HD2	2	0.14
(1,2225)	1:B:84:GLU:HG3	1:B:88:ARG:HD3	2	0.14
(1,2171)	1:B:78:TYR:H	1:B:78:TYR:HD1	7	0.14
(1,1934)	1:B:59:LEU:HB2	1:B:79:TYR:HE1	11	0.14
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB1	14	0.14
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB2	14	0.14
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB3	14	0.14
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB1	14	0.14
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB2	14	0.14
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB3	14	0.14
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB1	14	0.14
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB2	14	0.14
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB3	14	0.14
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD11	4	0.14
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD12	4	0.14
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD13	4	0.14
(1,1849)	1:B:50:MET:H	1:B:50:MET:HG2	6	0.14
(1,1747)	1:B:42:GLU:HG2	1:B:52:LEU:HG	20	0.14
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	5	0.14
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	5	0.14
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	5	0.14
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	18	0.14
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	18	0.14
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	18	0.14
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	4	0.14
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	4	0.14
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	4	0.14
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	4	0.14
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	4	0.14
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	4	0.14

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	4	0.14
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	4	0.14
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	4	0.14
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD11	5	0.14
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD12	5	0.14
(1,1687)	1:B:40:ALA:HB1	1:B:52:LEU:HD13	5	0.14
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD11	5	0.14
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD12	5	0.14
(1,1687)	1:B:40:ALA:HB2	1:B:52:LEU:HD13	5	0.14
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD11	5	0.14
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD12	5	0.14
(1,1687)	1:B:40:ALA:HB3	1:B:52:LEU:HD13	5	0.14
(1,1646)	1:B:36:GLN:H	1:B:36:GLN:HB2	12	0.14
(1,1646)	1:B:36:GLN:H	1:B:36:GLN:HB2	13	0.14
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB1	4	0.14
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB2	4	0.14
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB3	4	0.14
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB1	4	0.14
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB2	4	0.14
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB3	4	0.14
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB1	4	0.14
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB2	4	0.14
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB3	4	0.14
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB1	7	0.14
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB2	7	0.14
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB3	7	0.14
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB1	7	0.14
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB2	7	0.14
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB3	7	0.14
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB1	7	0.14
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB2	7	0.14
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB3	7	0.14
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	17	0.14
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	17	0.14
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	17	0.14
(1,1494)	1:B:29:GLN:H	1:B:29:GLN:HG2	8	0.14
(1,1460)	1:B:27:ARG:HD2	1:B:58:ASN:HA	7	0.14
(1,1361)	1:B:17:ARG:HA	1:B:65:GLY:HA2	17	0.14
(1,130)	1:A:5:SER:HB2	1:A:6:ASP:H	15	0.14
(1,1296)	1:B:10:ALA:HB1	1:B:13:ASP:HB2	4	0.14
(1,1296)	1:B:10:ALA:HB2	1:B:13:ASP:HB2	4	0.14
(1,1296)	1:B:10:ALA:HB3	1:B:13:ASP:HB2	4	0.14

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1296)	1:B:10:ALA:HB1	1:B:13:ASP:HB2	8	0.14
(1,1296)	1:B:10:ALA:HB2	1:B:13:ASP:HB2	8	0.14
(1,1296)	1:B:10:ALA:HB3	1:B:13:ASP:HB2	8	0.14
(1,1210)	1:A:95:VAL:HG11	1:A:99:GLU:HB2	13	0.14
(1,1210)	1:A:95:VAL:HG12	1:A:99:GLU:HB2	13	0.14
(1,1210)	1:A:95:VAL:HG13	1:A:99:GLU:HB2	13	0.14
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB1	11	0.14
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB2	11	0.14
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB3	11	0.14
(1,1059)	1:A:81:ILE:HG12	1:A:87:ALA:HA	16	0.14
(1,1047)	1:A:80:ARG:H	1:A:80:ARG:HG2	8	0.14
(1,729)	1:A:52:LEU:HA	1:A:52:LEU:HD11	7	0.13
(1,729)	1:A:52:LEU:HA	1:A:52:LEU:HD12	7	0.13
(1,729)	1:A:52:LEU:HA	1:A:52:LEU:HD13	7	0.13
(1,691)	1:A:48:THR:HB	1:A:50:MET:HG2	2	0.13
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD21	11	0.13
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD22	11	0.13
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD23	11	0.13
(1,514)	1:A:36:GLN:H	1:A:36:GLN:HB2	20	0.13
(1,440)	1:A:31:LEU:HD21	1:A:90:PHE:HE1	11	0.13
(1,440)	1:A:31:LEU:HD22	1:A:90:PHE:HE1	11	0.13
(1,440)	1:A:31:LEU:HD23	1:A:90:PHE:HE1	11	0.13
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	4	0.13
(1,328)	1:A:27:ARG:HD2	1:A:58:ASN:HA	2	0.13
(1,318)	1:A:26:ARG:HA	1:A:29:GLN:HG2	19	0.13
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	10	0.13
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	10	0.13
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	10	0.13
(1,2390)	1:B:107:HIS:HB2	1:B:108:HIS:H	5	0.13
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB2	20	0.13
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB3	20	0.13
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB2	20	0.13
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB3	20	0.13
(1,2179)	1:B:80:ARG:H	1:B:80:ARG:HG2	16	0.13
(1,2176)	1:B:80:ARG:HB2	1:B:80:ARG:HE	2	0.13
(1,1972)	1:B:62:LEU:HB2	1:B:68:VAL:HG11	7	0.13
(1,1972)	1:B:62:LEU:HB2	1:B:68:VAL:HG12	7	0.13
(1,1972)	1:B:62:LEU:HB2	1:B:68:VAL:HG13	7	0.13
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	18	0.13
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	18	0.13
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	18	0.13
(1,1726)	1:B:41:VAL:HG21	1:B:77:GLN:HG2	12	0.13

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1726)	1:B:41:VAL:HG22	1:B:77:GLN:HG2	12	0.13
(1,1726)	1:B:41:VAL:HG23	1:B:77:GLN:HG2	12	0.13
(1,1691)	1:B:40:ALA:HB1	1:B:78:TYR:HE1	2	0.13
(1,1691)	1:B:40:ALA:HB2	1:B:78:TYR:HE1	2	0.13
(1,1691)	1:B:40:ALA:HB3	1:B:78:TYR:HE1	2	0.13
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	1	0.13
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	1	0.13
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	1	0.13
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD11	8	0.13
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD12	8	0.13
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD13	8	0.13
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD11	8	0.13
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD12	8	0.13
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD13	8	0.13
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD2	19	0.13
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD3	19	0.13
(1,144)	1:A:7:ARG:H	1:A:7:ARG:HG2	8	0.13
(1,144)	1:A:7:ARG:H	1:A:7:ARG:HG2	18	0.13
(1,1421)	1:B:22:LEU:HB2	1:B:23:ALA:H	15	0.13
(1,1411)	1:B:21:ALA:HB1	1:B:65:GLY:H	13	0.13
(1,1411)	1:B:21:ALA:HB2	1:B:65:GLY:H	13	0.13
(1,1411)	1:B:21:ALA:HB3	1:B:65:GLY:H	13	0.13
(1,1375)	1:B:18:VAL:HG11	1:B:22:LEU:H	20	0.13
(1,1375)	1:B:18:VAL:HG12	1:B:22:LEU:H	20	0.13
(1,1375)	1:B:18:VAL:HG13	1:B:22:LEU:H	20	0.13
(1,1292)	1:B:10:ALA:HA	1:B:13:ASP:HB2	12	0.13
(1,1252)	1:A:101:LEU:HD21	1:A:102:GLU:H	4	0.13
(1,1252)	1:A:101:LEU:HD22	1:A:102:GLU:H	4	0.13
(1,1252)	1:A:101:LEU:HD23	1:A:102:GLU:H	4	0.13
(1,1166)	1:A:91:ALA:HA	1:A:94:GLN:HG2	17	0.13
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG11	18	0.13
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG12	18	0.13
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG13	18	0.13
(1,1044)	1:A:80:ARG:HB2	1:A:80:ARG:HE	10	0.13
(1,1020)	1:A:76:ARG:HD2	1:A:78:TYR:HE1	2	0.13
(1,1020)	1:A:76:ARG:HD3	1:A:78:TYR:HE1	2	0.13
(1,996)	1:A:73:GLU:HG2	1:A:78:TYR:HD1	2	0.12
(1,996)	1:A:73:GLU:HG3	1:A:78:TYR:HD1	2	0.12
(1,888)	1:A:67:LEU:HA	1:A:67:LEU:HD11	12	0.12
(1,888)	1:A:67:LEU:HA	1:A:67:LEU:HD12	12	0.12
(1,888)	1:A:67:LEU:HA	1:A:67:LEU:HD13	12	0.12
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB2	9	0.12

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB3	9	0.12
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB2	9	0.12
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB3	9	0.12
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB2	9	0.12
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB3	9	0.12
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	4	0.12
(1,530)	1:A:39:ARG:HA	1:A:39:ARG:HD2	13	0.12
(1,514)	1:A:36:GLN:H	1:A:36:GLN:HB2	4	0.12
(1,514)	1:A:36:GLN:H	1:A:36:GLN:HB2	9	0.12
(1,511)	1:A:36:GLN:HB2	1:A:37:GLY:H	11	0.12
(1,486)	1:A:34:LEU:HB2	1:A:80:ARG:HA	8	0.12
(1,354)	1:A:29:GLN:HB2	1:A:48:THR:HB	13	0.12
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	11	0.12
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	11	0.12
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	11	0.12
(1,2390)	1:B:107:HIS:HB2	1:B:108:HIS:H	18	0.12
(1,2374)	1:B:99:GLU:HG2	1:B:100:HIS:H	1	0.12
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD21	17	0.12
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD22	17	0.12
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD23	17	0.12
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD21	17	0.12
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD22	17	0.12
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD23	17	0.12
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD21	17	0.12
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD22	17	0.12
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD23	17	0.12
(1,2342)	1:B:95:VAL:HG11	1:B:99:GLU:HB2	18	0.12
(1,2342)	1:B:95:VAL:HG12	1:B:99:GLU:HB2	18	0.12
(1,2342)	1:B:95:VAL:HG13	1:B:99:GLU:HB2	18	0.12
(1,2276)	1:B:89:LEU:HD21	1:B:93:VAL:HB	18	0.12
(1,2276)	1:B:89:LEU:HD22	1:B:93:VAL:HB	18	0.12
(1,2276)	1:B:89:LEU:HD23	1:B:93:VAL:HB	18	0.12
(1,2113)	1:B:72:ARG:HA	1:B:77:GLN:HG2	1	0.12
(1,2031)	1:B:67:LEU:HD11	1:B:86:VAL:HA	13	0.12
(1,2031)	1:B:67:LEU:HD12	1:B:86:VAL:HA	13	0.12
(1,2031)	1:B:67:LEU:HD13	1:B:86:VAL:HA	13	0.12
(1,2029)	1:B:67:LEU:HB2	1:B:68:VAL:HG21	3	0.12
(1,2029)	1:B:67:LEU:HB2	1:B:68:VAL:HG22	3	0.12
(1,2029)	1:B:67:LEU:HB2	1:B:68:VAL:HG23	3	0.12
(1,2029)	1:B:67:LEU:HB3	1:B:68:VAL:HG21	3	0.12
(1,2029)	1:B:67:LEU:HB3	1:B:68:VAL:HG22	3	0.12
(1,2029)	1:B:67:LEU:HB3	1:B:68:VAL:HG23	3	0.12

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	10	0.12
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	10	0.12
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB2	17	0.12
(1,1873)	1:B:52:LEU:HD11	1:B:56:SER:HB3	17	0.12
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB2	17	0.12
(1,1873)	1:B:52:LEU:HD12	1:B:56:SER:HB3	17	0.12
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB2	17	0.12
(1,1873)	1:B:52:LEU:HD13	1:B:56:SER:HB3	17	0.12
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD11	19	0.12
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD12	19	0.12
(1,1861)	1:B:52:LEU:HA	1:B:52:LEU:HD13	19	0.12
(1,1845)	1:B:50:MET:HG2	1:B:54:THR:HG21	16	0.12
(1,1845)	1:B:50:MET:HG2	1:B:54:THR:HG22	16	0.12
(1,1845)	1:B:50:MET:HG2	1:B:54:THR:HG23	16	0.12
(1,1688)	1:B:40:ALA:HB1	1:B:76:ARG:HD2	2	0.12
(1,1688)	1:B:40:ALA:HB1	1:B:76:ARG:HD3	2	0.12
(1,1688)	1:B:40:ALA:HB2	1:B:76:ARG:HD2	2	0.12
(1,1688)	1:B:40:ALA:HB2	1:B:76:ARG:HD3	2	0.12
(1,1688)	1:B:40:ALA:HB3	1:B:76:ARG:HD2	2	0.12
(1,1688)	1:B:40:ALA:HB3	1:B:76:ARG:HD3	2	0.12
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	6	0.12
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	6	0.12
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	6	0.12
(1,150)	1:A:8:LYS:HB2	1:A:9:ALA:H	4	0.12
(1,150)	1:A:8:LYS:HB3	1:A:9:ALA:H	4	0.12
(1,1411)	1:B:21:ALA:HB1	1:B:65:GLY:H	20	0.12
(1,1411)	1:B:21:ALA:HB2	1:B:65:GLY:H	20	0.12
(1,1411)	1:B:21:ALA:HB3	1:B:65:GLY:H	20	0.12
(1,1258)	1:A:107:HIS:HB2	1:A:108:HIS:H	16	0.12
(1,1242)	1:A:99:GLU:HG2	1:A:100:HIS:H	19	0.12
(1,120)	1:B:88:ARG:HB2	1:A:92:LEU:HD11	9	0.12
(1,120)	1:B:88:ARG:HB2	1:A:92:LEU:HD12	9	0.12
(1,120)	1:B:88:ARG:HB2	1:A:92:LEU:HD13	9	0.12
(1,1166)	1:A:91:ALA:HA	1:A:94:GLN:HG2	3	0.12
(1,972)	1:A:71:ARG:HG2	1:A:78:TYR:HB2	7	0.11
(1,899)	1:A:67:LEU:HD11	1:A:86:VAL:HA	4	0.11
(1,899)	1:A:67:LEU:HD12	1:A:86:VAL:HA	4	0.11
(1,899)	1:A:67:LEU:HD13	1:A:86:VAL:HA	4	0.11
(1,899)	1:A:67:LEU:HD11	1:A:86:VAL:HA	11	0.11
(1,899)	1:A:67:LEU:HD12	1:A:86:VAL:HA	11	0.11
(1,899)	1:A:67:LEU:HD13	1:A:86:VAL:HA	11	0.11
(1,816)	1:A:60:GLN:HA	1:A:60:GLN:HE21	5	0.11

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,71)	1:B:12:LEU:HD11	1:A:29:GLN:HE21	18	0.11
(1,71)	1:B:12:LEU:HD12	1:A:29:GLN:HE21	18	0.11
(1,71)	1:B:12:LEU:HD13	1:A:29:GLN:HE21	18	0.11
(1,615)	1:A:42:GLU:HG2	1:A:52:LEU:HG	2	0.11
(1,530)	1:A:39:ARG:HA	1:A:39:ARG:HD2	1	0.11
(1,522)	1:A:38:GLU:HB2	1:A:80:ARG:HE	18	0.11
(1,522)	1:A:38:GLU:HB3	1:A:80:ARG:HE	18	0.11
(1,464)	1:A:33:LEU:HD11	1:A:36:GLN:HG2	2	0.11
(1,464)	1:A:33:LEU:HD12	1:A:36:GLN:HG2	2	0.11
(1,464)	1:A:33:LEU:HD13	1:A:36:GLN:HG2	2	0.11
(1,460)	1:A:33:LEU:HB2	1:A:34:LEU:H	9	0.11
(1,408)	1:A:31:LEU:HA	1:A:62:LEU:HD11	7	0.11
(1,408)	1:A:31:LEU:HA	1:A:62:LEU:HD12	7	0.11
(1,408)	1:A:31:LEU:HA	1:A:62:LEU:HD13	7	0.11
(1,362)	1:A:29:GLN:H	1:A:29:GLN:HG2	10	0.11
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	7	0.11
(1,319)	1:A:26:ARG:H	1:A:26:ARG:HG2	6	0.11
(1,319)	1:A:26:ARG:H	1:A:26:ARG:HG3	6	0.11
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD21	7	0.11
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD22	7	0.11
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD23	7	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD21	7	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD22	7	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD23	7	0.11
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD21	7	0.11
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD22	7	0.11
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD23	7	0.11
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD21	11	0.11
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD22	11	0.11
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD23	11	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD21	11	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD22	11	0.11
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD23	11	0.11
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD21	11	0.11
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD22	11	0.11
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD23	11	0.11
(1,2343)	1:B:95:VAL:HG11	1:B:99:GLU:HG2	16	0.11
(1,2343)	1:B:95:VAL:HG12	1:B:99:GLU:HG2	16	0.11
(1,2343)	1:B:95:VAL:HG13	1:B:99:GLU:HG2	16	0.11
(1,2298)	1:B:91:ALA:HA	1:B:94:GLN:HG2	13	0.11
(1,2154)	1:B:76:ARG:HG2	1:B:78:TYR:HE1	9	0.11
(1,2139)	1:B:75:THR:H	1:B:76:ARG:HG2	2	0.11

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2131)	1:B:73:GLU:H	1:B:76:ARG:HG2	2	0.11
(1,2100)	1:B:71:ARG:HB2	1:B:72:ARG:H	10	0.11
(1,2100)	1:B:71:ARG:HB2	1:B:72:ARG:H	11	0.11
(1,1835)	1:B:50:MET:HB2	1:B:54:THR:HG21	1	0.11
(1,1835)	1:B:50:MET:HB2	1:B:54:THR:HG22	1	0.11
(1,1835)	1:B:50:MET:HB2	1:B:54:THR:HG23	1	0.11
(1,1706)	1:B:41:VAL:HB	1:B:79:TYR:HE1	15	0.11
(1,1690)	1:B:40:ALA:HB1	1:B:78:TYR:HD1	9	0.11
(1,1690)	1:B:40:ALA:HB2	1:B:78:TYR:HD1	9	0.11
(1,1690)	1:B:40:ALA:HB3	1:B:78:TYR:HD1	9	0.11
(1,1662)	1:B:39:ARG:HA	1:B:39:ARG:HD2	4	0.11
(1,1662)	1:B:39:ARG:HA	1:B:39:ARG:HD2	19	0.11
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	10	0.11
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	10	0.11
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	10	0.11
(1,1451)	1:B:26:ARG:H	1:B:26:ARG:HG2	12	0.11
(1,1451)	1:B:26:ARG:H	1:B:26:ARG:HG3	12	0.11
(1,144)	1:A:7:ARG:H	1:A:7:ARG:HG2	16	0.11
(1,144)	1:A:7:ARG:H	1:A:7:ARG:HG2	19	0.11
(1,1276)	1:B:7:ARG:H	1:B:7:ARG:HG2	17	0.11
(1,1220)	1:A:96:VAL:HA	1:A:100:HIS:HD2	15	0.11
(1,968)	1:A:71:ARG:HB2	1:A:72:ARG:H	18	0.1
(1,897)	1:A:67:LEU:HB2	1:A:68:VAL:HG21	14	0.1
(1,897)	1:A:67:LEU:HB2	1:A:68:VAL:HG22	14	0.1
(1,897)	1:A:67:LEU:HB2	1:A:68:VAL:HG23	14	0.1
(1,897)	1:A:67:LEU:HB3	1:A:68:VAL:HG21	14	0.1
(1,897)	1:A:67:LEU:HB3	1:A:68:VAL:HG22	14	0.1
(1,897)	1:A:67:LEU:HB3	1:A:68:VAL:HG23	14	0.1
(1,819)	1:A:60:GLN:HA	1:A:63:LYS:HG2	11	0.1
(1,819)	1:A:60:GLN:HA	1:A:63:LYS:HG3	11	0.1
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB1	17	0.1
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB2	17	0.1
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB3	17	0.1
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB1	17	0.1
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB2	17	0.1
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB3	17	0.1
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB1	17	0.1
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB2	17	0.1
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB3	17	0.1
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB1	18	0.1
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB2	18	0.1
(1,740)	1:A:52:LEU:HD11	1:A:55:ALA:HB3	18	0.1

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB1	18	0.1
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB2	18	0.1
(1,740)	1:A:52:LEU:HD12	1:A:55:ALA:HB3	18	0.1
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB1	18	0.1
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB2	18	0.1
(1,740)	1:A:52:LEU:HD13	1:A:55:ALA:HB3	18	0.1
(1,7)	1:A:12:LEU:HD11	1:B:29:GLN:HB2	14	0.1
(1,7)	1:A:12:LEU:HD12	1:B:29:GLN:HB2	14	0.1
(1,7)	1:A:12:LEU:HD13	1:B:29:GLN:HB2	14	0.1
(1,594)	1:A:41:VAL:HG21	1:A:77:GLN:HG2	13	0.1
(1,594)	1:A:41:VAL:HG22	1:A:77:GLN:HG2	13	0.1
(1,594)	1:A:41:VAL:HG23	1:A:77:GLN:HG2	13	0.1
(1,558)	1:A:40:ALA:HB1	1:A:78:TYR:HD1	11	0.1
(1,558)	1:A:40:ALA:HB2	1:A:78:TYR:HD1	11	0.1
(1,558)	1:A:40:ALA:HB3	1:A:78:TYR:HD1	11	0.1
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD11	13	0.1
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD12	13	0.1
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD13	13	0.1
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD11	13	0.1
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD12	13	0.1
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD13	13	0.1
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD11	13	0.1
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD12	13	0.1
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD13	13	0.1
(1,530)	1:A:39:ARG:HA	1:A:39:ARG:HD2	15	0.1
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB1	19	0.1
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB2	19	0.1
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB3	19	0.1
(1,455)	1:A:33:LEU:HA	1:A:33:LEU:HD11	17	0.1
(1,455)	1:A:33:LEU:HA	1:A:33:LEU:HD12	17	0.1
(1,455)	1:A:33:LEU:HA	1:A:33:LEU:HD13	17	0.1
(1,4)	1:A:11:LEU:HD11	1:B:98:ASP:H	8	0.1
(1,4)	1:A:11:LEU:HD12	1:B:98:ASP:H	8	0.1
(1,4)	1:A:11:LEU:HD13	1:B:98:ASP:H	8	0.1
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	19	0.1
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	19	0.1
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	19	0.1
(1,2573)	1:B:66:GLY:H	1:B:63:LYS:O	3	0.1
(1,2459)	1:A:66:GLY:H	1:A:63:LYS:O	14	0.1
(1,2459)	1:A:66:GLY:H	1:A:63:LYS:O	15	0.1
(1,2384)	1:B:101:LEU:HD21	1:B:102:GLU:H	12	0.1
(1,2384)	1:B:101:LEU:HD22	1:B:102:GLU:H	12	0.1

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2384)	1:B:101:LEU:HD23	1:B:102:GLU:H	12	0.1
(1,231)	1:A:17:ARG:H	1:A:17:ARG:HG2	1	0.1
(1,2131)	1:B:73:GLU:H	1:B:76:ARG:HG2	5	0.1
(1,2128)	1:B:73:GLU:HG2	1:B:78:TYR:HD1	8	0.1
(1,2128)	1:B:73:GLU:HG3	1:B:78:TYR:HD1	8	0.1
(1,2031)	1:B:67:LEU:HD11	1:B:86:VAL:HA	14	0.1
(1,2031)	1:B:67:LEU:HD12	1:B:86:VAL:HA	14	0.1
(1,2031)	1:B:67:LEU:HD13	1:B:86:VAL:HA	14	0.1
(1,2)	1:A:11:LEU:HD11	1:B:98:ASP:HB3	3	0.1
(1,2)	1:A:11:LEU:HD12	1:B:98:ASP:HB3	3	0.1
(1,2)	1:A:11:LEU:HD13	1:B:98:ASP:HB3	3	0.1
(1,1854)	1:B:51:ASN:HB2	1:B:53:THR:H	13	0.1
(1,1845)	1:B:50:MET:HG2	1:B:54:THR:HG21	9	0.1
(1,1845)	1:B:50:MET:HG2	1:B:54:THR:HG22	9	0.1
(1,1845)	1:B:50:MET:HG2	1:B:54:THR:HG23	9	0.1
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	4	0.1
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	4	0.1
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	4	0.1
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD11	4	0.1
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD12	4	0.1
(1,1738)	1:B:42:GLU:HA	1:B:52:LEU:HD13	4	0.1
(1,1662)	1:B:39:ARG:HA	1:B:39:ARG:HD2	1	0.1
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD21	10	0.1
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD22	10	0.1
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD23	10	0.1
(1,1441)	1:B:24:ASN:H	1:B:24:ASN:HB2	17	0.1
(1,144)	1:A:7:ARG:H	1:A:7:ARG:HG2	6	0.1
(1,1367)	1:B:17:ARG:HD2	1:B:64:SER:HB2	7	0.1
(1,1367)	1:B:17:ARG:HD2	1:B:64:SER:HB3	7	0.1
(1,1367)	1:B:17:ARG:HD3	1:B:64:SER:HB2	7	0.1
(1,1367)	1:B:17:ARG:HD3	1:B:64:SER:HB3	7	0.1
(1,1363)	1:B:17:ARG:H	1:B:17:ARG:HG2	15	0.1
(1,1304)	1:B:11:LEU:HA	1:B:14:GLN:HG2	18	0.1
(1,1269)	1:B:7:ARG:HA	1:B:7:ARG:HG2	8	0.1
(1,1242)	1:A:99:GLU:HG2	1:A:100:HIS:H	1	0.1
(1,1242)	1:A:99:GLU:HG2	1:A:100:HIS:H	11	0.1
(1,1225)	1:A:96:VAL:HG21	1:A:100:HIS:HD2	17	0.1
(1,1225)	1:A:96:VAL:HG22	1:A:100:HIS:HD2	17	0.1
(1,1225)	1:A:96:VAL:HG23	1:A:100:HIS:HD2	17	0.1
(1,1208)	1:A:95:VAL:HG11	1:A:98:ASP:HB2	6	0.1
(1,1208)	1:A:95:VAL:HG12	1:A:98:ASP:HB2	6	0.1
(1,1208)	1:A:95:VAL:HG13	1:A:98:ASP:HB2	6	0.1

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG11	1	0.1
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG12	1	0.1
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG13	1	0.1
(1,1003)	1:A:74:GLY:HA2	1:A:76:ARG:H	4	0.1
(1,990)	1:A:72:ARG:H	1:A:72:ARG:HD2	20	0.09
(1,990)	1:A:72:ARG:H	1:A:72:ARG:HD3	20	0.09
(1,968)	1:A:71:ARG:HB2	1:A:72:ARG:H	10	0.09
(1,963)	1:A:70:ALA:HB1	1:A:79:TYR:HE1	5	0.09
(1,963)	1:A:70:ALA:HB2	1:A:79:TYR:HE1	5	0.09
(1,963)	1:A:70:ALA:HB3	1:A:79:TYR:HE1	5	0.09
(1,944)	1:A:69:GLU:HG3	1:A:82:ALA:HB1	3	0.09
(1,944)	1:A:69:GLU:HG3	1:A:82:ALA:HB2	3	0.09
(1,944)	1:A:69:GLU:HG3	1:A:82:ALA:HB3	3	0.09
(1,944)	1:A:69:GLU:HG3	1:A:82:ALA:HB1	8	0.09
(1,944)	1:A:69:GLU:HG3	1:A:82:ALA:HB2	8	0.09
(1,944)	1:A:69:GLU:HG3	1:A:82:ALA:HB3	8	0.09
(1,897)	1:A:67:LEU:HB2	1:A:68:VAL:HG21	15	0.09
(1,897)	1:A:67:LEU:HB2	1:A:68:VAL:HG22	15	0.09
(1,897)	1:A:67:LEU:HB2	1:A:68:VAL:HG23	15	0.09
(1,897)	1:A:67:LEU:HB3	1:A:68:VAL:HG21	15	0.09
(1,897)	1:A:67:LEU:HB3	1:A:68:VAL:HG22	15	0.09
(1,897)	1:A:67:LEU:HB3	1:A:68:VAL:HG23	15	0.09
(1,89)	1:B:14:GLN:HB2	1:A:101:LEU:HD21	6	0.09
(1,89)	1:B:14:GLN:HB2	1:A:101:LEU:HD22	6	0.09
(1,89)	1:B:14:GLN:HB2	1:A:101:LEU:HD23	6	0.09
(1,89)	1:B:14:GLN:HB3	1:A:101:LEU:HD21	6	0.09
(1,89)	1:B:14:GLN:HB3	1:A:101:LEU:HD22	6	0.09
(1,89)	1:B:14:GLN:HB3	1:A:101:LEU:HD23	6	0.09
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	20	0.09
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	20	0.09
(1,835)	1:A:62:LEU:HA	1:A:67:LEU:HD21	14	0.09
(1,835)	1:A:62:LEU:HA	1:A:67:LEU:HD22	14	0.09
(1,835)	1:A:62:LEU:HA	1:A:67:LEU:HD23	14	0.09
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB2	8	0.09
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB3	8	0.09
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB2	8	0.09
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB3	8	0.09
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB2	8	0.09
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB3	8	0.09
(1,705)	1:A:50:MET:HB2	1:A:55:ALA:H	12	0.09
(1,7)	1:A:12:LEU:HD11	1:B:29:GLN:HB2	16	0.09
(1,7)	1:A:12:LEU:HD12	1:B:29:GLN:HB2	16	0.09

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,7)	1:A:12:LEU:HD13	1:B:29:GLN:HB2	16	0.09
(1,558)	1:A:40:ALA:HB1	1:A:78:TYR:HD1	7	0.09
(1,558)	1:A:40:ALA:HB2	1:A:78:TYR:HD1	7	0.09
(1,558)	1:A:40:ALA:HB3	1:A:78:TYR:HD1	7	0.09
(1,511)	1:A:36:GLN:HB2	1:A:37:GLY:H	18	0.09
(1,472)	1:A:33:LEU:HD11	1:A:47:ALA:HB1	1	0.09
(1,472)	1:A:33:LEU:HD11	1:A:47:ALA:HB2	1	0.09
(1,472)	1:A:33:LEU:HD11	1:A:47:ALA:HB3	1	0.09
(1,472)	1:A:33:LEU:HD12	1:A:47:ALA:HB1	1	0.09
(1,472)	1:A:33:LEU:HD12	1:A:47:ALA:HB2	1	0.09
(1,472)	1:A:33:LEU:HD12	1:A:47:ALA:HB3	1	0.09
(1,472)	1:A:33:LEU:HD13	1:A:47:ALA:HB1	1	0.09
(1,472)	1:A:33:LEU:HD13	1:A:47:ALA:HB2	1	0.09
(1,472)	1:A:33:LEU:HD13	1:A:47:ALA:HB3	1	0.09
(1,465)	1:A:33:LEU:HD11	1:A:36:GLN:H	17	0.09
(1,465)	1:A:33:LEU:HD12	1:A:36:GLN:H	17	0.09
(1,465)	1:A:33:LEU:HD13	1:A:36:GLN:H	17	0.09
(1,463)	1:A:33:LEU:HD11	1:A:36:GLN:HE21	18	0.09
(1,463)	1:A:33:LEU:HD12	1:A:36:GLN:HE21	18	0.09
(1,463)	1:A:33:LEU:HD13	1:A:36:GLN:HE21	18	0.09
(1,462)	1:A:33:LEU:HD11	1:A:36:GLN:HB2	17	0.09
(1,462)	1:A:33:LEU:HD12	1:A:36:GLN:HB2	17	0.09
(1,462)	1:A:33:LEU:HD13	1:A:36:GLN:HB2	17	0.09
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD21	9	0.09
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD22	9	0.09
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD23	9	0.09
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD21	9	0.09
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD22	9	0.09
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD23	9	0.09
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD21	9	0.09
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD22	9	0.09
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD23	9	0.09
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	15	0.09
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	15	0.09
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	15	0.09
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	16	0.09
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	16	0.09
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	16	0.09
(1,245)	1:A:18:VAL:HG11	1:A:65:GLY:HA2	5	0.09
(1,245)	1:A:18:VAL:HG12	1:A:65:GLY:HA2	5	0.09
(1,245)	1:A:18:VAL:HG13	1:A:65:GLY:HA2	5	0.09
(1,2390)	1:B:107:HIS:HB2	1:B:108:HIS:H	3	0.09

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA2	8	0.09
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA2	20	0.09
(1,2287)	1:B:90:PHE:HB2	1:B:93:VAL:HG11	7	0.09
(1,2287)	1:B:90:PHE:HB2	1:B:93:VAL:HG12	7	0.09
(1,2287)	1:B:90:PHE:HB2	1:B:93:VAL:HG13	7	0.09
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	18	0.09
(1,2151)	1:B:76:ARG:HD2	1:B:77:GLN:H	17	0.09
(1,2151)	1:B:76:ARG:HD3	1:B:77:GLN:H	17	0.09
(1,2145)	1:B:76:ARG:HB2	1:B:78:TYR:HD1	3	0.09
(1,2145)	1:B:76:ARG:HB2	1:B:78:TYR:HD1	10	0.09
(1,2020)	1:B:67:LEU:HA	1:B:67:LEU:HD11	6	0.09
(1,2020)	1:B:67:LEU:HA	1:B:67:LEU:HD12	6	0.09
(1,2020)	1:B:67:LEU:HA	1:B:67:LEU:HD13	6	0.09
(1,1991)	1:B:63:LYS:HB2	1:B:69:GLU:HA	6	0.09
(1,1837)	1:B:50:MET:HB2	1:B:55:ALA:H	3	0.09
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD11	7	0.09
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD12	7	0.09
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD13	7	0.09
(1,1681)	1:B:40:ALA:HB1	1:B:42:GLU:HG2	18	0.09
(1,1681)	1:B:40:ALA:HB2	1:B:42:GLU:HG2	18	0.09
(1,1681)	1:B:40:ALA:HB3	1:B:42:GLU:HG2	18	0.09
(1,1657)	1:B:38:GLU:HG2	1:B:78:TYR:HB2	1	0.09
(1,1657)	1:B:38:GLU:HG3	1:B:78:TYR:HB2	1	0.09
(1,1657)	1:B:38:GLU:HG2	1:B:78:TYR:HB2	8	0.09
(1,1657)	1:B:38:GLU:HG3	1:B:78:TYR:HB2	8	0.09
(1,1643)	1:B:36:GLN:HB2	1:B:37:GLY:H	13	0.09
(1,1618)	1:B:34:LEU:HB2	1:B:80:ARG:HA	15	0.09
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB1	11	0.09
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB2	11	0.09
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB3	11	0.09
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB1	11	0.09
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB2	11	0.09
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB3	11	0.09
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB1	11	0.09
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB2	11	0.09
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB3	11	0.09
(1,160)	1:A:10:ALA:HA	1:A:13:ASP:HB2	14	0.09
(1,1592)	1:B:33:LEU:HB2	1:B:34:LEU:H	16	0.09
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG21	2	0.09
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG22	2	0.09
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG23	2	0.09
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG21	13	0.09

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG22	13	0.09
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG23	13	0.09
(1,1411)	1:B:21:ALA:HB1	1:B:65:GLY:H	5	0.09
(1,1411)	1:B:21:ALA:HB2	1:B:65:GLY:H	5	0.09
(1,1411)	1:B:21:ALA:HB3	1:B:65:GLY:H	5	0.09
(1,1363)	1:B:17:ARG:H	1:B:17:ARG:HG2	13	0.09
(1,1283)	1:B:8:LYS:HE2	1:B:12:LEU:HD11	14	0.09
(1,1283)	1:B:8:LYS:HE2	1:B:12:LEU:HD12	14	0.09
(1,1283)	1:B:8:LYS:HE2	1:B:12:LEU:HD13	14	0.09
(1,1283)	1:B:8:LYS:HE3	1:B:12:LEU:HD11	14	0.09
(1,1283)	1:B:8:LYS:HE3	1:B:12:LEU:HD12	14	0.09
(1,1283)	1:B:8:LYS:HE3	1:B:12:LEU:HD13	14	0.09
(1,1276)	1:B:7:ARG:H	1:B:7:ARG:HG2	3	0.09
(1,1276)	1:B:7:ARG:H	1:B:7:ARG:HG2	10	0.09
(1,1230)	1:A:97:ALA:HA	1:A:101:LEU:HD21	16	0.09
(1,1230)	1:A:97:ALA:HA	1:A:101:LEU:HD22	16	0.09
(1,1230)	1:A:97:ALA:HA	1:A:101:LEU:HD23	16	0.09
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB1	7	0.09
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB2	7	0.09
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB3	7	0.09
(1,1035)	1:A:77:GLN:HG2	1:A:79:TYR:HE1	11	0.09
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	2	0.08
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	2	0.08
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	2	0.08
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	2	0.08
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	2	0.08
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	2	0.08
(1,796)	1:A:59:LEU:HA	1:A:62:LEU:HD11	5	0.08
(1,796)	1:A:59:LEU:HA	1:A:62:LEU:HD12	5	0.08
(1,796)	1:A:59:LEU:HA	1:A:62:LEU:HD13	5	0.08
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	3	0.08
(1,615)	1:A:42:GLU:HG2	1:A:52:LEU:HG	16	0.08
(1,549)	1:A:40:ALA:HB1	1:A:42:GLU:HG2	4	0.08
(1,549)	1:A:40:ALA:HB2	1:A:42:GLU:HG2	4	0.08
(1,549)	1:A:40:ALA:HB3	1:A:42:GLU:HG2	4	0.08
(1,549)	1:A:40:ALA:HB1	1:A:42:GLU:HG2	16	0.08
(1,549)	1:A:40:ALA:HB2	1:A:42:GLU:HG2	16	0.08
(1,549)	1:A:40:ALA:HB3	1:A:42:GLU:HG2	16	0.08
(1,538)	1:A:39:ARG:HG2	1:A:40:ALA:H	11	0.08
(1,537)	1:A:39:ARG:HD2	1:A:43:ALA:HB1	16	0.08
(1,537)	1:A:39:ARG:HD2	1:A:43:ALA:HB2	16	0.08
(1,537)	1:A:39:ARG:HD2	1:A:43:ALA:HB3	16	0.08

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,530)	1:A:39:ARG:HA	1:A:39:ARG:HD2	10	0.08
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB1	11	0.08
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB2	11	0.08
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB3	11	0.08
(1,462)	1:A:33:LEU:HD11	1:A:36:GLN:HB2	8	0.08
(1,462)	1:A:33:LEU:HD12	1:A:36:GLN:HB2	8	0.08
(1,462)	1:A:33:LEU:HD13	1:A:36:GLN:HB2	8	0.08
(1,462)	1:A:33:LEU:HD11	1:A:36:GLN:HB2	15	0.08
(1,462)	1:A:33:LEU:HD12	1:A:36:GLN:HB2	15	0.08
(1,462)	1:A:33:LEU:HD13	1:A:36:GLN:HB2	15	0.08
(1,313)	1:A:25:GLY:HA2	1:A:28:LEU:HD11	6	0.08
(1,313)	1:A:25:GLY:HA2	1:A:28:LEU:HD12	6	0.08
(1,313)	1:A:25:GLY:HA2	1:A:28:LEU:HD13	6	0.08
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	7	0.08
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	7	0.08
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	7	0.08
(1,308)	1:A:23:ALA:H	1:A:24:ASN:H	19	0.08
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	3	0.08
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	3	0.08
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	3	0.08
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	12	0.08
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	12	0.08
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	12	0.08
(1,2151)	1:B:76:ARG:HD2	1:B:77:GLN:H	4	0.08
(1,2151)	1:B:76:ARG:HD3	1:B:77:GLN:H	4	0.08
(1,2100)	1:B:71:ARG:HB2	1:B:72:ARG:H	1	0.08
(1,2095)	1:B:70:ALA:HB1	1:B:79:TYR:HE1	5	0.08
(1,2095)	1:B:70:ALA:HB2	1:B:79:TYR:HE1	5	0.08
(1,2095)	1:B:70:ALA:HB3	1:B:79:TYR:HE1	5	0.08
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	2	0.08
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	2	0.08
(1,1991)	1:B:63:LYS:HB2	1:B:69:GLU:HA	16	0.08
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE2	4	0.08
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE3	4	0.08
(1,1967)	1:B:62:LEU:HA	1:B:67:LEU:HD21	13	0.08
(1,1967)	1:B:62:LEU:HA	1:B:67:LEU:HD22	13	0.08
(1,1967)	1:B:62:LEU:HA	1:B:67:LEU:HD23	13	0.08
(1,1951)	1:B:60:GLN:HA	1:B:63:LYS:HG2	12	0.08
(1,1951)	1:B:60:GLN:HA	1:B:63:LYS:HG3	12	0.08
(1,1879)	1:B:53:THR:HB	1:B:54:THR:H	20	0.08
(1,1681)	1:B:40:ALA:HB1	1:B:42:GLU:HG2	15	0.08
(1,1681)	1:B:40:ALA:HB2	1:B:42:GLU:HG2	15	0.08

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1681)	1:B:40:ALA:HB3	1:B:42:GLU:HG2	15	0.08
(1,1675)	1:B:40:ALA:HA	1:B:78:TYR:HA	9	0.08
(1,1675)	1:B:40:ALA:HA	1:B:78:TYR:HA	19	0.08
(1,1670)	1:B:39:ARG:HG2	1:B:40:ALA:H	18	0.08
(1,1662)	1:B:39:ARG:HA	1:B:39:ARG:HD2	17	0.08
(1,164)	1:A:10:ALA:HB1	1:A:13:ASP:HB2	13	0.08
(1,164)	1:A:10:ALA:HB2	1:A:13:ASP:HB2	13	0.08
(1,164)	1:A:10:ALA:HB3	1:A:13:ASP:HB2	13	0.08
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB1	18	0.08
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB2	18	0.08
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB3	18	0.08
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB1	18	0.08
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB2	18	0.08
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB3	18	0.08
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB1	18	0.08
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB2	18	0.08
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB3	18	0.08
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	20	0.08
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	20	0.08
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	20	0.08
(1,1563)	1:B:31:LEU:HD21	1:B:67:LEU:HD11	3	0.08
(1,1563)	1:B:31:LEU:HD21	1:B:67:LEU:HD12	3	0.08
(1,1563)	1:B:31:LEU:HD21	1:B:67:LEU:HD13	3	0.08
(1,1563)	1:B:31:LEU:HD22	1:B:67:LEU:HD11	3	0.08
(1,1563)	1:B:31:LEU:HD22	1:B:67:LEU:HD12	3	0.08
(1,1563)	1:B:31:LEU:HD22	1:B:67:LEU:HD13	3	0.08
(1,1563)	1:B:31:LEU:HD23	1:B:67:LEU:HD11	3	0.08
(1,1563)	1:B:31:LEU:HD23	1:B:67:LEU:HD12	3	0.08
(1,1563)	1:B:31:LEU:HD23	1:B:67:LEU:HD13	3	0.08
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG21	3	0.08
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG22	3	0.08
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG23	3	0.08
(1,1446)	1:B:25:GLY:HA3	1:B:28:LEU:HD11	19	0.08
(1,1446)	1:B:25:GLY:HA3	1:B:28:LEU:HD12	19	0.08
(1,1446)	1:B:25:GLY:HA3	1:B:28:LEU:HD13	19	0.08
(1,144)	1:A:7:ARG:H	1:A:7:ARG:HG2	10	0.08
(1,144)	1:A:7:ARG:H	1:A:7:ARG:HG2	11	0.08
(1,141)	1:A:7:ARG:HB2	1:A:8:LYS:H	19	0.08
(1,1377)	1:B:18:VAL:HG11	1:B:65:GLY:HA2	15	0.08
(1,1377)	1:B:18:VAL:HG12	1:B:65:GLY:HA2	15	0.08
(1,1377)	1:B:18:VAL:HG13	1:B:65:GLY:HA2	15	0.08
(1,1367)	1:B:17:ARG:HD2	1:B:64:SER:HB2	17	0.08

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1367)	1:B:17:ARG:HD2	1:B:64:SER:HB3	17	0.08
(1,1367)	1:B:17:ARG:HD3	1:B:64:SER:HB2	17	0.08
(1,1367)	1:B:17:ARG:HD3	1:B:64:SER:HB3	17	0.08
(1,1363)	1:B:17:ARG:H	1:B:17:ARG:HG2	1	0.08
(1,1276)	1:B:7:ARG:H	1:B:7:ARG:HG2	16	0.08
(1,1269)	1:B:7:ARG:HA	1:B:7:ARG:HG2	7	0.08
(1,1262)	1:B:5:SER:HB2	1:B:6:ASP:H	1	0.08
(1,1248)	1:A:101:LEU:HA	1:A:101:LEU:HD21	8	0.08
(1,1248)	1:A:101:LEU:HA	1:A:101:LEU:HD22	8	0.08
(1,1248)	1:A:101:LEU:HA	1:A:101:LEU:HD23	8	0.08
(1,1220)	1:A:96:VAL:HA	1:A:100:HIS:HD2	12	0.08
(1,1186)	1:A:93:VAL:H	1:A:93:VAL:HG11	2	0.08
(1,1186)	1:A:93:VAL:H	1:A:93:VAL:HG12	2	0.08
(1,1186)	1:A:93:VAL:H	1:A:93:VAL:HG13	2	0.08
(1,1166)	1:A:91:ALA:HA	1:A:94:GLN:HG2	4	0.08
(1,1166)	1:A:91:ALA:HA	1:A:94:GLN:HG2	5	0.08
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG11	12	0.08
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG12	12	0.08
(1,1155)	1:A:90:PHE:HB2	1:A:93:VAL:HG13	12	0.08
(1,969)	1:A:71:ARG:HB2	1:A:79:TYR:HA	14	0.07
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG21	14	0.07
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG22	14	0.07
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG23	14	0.07
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG21	15	0.07
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG22	15	0.07
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG23	15	0.07
(1,859)	1:A:63:LYS:HB2	1:A:69:GLU:HA	16	0.07
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE2	1	0.07
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE3	1	0.07
(1,835)	1:A:62:LEU:HA	1:A:67:LEU:HD21	15	0.07
(1,835)	1:A:62:LEU:HA	1:A:67:LEU:HD22	15	0.07
(1,835)	1:A:62:LEU:HA	1:A:67:LEU:HD23	15	0.07
(1,816)	1:A:60:GLN:HA	1:A:60:GLN:HE21	18	0.07
(1,810)	1:A:59:LEU:HD21	1:A:79:TYR:HE1	19	0.07
(1,810)	1:A:59:LEU:HD22	1:A:79:TYR:HE1	19	0.07
(1,810)	1:A:59:LEU:HD23	1:A:79:TYR:HE1	19	0.07
(1,749)	1:A:53:THR:HG21	1:A:54:THR:H	5	0.07
(1,749)	1:A:53:THR:HG22	1:A:54:THR:H	5	0.07
(1,749)	1:A:53:THR:HG23	1:A:54:THR:H	5	0.07
(1,749)	1:A:53:THR:HG21	1:A:54:THR:H	13	0.07
(1,749)	1:A:53:THR:HG22	1:A:54:THR:H	13	0.07
(1,749)	1:A:53:THR:HG23	1:A:54:THR:H	13	0.07

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	10	0.07
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	9	0.07
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	9	0.07
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	9	0.07
(1,615)	1:A:42:GLU:HG2	1:A:52:LEU:HG	13	0.07
(1,612)	1:A:42:GLU:HG2	1:A:43:ALA:H	18	0.07
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB1	17	0.07
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB2	17	0.07
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB3	17	0.07
(1,524)	1:A:38:GLU:HG2	1:A:39:ARG:H	5	0.07
(1,524)	1:A:38:GLU:HG3	1:A:39:ARG:H	5	0.07
(1,524)	1:A:38:GLU:HG2	1:A:39:ARG:H	8	0.07
(1,524)	1:A:38:GLU:HG3	1:A:39:ARG:H	8	0.07
(1,50)	1:A:20:LYS:HA	1:B:23:ALA:HB1	3	0.07
(1,50)	1:A:20:LYS:HA	1:B:23:ALA:HB2	3	0.07
(1,50)	1:A:20:LYS:HA	1:B:23:ALA:HB3	3	0.07
(1,476)	1:A:33:LEU:HG	1:A:39:ARG:HE	15	0.07
(1,473)	1:A:33:LEU:HD11	1:A:47:ALA:H	18	0.07
(1,473)	1:A:33:LEU:HD12	1:A:47:ALA:H	18	0.07
(1,473)	1:A:33:LEU:HD13	1:A:47:ALA:H	18	0.07
(1,467)	1:A:33:LEU:HD11	1:A:39:ARG:HD2	5	0.07
(1,467)	1:A:33:LEU:HD12	1:A:39:ARG:HD2	5	0.07
(1,467)	1:A:33:LEU:HD13	1:A:39:ARG:HD2	5	0.07
(1,461)	1:A:33:LEU:HD11	1:A:34:LEU:H	8	0.07
(1,461)	1:A:33:LEU:HD12	1:A:34:LEU:H	8	0.07
(1,461)	1:A:33:LEU:HD13	1:A:34:LEU:H	8	0.07
(1,431)	1:A:31:LEU:HD21	1:A:67:LEU:HD11	14	0.07
(1,431)	1:A:31:LEU:HD21	1:A:67:LEU:HD12	14	0.07
(1,431)	1:A:31:LEU:HD21	1:A:67:LEU:HD13	14	0.07
(1,431)	1:A:31:LEU:HD22	1:A:67:LEU:HD11	14	0.07
(1,431)	1:A:31:LEU:HD22	1:A:67:LEU:HD12	14	0.07
(1,431)	1:A:31:LEU:HD22	1:A:67:LEU:HD13	14	0.07
(1,431)	1:A:31:LEU:HD23	1:A:67:LEU:HD11	14	0.07
(1,431)	1:A:31:LEU:HD23	1:A:67:LEU:HD12	14	0.07
(1,431)	1:A:31:LEU:HD23	1:A:67:LEU:HD13	14	0.07
(1,408)	1:A:31:LEU:HA	1:A:62:LEU:HD11	12	0.07
(1,408)	1:A:31:LEU:HA	1:A:62:LEU:HD12	12	0.07
(1,408)	1:A:31:LEU:HA	1:A:62:LEU:HD13	12	0.07
(1,389)	1:A:30:ILE:HG21	1:A:33:LEU:HB2	6	0.07
(1,389)	1:A:30:ILE:HG22	1:A:33:LEU:HB2	6	0.07
(1,389)	1:A:30:ILE:HG23	1:A:33:LEU:HB2	6	0.07
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD21	16	0.07

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD22	16	0.07
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD23	16	0.07
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD21	16	0.07
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD22	16	0.07
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD23	16	0.07
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD21	16	0.07
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD22	16	0.07
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD23	16	0.07
(1,2535)	1:B:41:VAL:H	1:B:77:GLN:O	7	0.07
(1,2515)	1:B:18:VAL:H	1:B:14:GLN:O	4	0.07
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD21	19	0.07
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD22	19	0.07
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD23	19	0.07
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD21	19	0.07
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD22	19	0.07
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD23	19	0.07
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD21	19	0.07
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD22	19	0.07
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD23	19	0.07
(1,2357)	1:B:96:VAL:HG21	1:B:100:HIS:HD2	15	0.07
(1,2357)	1:B:96:VAL:HG22	1:B:100:HIS:HD2	15	0.07
(1,2357)	1:B:96:VAL:HG23	1:B:100:HIS:HD2	15	0.07
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB2	5	0.07
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB3	5	0.07
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB2	5	0.07
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB3	5	0.07
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB2	11	0.07
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB3	11	0.07
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB2	11	0.07
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB3	11	0.07
(1,2318)	1:B:93:VAL:H	1:B:93:VAL:HG11	3	0.07
(1,2318)	1:B:93:VAL:H	1:B:93:VAL:HG12	3	0.07
(1,2318)	1:B:93:VAL:H	1:B:93:VAL:HG13	3	0.07
(1,2318)	1:B:93:VAL:H	1:B:93:VAL:HG11	8	0.07
(1,2318)	1:B:93:VAL:H	1:B:93:VAL:HG12	8	0.07
(1,2318)	1:B:93:VAL:H	1:B:93:VAL:HG13	8	0.07
(1,2318)	1:B:93:VAL:H	1:B:93:VAL:HG11	18	0.07
(1,2318)	1:B:93:VAL:H	1:B:93:VAL:HG12	18	0.07
(1,2318)	1:B:93:VAL:H	1:B:93:VAL:HG13	18	0.07
(1,2191)	1:B:81:ILE:HG12	1:B:87:ALA:HA	13	0.07
(1,2157)	1:B:76:ARG:H	1:B:76:ARG:HG2	2	0.07
(1,2119)	1:B:72:ARG:HD2	1:B:77:GLN:HG2	4	0.07

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2119)	1:B:72:ARG:HD3	1:B:77:GLN:HG2	4	0.07
(1,2105)	1:B:71:ARG:H	1:B:71:ARG:HG2	11	0.07
(1,2094)	1:B:70:ALA:HB1	1:B:79:TYR:HD1	8	0.07
(1,2094)	1:B:70:ALA:HB2	1:B:79:TYR:HD1	8	0.07
(1,2094)	1:B:70:ALA:HB3	1:B:79:TYR:HD1	8	0.07
(1,2031)	1:B:67:LEU:HD11	1:B:86:VAL:HA	15	0.07
(1,2031)	1:B:67:LEU:HD12	1:B:86:VAL:HA	15	0.07
(1,2031)	1:B:67:LEU:HD13	1:B:86:VAL:HA	15	0.07
(1,2031)	1:B:67:LEU:HD11	1:B:86:VAL:HA	17	0.07
(1,2031)	1:B:67:LEU:HD12	1:B:86:VAL:HA	17	0.07
(1,2031)	1:B:67:LEU:HD13	1:B:86:VAL:HA	17	0.07
(1,203)	1:A:14:GLN:HB2	1:A:14:GLN:HE21	8	0.07
(1,203)	1:A:14:GLN:HB3	1:A:14:GLN:HE21	8	0.07
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD2	7	0.07
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD3	7	0.07
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	5	0.07
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	5	0.07
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	5	0.07
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	5	0.07
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	5	0.07
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	5	0.07
(1,1849)	1:B:50:MET:H	1:B:50:MET:HG2	18	0.07
(1,1750)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	4	0.07
(1,1750)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	4	0.07
(1,1750)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	4	0.07
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	15	0.07
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	15	0.07
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	15	0.07
(1,1706)	1:B:41:VAL:HB	1:B:79:TYR:HE1	3	0.07
(1,1662)	1:B:39:ARG:HA	1:B:39:ARG:HD2	10	0.07
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB1	18	0.07
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB2	18	0.07
(1,1601)	1:B:33:LEU:HD11	1:B:43:ALA:HB3	18	0.07
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB1	18	0.07
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB2	18	0.07
(1,1601)	1:B:33:LEU:HD12	1:B:43:ALA:HB3	18	0.07
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB1	18	0.07
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB2	18	0.07
(1,1601)	1:B:33:LEU:HD13	1:B:43:ALA:HB3	18	0.07
(1,1592)	1:B:33:LEU:HB2	1:B:34:LEU:H	8	0.07
(1,1499)	1:B:30:ILE:HA	1:B:33:LEU:HD11	15	0.07
(1,1499)	1:B:30:ILE:HA	1:B:33:LEU:HD12	15	0.07

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1499)	1:B:30:ILE:HA	1:B:33:LEU:HD13	15	0.07
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	19	0.07
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	19	0.07
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	19	0.07
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	19	0.07
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	19	0.07
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	19	0.07
(1,1367)	1:B:17:ARG:HD2	1:B:64:SER:HB2	6	0.07
(1,1367)	1:B:17:ARG:HD2	1:B:64:SER:HB3	6	0.07
(1,1367)	1:B:17:ARG:HD3	1:B:64:SER:HB2	6	0.07
(1,1367)	1:B:17:ARG:HD3	1:B:64:SER:HB3	6	0.07
(1,1363)	1:B:17:ARG:H	1:B:17:ARG:HG2	11	0.07
(1,1333)	1:B:14:GLN:HA	1:B:17:ARG:HD2	4	0.07
(1,1333)	1:B:14:GLN:HA	1:B:17:ARG:HD3	4	0.07
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD11	18	0.07
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD12	18	0.07
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD13	18	0.07
(1,1257)	1:A:102:GLU:H	1:A:102:GLU:HG2	4	0.07
(1,1257)	1:A:102:GLU:H	1:A:102:GLU:HG3	4	0.07
(1,1252)	1:A:101:LEU:HD21	1:A:102:GLU:H	14	0.07
(1,1252)	1:A:101:LEU:HD22	1:A:102:GLU:H	14	0.07
(1,1252)	1:A:101:LEU:HD23	1:A:102:GLU:H	14	0.07
(1,1242)	1:A:99:GLU:HG2	1:A:100:HIS:H	5	0.07
(1,1186)	1:A:93:VAL:H	1:A:93:VAL:HG11	10	0.07
(1,1186)	1:A:93:VAL:H	1:A:93:VAL:HG12	10	0.07
(1,1186)	1:A:93:VAL:H	1:A:93:VAL:HG13	10	0.07
(1,11)	1:A:12:LEU:HD11	1:B:32:ASP:HB2	16	0.07
(1,11)	1:A:12:LEU:HD11	1:B:32:ASP:HB3	16	0.07
(1,11)	1:A:12:LEU:HD12	1:B:32:ASP:HB2	16	0.07
(1,11)	1:A:12:LEU:HD12	1:B:32:ASP:HB3	16	0.07
(1,11)	1:A:12:LEU:HD13	1:B:32:ASP:HB2	16	0.07
(1,11)	1:A:12:LEU:HD13	1:B:32:ASP:HB3	16	0.07
(1,1095)	1:A:84:GLU:HG2	1:A:88:ARG:HG2	3	0.07
(1,1095)	1:A:84:GLU:HG3	1:A:88:ARG:HG2	3	0.07
(1,1035)	1:A:77:GLN:HG2	1:A:79:TYR:HE1	17	0.07
(1,1035)	1:A:77:GLN:HG2	1:A:79:TYR:HE1	19	0.07
(1,1033)	1:A:77:GLN:HG2	1:A:77:GLN:HE21	3	0.07
(1,1033)	1:A:77:GLN:HG2	1:A:77:GLN:HE21	4	0.07
(1,1019)	1:A:76:ARG:HD2	1:A:77:GLN:H	15	0.07
(1,1019)	1:A:76:ARG:HD3	1:A:77:GLN:H	15	0.07
(1,969)	1:A:71:ARG:HB2	1:A:79:TYR:HA	9	0.06
(1,968)	1:A:71:ARG:HB2	1:A:72:ARG:H	15	0.06

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,963)	1:A:70:ALA:HB1	1:A:79:TYR:HE1	2	0.06
(1,963)	1:A:70:ALA:HB2	1:A:79:TYR:HE1	2	0.06
(1,963)	1:A:70:ALA:HB3	1:A:79:TYR:HE1	2	0.06
(1,963)	1:A:70:ALA:HB1	1:A:79:TYR:HE1	4	0.06
(1,963)	1:A:70:ALA:HB2	1:A:79:TYR:HE1	4	0.06
(1,963)	1:A:70:ALA:HB3	1:A:79:TYR:HE1	4	0.06
(1,899)	1:A:67:LEU:HD11	1:A:86:VAL:HA	1	0.06
(1,899)	1:A:67:LEU:HD12	1:A:86:VAL:HA	1	0.06
(1,899)	1:A:67:LEU:HD13	1:A:86:VAL:HA	1	0.06
(1,899)	1:A:67:LEU:HD11	1:A:86:VAL:HA	16	0.06
(1,899)	1:A:67:LEU:HD12	1:A:86:VAL:HA	16	0.06
(1,899)	1:A:67:LEU:HD13	1:A:86:VAL:HA	16	0.06
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG21	4	0.06
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG22	4	0.06
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG23	4	0.06
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	20	0.06
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	20	0.06
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	20	0.06
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	20	0.06
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	20	0.06
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	20	0.06
(1,819)	1:A:60:GLN:HA	1:A:63:LYS:HG2	7	0.06
(1,819)	1:A:60:GLN:HA	1:A:63:LYS:HG3	7	0.06
(1,816)	1:A:60:GLN:HA	1:A:60:GLN:HE21	20	0.06
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB2	16	0.06
(1,741)	1:A:52:LEU:HD11	1:A:56:SER:HB3	16	0.06
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB2	16	0.06
(1,741)	1:A:52:LEU:HD12	1:A:56:SER:HB3	16	0.06
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB2	16	0.06
(1,741)	1:A:52:LEU:HD13	1:A:56:SER:HB3	16	0.06
(1,646)	1:A:44:ILE:HD11	1:A:79:TYR:HD1	11	0.06
(1,646)	1:A:44:ILE:HD12	1:A:79:TYR:HD1	11	0.06
(1,646)	1:A:44:ILE:HD13	1:A:79:TYR:HD1	11	0.06
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB1	16	0.06
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB2	16	0.06
(1,613)	1:A:42:GLU:HG2	1:A:45:ALA:HB3	16	0.06
(1,594)	1:A:41:VAL:HG21	1:A:77:GLN:HG2	12	0.06
(1,594)	1:A:41:VAL:HG22	1:A:77:GLN:HG2	12	0.06
(1,594)	1:A:41:VAL:HG23	1:A:77:GLN:HG2	12	0.06
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	10	0.06
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	10	0.06
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	10	0.06

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	10	0.06
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	10	0.06
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	10	0.06
(1,431)	1:A:31:LEU:HD21	1:A:67:LEU:HD11	15	0.06
(1,431)	1:A:31:LEU:HD21	1:A:67:LEU:HD12	15	0.06
(1,431)	1:A:31:LEU:HD21	1:A:67:LEU:HD13	15	0.06
(1,431)	1:A:31:LEU:HD22	1:A:67:LEU:HD11	15	0.06
(1,431)	1:A:31:LEU:HD22	1:A:67:LEU:HD12	15	0.06
(1,431)	1:A:31:LEU:HD22	1:A:67:LEU:HD13	15	0.06
(1,431)	1:A:31:LEU:HD23	1:A:67:LEU:HD11	15	0.06
(1,431)	1:A:31:LEU:HD23	1:A:67:LEU:HD12	15	0.06
(1,431)	1:A:31:LEU:HD23	1:A:67:LEU:HD13	15	0.06
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD1	13	0.06
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD2	13	0.06
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD1	13	0.06
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD2	13	0.06
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD1	13	0.06
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD2	13	0.06
(1,330)	1:A:27:ARG:HD2	1:A:62:LEU:H	12	0.06
(1,30)	1:A:14:GLN:HG2	1:B:97:ALA:HA	10	0.06
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD21	14	0.06
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD22	14	0.06
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD23	14	0.06
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD21	14	0.06
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD22	14	0.06
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD23	14	0.06
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD21	14	0.06
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD22	14	0.06
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD23	14	0.06
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD21	18	0.06
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD22	18	0.06
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD23	18	0.06
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD21	18	0.06
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD22	18	0.06
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD23	18	0.06
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD21	18	0.06
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD22	18	0.06
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD23	18	0.06
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	17	0.06
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	17	0.06
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	17	0.06
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	20	0.06

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	20	0.06
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	20	0.06
(1,2613)	1:B:97:ALA:H	1:B:93:VAL:O	18	0.06
(1,2583)	1:B:76:ARG:H	1:B:73:GLU:O	9	0.06
(1,2574)	1:B:66:GLY:N	1:B:63:LYS:O	3	0.06
(1,2533)	1:B:39:ARG:H	1:B:79:TYR:O	19	0.06
(1,2521)	1:B:21:ALA:H	1:B:17:ARG:O	4	0.06
(1,2507)	1:B:14:GLN:H	1:B:10:ALA:O	9	0.06
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	13	0.06
(1,2469)	1:A:76:ARG:H	1:A:73:GLU:O	4	0.06
(1,2461)	1:A:67:LEU:H	1:A:62:LEU:O	5	0.06
(1,2460)	1:A:66:GLY:N	1:A:63:LYS:O	15	0.06
(1,2407)	1:A:21:ALA:H	1:A:17:ARG:O	2	0.06
(1,2390)	1:B:107:HIS:HB2	1:B:108:HIS:H	6	0.06
(1,2374)	1:B:99:GLU:HG2	1:B:100:HIS:H	15	0.06
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD21	6	0.06
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD22	6	0.06
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD23	6	0.06
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD21	6	0.06
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD22	6	0.06
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD23	6	0.06
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD21	6	0.06
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD22	6	0.06
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD23	6	0.06
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB2	1	0.06
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB3	1	0.06
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB2	1	0.06
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB3	1	0.06
(1,231)	1:A:17:ARG:H	1:A:17:ARG:HG2	16	0.06
(1,2285)	1:B:90:PHE:HA	1:B:93:VAL:HG11	8	0.06
(1,2285)	1:B:90:PHE:HA	1:B:93:VAL:HG12	8	0.06
(1,2285)	1:B:90:PHE:HA	1:B:93:VAL:HG13	8	0.06
(1,2176)	1:B:80:ARG:HB2	1:B:80:ARG:HE	1	0.06
(1,2151)	1:B:76:ARG:HD2	1:B:77:GLN:H	19	0.06
(1,2151)	1:B:76:ARG:HD3	1:B:77:GLN:H	19	0.06
(1,2129)	1:B:73:GLU:HG2	1:B:78:TYR:HE1	12	0.06
(1,2129)	1:B:73:GLU:HG3	1:B:78:TYR:HE1	12	0.06
(1,2031)	1:B:67:LEU:HD11	1:B:86:VAL:HA	6	0.06
(1,2031)	1:B:67:LEU:HD12	1:B:86:VAL:HA	6	0.06
(1,2031)	1:B:67:LEU:HD13	1:B:86:VAL:HA	6	0.06
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB2	6	0.06
(1,2013)	1:B:65:GLY:HA2	1:B:67:LEU:HB3	6	0.06

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD2	14	0.06
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD3	14	0.06
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE2	19	0.06
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE3	19	0.06
(1,1942)	1:B:59:LEU:HD21	1:B:79:TYR:HE1	10	0.06
(1,1942)	1:B:59:LEU:HD22	1:B:79:TYR:HE1	10	0.06
(1,1942)	1:B:59:LEU:HD23	1:B:79:TYR:HE1	10	0.06
(1,1942)	1:B:59:LEU:HD21	1:B:79:TYR:HE1	15	0.06
(1,1942)	1:B:59:LEU:HD22	1:B:79:TYR:HE1	15	0.06
(1,1942)	1:B:59:LEU:HD23	1:B:79:TYR:HE1	15	0.06
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	4	0.06
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	4	0.06
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	4	0.06
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	4	0.06
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	4	0.06
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	4	0.06
(1,1881)	1:B:53:THR:HG21	1:B:54:THR:H	9	0.06
(1,1881)	1:B:53:THR:HG22	1:B:54:THR:H	9	0.06
(1,1881)	1:B:53:THR:HG23	1:B:54:THR:H	9	0.06
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	1	0.06
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	1	0.06
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	1	0.06
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	10	0.06
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	10	0.06
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	10	0.06
(1,1744)	1:B:42:GLU:HG2	1:B:43:ALA:H	3	0.06
(1,1670)	1:B:39:ARG:HG2	1:B:40:ALA:H	5	0.06
(1,1643)	1:B:36:GLN:HB2	1:B:37:GLY:H	16	0.06
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB1	6	0.06
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB2	6	0.06
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB3	6	0.06
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB1	6	0.06
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB2	6	0.06
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB3	6	0.06
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB1	6	0.06
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB2	6	0.06
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB3	6	0.06
(1,1594)	1:B:33:LEU:HD11	1:B:36:GLN:HB2	13	0.06
(1,1594)	1:B:33:LEU:HD12	1:B:36:GLN:HB2	13	0.06
(1,1594)	1:B:33:LEU:HD13	1:B:36:GLN:HB2	13	0.06
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	5	0.06
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	5	0.06

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	5	0.06
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	8	0.06
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	8	0.06
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	8	0.06
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	8	0.06
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	8	0.06
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	8	0.06
(1,1570)	1:B:31:LEU:HD21	1:B:86:VAL:HG11	2	0.06
(1,1570)	1:B:31:LEU:HD21	1:B:86:VAL:HG12	2	0.06
(1,1570)	1:B:31:LEU:HD21	1:B:86:VAL:HG13	2	0.06
(1,1570)	1:B:31:LEU:HD22	1:B:86:VAL:HG11	2	0.06
(1,1570)	1:B:31:LEU:HD22	1:B:86:VAL:HG12	2	0.06
(1,1570)	1:B:31:LEU:HD22	1:B:86:VAL:HG13	2	0.06
(1,1570)	1:B:31:LEU:HD23	1:B:86:VAL:HG11	2	0.06
(1,1570)	1:B:31:LEU:HD23	1:B:86:VAL:HG12	2	0.06
(1,1570)	1:B:31:LEU:HD23	1:B:86:VAL:HG13	2	0.06
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	1	0.06
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	1	0.06
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	1	0.06
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	1	0.06
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	1	0.06
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	1	0.06
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB1	14	0.06
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB2	14	0.06
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB3	14	0.06
(1,1377)	1:B:18:VAL:HG11	1:B:65:GLY:HA2	7	0.06
(1,1377)	1:B:18:VAL:HG12	1:B:65:GLY:HA2	7	0.06
(1,1377)	1:B:18:VAL:HG13	1:B:65:GLY:HA2	7	0.06
(1,1333)	1:B:14:GLN:HA	1:B:17:ARG:HD2	2	0.06
(1,1333)	1:B:14:GLN:HA	1:B:17:ARG:HD3	2	0.06
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB1	14	0.06
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB2	14	0.06
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB3	14	0.06
(1,1283)	1:B:8:LYS:HE2	1:B:12:LEU:HD11	8	0.06
(1,1283)	1:B:8:LYS:HE2	1:B:12:LEU:HD12	8	0.06
(1,1283)	1:B:8:LYS:HE2	1:B:12:LEU:HD13	8	0.06
(1,1283)	1:B:8:LYS:HE3	1:B:12:LEU:HD11	8	0.06
(1,1283)	1:B:8:LYS:HE3	1:B:12:LEU:HD12	8	0.06
(1,1283)	1:B:8:LYS:HE3	1:B:12:LEU:HD13	8	0.06
(1,1273)	1:B:7:ARG:HB2	1:B:8:LYS:H	16	0.06
(1,1258)	1:A:107:HIS:HB2	1:A:108:HIS:H	7	0.06
(1,1153)	1:A:90:PHE:HA	1:A:93:VAL:HG11	2	0.06

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1153)	1:A:90:PHE:HA	1:A:93:VAL:HG12	2	0.06
(1,1153)	1:A:90:PHE:HA	1:A:93:VAL:HG13	2	0.06
(1,1153)	1:A:90:PHE:HA	1:A:93:VAL:HG11	10	0.06
(1,1153)	1:A:90:PHE:HA	1:A:93:VAL:HG12	10	0.06
(1,1153)	1:A:90:PHE:HA	1:A:93:VAL:HG13	10	0.06
(1,1059)	1:A:81:ILE:HG12	1:A:87:ALA:HA	9	0.06
(1,1033)	1:A:77:GLN:HG2	1:A:77:GLN:HE21	18	0.06
(1,1019)	1:A:76:ARG:HD2	1:A:77:GLN:H	1	0.06
(1,1019)	1:A:76:ARG:HD3	1:A:77:GLN:H	1	0.06
(1,1019)	1:A:76:ARG:HD2	1:A:77:GLN:H	19	0.06
(1,1019)	1:A:76:ARG:HD3	1:A:77:GLN:H	19	0.06
(1,98)	1:B:15:VAL:HG11	1:A:28:LEU:HD11	6	0.05
(1,98)	1:B:15:VAL:HG11	1:A:28:LEU:HD12	6	0.05
(1,98)	1:B:15:VAL:HG11	1:A:28:LEU:HD13	6	0.05
(1,98)	1:B:15:VAL:HG12	1:A:28:LEU:HD11	6	0.05
(1,98)	1:B:15:VAL:HG12	1:A:28:LEU:HD12	6	0.05
(1,98)	1:B:15:VAL:HG12	1:A:28:LEU:HD13	6	0.05
(1,98)	1:B:15:VAL:HG13	1:A:28:LEU:HD11	6	0.05
(1,98)	1:B:15:VAL:HG13	1:A:28:LEU:HD12	6	0.05
(1,98)	1:B:15:VAL:HG13	1:A:28:LEU:HD13	6	0.05
(1,976)	1:A:72:ARG:HA	1:A:72:ARG:HD2	6	0.05
(1,976)	1:A:72:ARG:HA	1:A:72:ARG:HD3	6	0.05
(1,969)	1:A:71:ARG:HB2	1:A:79:TYR:HA	8	0.05
(1,94)	1:B:14:GLN:HG3	1:A:97:ALA:HB1	7	0.05
(1,94)	1:B:14:GLN:HG3	1:A:97:ALA:HB2	7	0.05
(1,94)	1:B:14:GLN:HG3	1:A:97:ALA:HB3	7	0.05
(1,899)	1:A:67:LEU:HD11	1:A:86:VAL:HA	5	0.05
(1,899)	1:A:67:LEU:HD12	1:A:86:VAL:HA	5	0.05
(1,899)	1:A:67:LEU:HD13	1:A:86:VAL:HA	5	0.05
(1,899)	1:A:67:LEU:HD11	1:A:86:VAL:HA	10	0.05
(1,899)	1:A:67:LEU:HD12	1:A:86:VAL:HA	10	0.05
(1,899)	1:A:67:LEU:HD13	1:A:86:VAL:HA	10	0.05
(1,899)	1:A:67:LEU:HD11	1:A:86:VAL:HA	19	0.05
(1,899)	1:A:67:LEU:HD12	1:A:86:VAL:HA	19	0.05
(1,899)	1:A:67:LEU:HD13	1:A:86:VAL:HA	19	0.05
(1,899)	1:A:67:LEU:HD11	1:A:86:VAL:HA	20	0.05
(1,899)	1:A:67:LEU:HD12	1:A:86:VAL:HA	20	0.05
(1,899)	1:A:67:LEU:HD13	1:A:86:VAL:HA	20	0.05
(1,891)	1:A:67:LEU:HA	1:A:86:VAL:HG11	10	0.05
(1,891)	1:A:67:LEU:HA	1:A:86:VAL:HG12	10	0.05
(1,891)	1:A:67:LEU:HA	1:A:86:VAL:HG13	10	0.05
(1,888)	1:A:67:LEU:HA	1:A:67:LEU:HD11	11	0.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,888)	1:A:67:LEU:HA	1:A:67:LEU:HD12	11	0.05
(1,888)	1:A:67:LEU:HA	1:A:67:LEU:HD13	11	0.05
(1,865)	1:A:63:LYS:HE2	1:A:70:ALA:H	11	0.05
(1,865)	1:A:63:LYS:HE3	1:A:70:ALA:H	11	0.05
(1,863)	1:A:63:LYS:HE2	1:A:69:GLU:HA	11	0.05
(1,863)	1:A:63:LYS:HE3	1:A:69:GLU:HA	11	0.05
(1,855)	1:A:63:LYS:HB2	1:A:64:SER:H	17	0.05
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE2	2	0.05
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE3	2	0.05
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	4	0.05
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	4	0.05
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	4	0.05
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	4	0.05
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	4	0.05
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	4	0.05
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	7	0.05
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	7	0.05
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	7	0.05
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	7	0.05
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	7	0.05
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	7	0.05
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	12	0.05
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	12	0.05
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	12	0.05
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	12	0.05
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	12	0.05
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	12	0.05
(1,749)	1:A:53:THR:HG21	1:A:54:THR:H	12	0.05
(1,749)	1:A:53:THR:HG22	1:A:54:THR:H	12	0.05
(1,749)	1:A:53:THR:HG23	1:A:54:THR:H	12	0.05
(1,749)	1:A:53:THR:HG21	1:A:54:THR:H	20	0.05
(1,749)	1:A:53:THR:HG22	1:A:54:THR:H	20	0.05
(1,749)	1:A:53:THR:HG23	1:A:54:THR:H	20	0.05
(1,722)	1:A:51:ASN:HB2	1:A:53:THR:H	1	0.05
(1,713)	1:A:50:MET:HG2	1:A:54:THR:HG21	19	0.05
(1,713)	1:A:50:MET:HG2	1:A:54:THR:HG22	19	0.05
(1,713)	1:A:50:MET:HG2	1:A:54:THR:HG23	19	0.05
(1,691)	1:A:48:THR:HB	1:A:50:MET:HG2	6	0.05
(1,691)	1:A:48:THR:HB	1:A:50:MET:HG2	7	0.05
(1,691)	1:A:48:THR:HB	1:A:50:MET:HG2	17	0.05
(1,619)	1:A:42:GLU:HG2	1:A:52:LEU:HD21	4	0.05
(1,619)	1:A:42:GLU:HG2	1:A:52:LEU:HD22	4	0.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,619)	1:A:42:GLU:HG2	1:A:52:LEU:HD23	4	0.05
(1,602)	1:A:42:GLU:HA	1:A:42:GLU:HG2	6	0.05
(1,602)	1:A:42:GLU:HA	1:A:42:GLU:HG2	9	0.05
(1,602)	1:A:42:GLU:HA	1:A:42:GLU:HG2	17	0.05
(1,574)	1:A:41:VAL:HB	1:A:79:TYR:HE1	2	0.05
(1,543)	1:A:40:ALA:HA	1:A:78:TYR:HA	10	0.05
(1,525)	1:A:38:GLU:HG2	1:A:78:TYR:HB2	19	0.05
(1,525)	1:A:38:GLU:HG3	1:A:78:TYR:HB2	19	0.05
(1,476)	1:A:33:LEU:HG	1:A:39:ARG:HE	8	0.05
(1,460)	1:A:33:LEU:HB2	1:A:34:LEU:H	8	0.05
(1,460)	1:A:33:LEU:HB2	1:A:34:LEU:H	11	0.05
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	8	0.05
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	8	0.05
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	8	0.05
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	8	0.05
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	8	0.05
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	8	0.05
(1,421)	1:A:31:LEU:HD11	1:A:67:LEU:HG	4	0.05
(1,421)	1:A:31:LEU:HD12	1:A:67:LEU:HG	4	0.05
(1,421)	1:A:31:LEU:HD13	1:A:67:LEU:HG	4	0.05
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	6	0.05
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	20	0.05
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	20	0.05
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	20	0.05
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD21	12	0.05
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD22	12	0.05
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD23	12	0.05
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD21	12	0.05
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD22	12	0.05
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD23	12	0.05
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD21	12	0.05
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD22	12	0.05
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD23	12	0.05
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	6	0.05
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	6	0.05
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	6	0.05
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	9	0.05
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	9	0.05
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	9	0.05
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	14	0.05
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	14	0.05
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	14	0.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	18	0.05
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	18	0.05
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	18	0.05
(1,277)	1:A:21:ALA:HB1	1:A:65:GLY:HA2	14	0.05
(1,277)	1:A:21:ALA:HB2	1:A:65:GLY:HA2	14	0.05
(1,277)	1:A:21:ALA:HB3	1:A:65:GLY:HA2	14	0.05
(1,2613)	1:B:97:ALA:H	1:B:93:VAL:O	8	0.05
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	13	0.05
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	18	0.05
(1,2521)	1:B:21:ALA:H	1:B:17:ARG:O	13	0.05
(1,2513)	1:B:17:ARG:H	1:B:13:ASP:O	7	0.05
(1,2507)	1:B:14:GLN:H	1:B:10:ALA:O	1	0.05
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	2	0.05
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	5	0.05
(1,2461)	1:A:67:LEU:H	1:A:62:LEU:O	11	0.05
(1,2460)	1:A:66:GLY:N	1:A:63:LYS:O	14	0.05
(1,2409)	1:A:22:LEU:H	1:A:18:VAL:O	6	0.05
(1,2407)	1:A:21:ALA:H	1:A:17:ARG:O	5	0.05
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	13	0.05
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	17	0.05
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	19	0.05
(1,2390)	1:B:107:HIS:HB2	1:B:108:HIS:H	17	0.05
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD21	5	0.05
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD22	5	0.05
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD23	5	0.05
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD21	5	0.05
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD22	5	0.05
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD23	5	0.05
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD21	5	0.05
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD22	5	0.05
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD23	5	0.05
(1,2362)	1:B:97:ALA:HA	1:B:101:LEU:HD21	2	0.05
(1,2362)	1:B:97:ALA:HA	1:B:101:LEU:HD22	2	0.05
(1,2362)	1:B:97:ALA:HA	1:B:101:LEU:HD23	2	0.05
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB2	3	0.05
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB3	3	0.05
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB2	3	0.05
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB3	3	0.05
(1,2343)	1:B:95:VAL:HG11	1:B:99:GLU:HG2	6	0.05
(1,2343)	1:B:95:VAL:HG12	1:B:99:GLU:HG2	6	0.05
(1,2343)	1:B:95:VAL:HG13	1:B:99:GLU:HG2	6	0.05
(1,2296)	1:B:91:ALA:HA	1:B:94:GLN:HE21	15	0.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2276)	1:B:89:LEU:HD21	1:B:93:VAL:HB	7	0.05
(1,2276)	1:B:89:LEU:HD22	1:B:93:VAL:HB	7	0.05
(1,2276)	1:B:89:LEU:HD23	1:B:93:VAL:HB	7	0.05
(1,2227)	1:B:84:GLU:HG2	1:B:88:ARG:HG2	6	0.05
(1,2227)	1:B:84:GLU:HG3	1:B:88:ARG:HG2	6	0.05
(1,2165)	1:B:77:GLN:HG2	1:B:77:GLN:HE21	9	0.05
(1,2151)	1:B:76:ARG:HD2	1:B:77:GLN:H	1	0.05
(1,2151)	1:B:76:ARG:HD3	1:B:77:GLN:H	1	0.05
(1,2151)	1:B:76:ARG:HD2	1:B:77:GLN:H	5	0.05
(1,2151)	1:B:76:ARG:HD3	1:B:77:GLN:H	5	0.05
(1,2151)	1:B:76:ARG:HD2	1:B:77:GLN:H	8	0.05
(1,2151)	1:B:76:ARG:HD3	1:B:77:GLN:H	8	0.05
(1,2125)	1:B:73:GLU:HB2	1:B:76:ARG:HG2	4	0.05
(1,2091)	1:B:70:ALA:HB1	1:B:77:GLN:HE22	4	0.05
(1,2091)	1:B:70:ALA:HB2	1:B:77:GLN:HE22	4	0.05
(1,2091)	1:B:70:ALA:HB3	1:B:77:GLN:HE22	4	0.05
(1,2077)	1:B:69:GLU:HG2	1:B:82:ALA:HA	20	0.05
(1,2075)	1:B:69:GLU:HG3	1:B:82:ALA:HA	3	0.05
(1,2031)	1:B:67:LEU:HD11	1:B:86:VAL:HA	2	0.05
(1,2031)	1:B:67:LEU:HD12	1:B:86:VAL:HA	2	0.05
(1,2031)	1:B:67:LEU:HD13	1:B:86:VAL:HA	2	0.05
(1,2031)	1:B:67:LEU:HD11	1:B:86:VAL:HA	7	0.05
(1,2031)	1:B:67:LEU:HD12	1:B:86:VAL:HA	7	0.05
(1,2031)	1:B:67:LEU:HD13	1:B:86:VAL:HA	7	0.05
(1,1948)	1:B:60:GLN:HA	1:B:60:GLN:HE21	15	0.05
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	18	0.05
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	18	0.05
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	18	0.05
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	18	0.05
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	18	0.05
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	18	0.05
(1,1782)	1:B:44:ILE:HG21	1:B:47:ALA:HB1	5	0.05
(1,1782)	1:B:44:ILE:HG21	1:B:47:ALA:HB2	5	0.05
(1,1782)	1:B:44:ILE:HG21	1:B:47:ALA:HB3	5	0.05
(1,1782)	1:B:44:ILE:HG22	1:B:47:ALA:HB1	5	0.05
(1,1782)	1:B:44:ILE:HG22	1:B:47:ALA:HB2	5	0.05
(1,1782)	1:B:44:ILE:HG22	1:B:47:ALA:HB3	5	0.05
(1,1782)	1:B:44:ILE:HG23	1:B:47:ALA:HB1	5	0.05
(1,1782)	1:B:44:ILE:HG23	1:B:47:ALA:HB2	5	0.05
(1,1782)	1:B:44:ILE:HG23	1:B:47:ALA:HB3	5	0.05
(1,1726)	1:B:41:VAL:HG21	1:B:77:GLN:HG2	5	0.05
(1,1726)	1:B:41:VAL:HG22	1:B:77:GLN:HG2	5	0.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1726)	1:B:41:VAL:HG23	1:B:77:GLN:HG2	5	0.05
(1,1690)	1:B:40:ALA:HB1	1:B:78:TYR:HD1	11	0.05
(1,1690)	1:B:40:ALA:HB2	1:B:78:TYR:HD1	11	0.05
(1,1690)	1:B:40:ALA:HB3	1:B:78:TYR:HD1	11	0.05
(1,1654)	1:B:38:GLU:HB2	1:B:80:ARG:HE	15	0.05
(1,1654)	1:B:38:GLU:HB3	1:B:80:ARG:HE	15	0.05
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	19	0.05
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	19	0.05
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	19	0.05
(1,1567)	1:B:31:LEU:HD21	1:B:81:ILE:HD11	13	0.05
(1,1567)	1:B:31:LEU:HD21	1:B:81:ILE:HD12	13	0.05
(1,1567)	1:B:31:LEU:HD21	1:B:81:ILE:HD13	13	0.05
(1,1567)	1:B:31:LEU:HD22	1:B:81:ILE:HD11	13	0.05
(1,1567)	1:B:31:LEU:HD22	1:B:81:ILE:HD12	13	0.05
(1,1567)	1:B:31:LEU:HD22	1:B:81:ILE:HD13	13	0.05
(1,1567)	1:B:31:LEU:HD23	1:B:81:ILE:HD11	13	0.05
(1,1567)	1:B:31:LEU:HD23	1:B:81:ILE:HD12	13	0.05
(1,1567)	1:B:31:LEU:HD23	1:B:81:ILE:HD13	13	0.05
(1,1567)	1:B:31:LEU:HD21	1:B:81:ILE:HD11	19	0.05
(1,1567)	1:B:31:LEU:HD21	1:B:81:ILE:HD12	19	0.05
(1,1567)	1:B:31:LEU:HD21	1:B:81:ILE:HD13	19	0.05
(1,1567)	1:B:31:LEU:HD22	1:B:81:ILE:HD11	19	0.05
(1,1567)	1:B:31:LEU:HD22	1:B:81:ILE:HD12	19	0.05
(1,1567)	1:B:31:LEU:HD22	1:B:81:ILE:HD13	19	0.05
(1,1567)	1:B:31:LEU:HD23	1:B:81:ILE:HD11	19	0.05
(1,1567)	1:B:31:LEU:HD23	1:B:81:ILE:HD12	19	0.05
(1,1567)	1:B:31:LEU:HD23	1:B:81:ILE:HD13	19	0.05
(1,1561)	1:B:31:LEU:HD21	1:B:67:LEU:HA	6	0.05
(1,1561)	1:B:31:LEU:HD22	1:B:67:LEU:HA	6	0.05
(1,1561)	1:B:31:LEU:HD23	1:B:67:LEU:HA	6	0.05
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	18	0.05
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	18	0.05
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	18	0.05
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	18	0.05
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	18	0.05
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	18	0.05
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD11	11	0.05
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD12	11	0.05
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD13	11	0.05
(1,1427)	1:B:22:LEU:HD11	1:B:93:VAL:HB	11	0.05
(1,1427)	1:B:22:LEU:HD12	1:B:93:VAL:HB	11	0.05
(1,1427)	1:B:22:LEU:HD13	1:B:93:VAL:HB	11	0.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1425)	1:B:22:LEU:HD11	1:B:89:LEU:HD21	6	0.05
(1,1425)	1:B:22:LEU:HD11	1:B:89:LEU:HD22	6	0.05
(1,1425)	1:B:22:LEU:HD11	1:B:89:LEU:HD23	6	0.05
(1,1425)	1:B:22:LEU:HD12	1:B:89:LEU:HD21	6	0.05
(1,1425)	1:B:22:LEU:HD12	1:B:89:LEU:HD22	6	0.05
(1,1425)	1:B:22:LEU:HD12	1:B:89:LEU:HD23	6	0.05
(1,1425)	1:B:22:LEU:HD13	1:B:89:LEU:HD21	6	0.05
(1,1425)	1:B:22:LEU:HD13	1:B:89:LEU:HD22	6	0.05
(1,1425)	1:B:22:LEU:HD13	1:B:89:LEU:HD23	6	0.05
(1,1418)	1:B:22:LEU:HA	1:B:28:LEU:HD21	9	0.05
(1,1418)	1:B:22:LEU:HA	1:B:28:LEU:HD22	9	0.05
(1,1418)	1:B:22:LEU:HA	1:B:28:LEU:HD23	9	0.05
(1,1411)	1:B:21:ALA:HB1	1:B:65:GLY:H	12	0.05
(1,1411)	1:B:21:ALA:HB2	1:B:65:GLY:H	12	0.05
(1,1411)	1:B:21:ALA:HB3	1:B:65:GLY:H	12	0.05
(1,1410)	1:B:21:ALA:HB1	1:B:65:GLY:HA3	10	0.05
(1,1410)	1:B:21:ALA:HB2	1:B:65:GLY:HA3	10	0.05
(1,1410)	1:B:21:ALA:HB3	1:B:65:GLY:HA3	10	0.05
(1,1402)	1:B:20:LYS:H	1:B:20:LYS:HD2	12	0.05
(1,1402)	1:B:20:LYS:H	1:B:20:LYS:HD3	12	0.05
(1,1377)	1:B:18:VAL:HG11	1:B:65:GLY:HA2	10	0.05
(1,1377)	1:B:18:VAL:HG12	1:B:65:GLY:HA2	10	0.05
(1,1377)	1:B:18:VAL:HG13	1:B:65:GLY:HA2	10	0.05
(1,137)	1:A:7:ARG:HA	1:A:7:ARG:HG2	17	0.05
(1,1361)	1:B:17:ARG:HA	1:B:65:GLY:HA2	2	0.05
(1,1333)	1:B:14:GLN:HA	1:B:17:ARG:HD2	8	0.05
(1,1333)	1:B:14:GLN:HA	1:B:17:ARG:HD3	8	0.05
(1,1283)	1:B:8:LYS:HE2	1:B:12:LEU:HD11	17	0.05
(1,1283)	1:B:8:LYS:HE2	1:B:12:LEU:HD12	17	0.05
(1,1283)	1:B:8:LYS:HE2	1:B:12:LEU:HD13	17	0.05
(1,1283)	1:B:8:LYS:HE3	1:B:12:LEU:HD11	17	0.05
(1,1283)	1:B:8:LYS:HE3	1:B:12:LEU:HD12	17	0.05
(1,1283)	1:B:8:LYS:HE3	1:B:12:LEU:HD13	17	0.05
(1,1262)	1:B:5:SER:HB2	1:B:6:ASP:H	10	0.05
(1,1251)	1:A:101:LEU:HB2	1:A:102:GLU:H	14	0.05
(1,1234)	1:A:97:ALA:HB1	1:A:101:LEU:HD21	4	0.05
(1,1234)	1:A:97:ALA:HB1	1:A:101:LEU:HD22	4	0.05
(1,1234)	1:A:97:ALA:HB1	1:A:101:LEU:HD23	4	0.05
(1,1234)	1:A:97:ALA:HB2	1:A:101:LEU:HD21	4	0.05
(1,1234)	1:A:97:ALA:HB2	1:A:101:LEU:HD22	4	0.05
(1,1234)	1:A:97:ALA:HB2	1:A:101:LEU:HD23	4	0.05
(1,1234)	1:A:97:ALA:HB3	1:A:101:LEU:HD21	4	0.05

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1234)	1:A:97:ALA:HB3	1:A:101:LEU:HD22	4	0.05
(1,1234)	1:A:97:ALA:HB3	1:A:101:LEU:HD23	4	0.05
(1,1234)	1:A:97:ALA:HB1	1:A:101:LEU:HD21	18	0.05
(1,1234)	1:A:97:ALA:HB1	1:A:101:LEU:HD22	18	0.05
(1,1234)	1:A:97:ALA:HB1	1:A:101:LEU:HD23	18	0.05
(1,1234)	1:A:97:ALA:HB2	1:A:101:LEU:HD21	18	0.05
(1,1234)	1:A:97:ALA:HB2	1:A:101:LEU:HD22	18	0.05
(1,1234)	1:A:97:ALA:HB2	1:A:101:LEU:HD23	18	0.05
(1,1234)	1:A:97:ALA:HB3	1:A:101:LEU:HD21	18	0.05
(1,1234)	1:A:97:ALA:HB3	1:A:101:LEU:HD22	18	0.05
(1,1234)	1:A:97:ALA:HB3	1:A:101:LEU:HD23	18	0.05
(1,1183)	1:A:93:VAL:HG11	1:A:94:GLN:H	15	0.05
(1,1183)	1:A:93:VAL:HG12	1:A:94:GLN:H	15	0.05
(1,1183)	1:A:93:VAL:HG13	1:A:94:GLN:H	15	0.05
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB1	11	0.05
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB2	11	0.05
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB3	11	0.05
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG11	14	0.05
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG12	14	0.05
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG13	14	0.05
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG11	14	0.05
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG12	14	0.05
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG13	14	0.05
(1,1093)	1:A:84:GLU:HG2	1:A:88:ARG:HD2	6	0.05
(1,1093)	1:A:84:GLU:HG2	1:A:88:ARG:HD3	6	0.05
(1,1093)	1:A:84:GLU:HG3	1:A:88:ARG:HD2	6	0.05
(1,1093)	1:A:84:GLU:HG3	1:A:88:ARG:HD3	6	0.05
(1,1052)	1:A:81:ILE:HD11	1:A:82:ALA:H	3	0.05
(1,1052)	1:A:81:ILE:HD12	1:A:82:ALA:H	3	0.05
(1,1052)	1:A:81:ILE:HD13	1:A:82:ALA:H	3	0.05
(1,1019)	1:A:76:ARG:HD2	1:A:77:GLN:H	3	0.05
(1,1019)	1:A:76:ARG:HD3	1:A:77:GLN:H	3	0.05
(1,999)	1:A:73:GLU:H	1:A:76:ARG:HG2	19	0.04
(1,969)	1:A:71:ARG:HB2	1:A:79:TYR:HA	1	0.04
(1,899)	1:A:67:LEU:HD11	1:A:86:VAL:HA	3	0.04
(1,899)	1:A:67:LEU:HD12	1:A:86:VAL:HA	3	0.04
(1,899)	1:A:67:LEU:HD13	1:A:86:VAL:HA	3	0.04
(1,899)	1:A:67:LEU:HD11	1:A:86:VAL:HA	17	0.04
(1,899)	1:A:67:LEU:HD12	1:A:86:VAL:HA	17	0.04
(1,899)	1:A:67:LEU:HD13	1:A:86:VAL:HA	17	0.04
(1,824)	1:A:60:GLN:HG2	1:A:61:ALA:HA	2	0.04
(1,824)	1:A:60:GLN:HG3	1:A:61:ALA:HA	2	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	5	0.04
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	5	0.04
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	5	0.04
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	5	0.04
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	5	0.04
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	5	0.04
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	10	0.04
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	10	0.04
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	10	0.04
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	10	0.04
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	10	0.04
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	10	0.04
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	19	0.04
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	19	0.04
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	19	0.04
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	19	0.04
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	19	0.04
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	19	0.04
(1,810)	1:A:59:LEU:HD21	1:A:79:TYR:HE1	7	0.04
(1,810)	1:A:59:LEU:HD22	1:A:79:TYR:HE1	7	0.04
(1,810)	1:A:59:LEU:HD23	1:A:79:TYR:HE1	7	0.04
(1,809)	1:A:59:LEU:HD21	1:A:79:TYR:HD1	13	0.04
(1,809)	1:A:59:LEU:HD22	1:A:79:TYR:HD1	13	0.04
(1,809)	1:A:59:LEU:HD23	1:A:79:TYR:HD1	13	0.04
(1,749)	1:A:53:THR:HG21	1:A:54:THR:H	6	0.04
(1,749)	1:A:53:THR:HG22	1:A:54:THR:H	6	0.04
(1,749)	1:A:53:THR:HG23	1:A:54:THR:H	6	0.04
(1,747)	1:A:53:THR:HB	1:A:54:THR:H	17	0.04
(1,715)	1:A:50:MET:H	1:A:50:MET:HB2	19	0.04
(1,7)	1:A:12:LEU:HD11	1:B:29:GLN:HB2	7	0.04
(1,7)	1:A:12:LEU:HD12	1:B:29:GLN:HB2	7	0.04
(1,7)	1:A:12:LEU:HD13	1:B:29:GLN:HB2	7	0.04
(1,617)	1:A:42:GLU:HG3	1:A:52:LEU:HD21	20	0.04
(1,617)	1:A:42:GLU:HG3	1:A:52:LEU:HD22	20	0.04
(1,617)	1:A:42:GLU:HG3	1:A:52:LEU:HD23	20	0.04
(1,615)	1:A:42:GLU:HG2	1:A:52:LEU:HG	12	0.04
(1,612)	1:A:42:GLU:HG2	1:A:43:ALA:H	4	0.04
(1,612)	1:A:42:GLU:HG2	1:A:43:ALA:H	11	0.04
(1,594)	1:A:41:VAL:HG21	1:A:77:GLN:HG2	8	0.04
(1,594)	1:A:41:VAL:HG22	1:A:77:GLN:HG2	8	0.04
(1,594)	1:A:41:VAL:HG23	1:A:77:GLN:HG2	8	0.04
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD11	13	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD12	13	0.04
(1,57)	1:A:88:ARG:HB2	1:B:92:LEU:HD13	13	0.04
(1,538)	1:A:39:ARG:HG2	1:A:40:ALA:H	5	0.04
(1,522)	1:A:38:GLU:HB2	1:A:80:ARG:HE	16	0.04
(1,522)	1:A:38:GLU:HB3	1:A:80:ARG:HE	16	0.04
(1,516)	1:A:37:GLY:HA2	1:A:38:GLU:HB2	9	0.04
(1,516)	1:A:37:GLY:HA2	1:A:38:GLU:HB3	9	0.04
(1,51)	1:A:20:LYS:HB2	1:B:23:ALA:HB1	4	0.04
(1,51)	1:A:20:LYS:HB2	1:B:23:ALA:HB2	4	0.04
(1,51)	1:A:20:LYS:HB2	1:B:23:ALA:HB3	4	0.04
(1,51)	1:A:20:LYS:HB3	1:B:23:ALA:HB1	4	0.04
(1,51)	1:A:20:LYS:HB3	1:B:23:ALA:HB2	4	0.04
(1,51)	1:A:20:LYS:HB3	1:B:23:ALA:HB3	4	0.04
(1,473)	1:A:33:LEU:HD11	1:A:47:ALA:H	6	0.04
(1,473)	1:A:33:LEU:HD12	1:A:47:ALA:H	6	0.04
(1,473)	1:A:33:LEU:HD13	1:A:47:ALA:H	6	0.04
(1,471)	1:A:33:LEU:HD11	1:A:44:ILE:H	15	0.04
(1,471)	1:A:33:LEU:HD12	1:A:44:ILE:H	15	0.04
(1,471)	1:A:33:LEU:HD13	1:A:44:ILE:H	15	0.04
(1,460)	1:A:33:LEU:HB2	1:A:34:LEU:H	4	0.04
(1,460)	1:A:33:LEU:HB2	1:A:34:LEU:H	18	0.04
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	18	0.04
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	18	0.04
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	18	0.04
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	18	0.04
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	18	0.04
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	18	0.04
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG21	7	0.04
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG22	7	0.04
(1,361)	1:A:29:GLN:HG2	1:A:48:THR:HG23	7	0.04
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD1	11	0.04
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD2	11	0.04
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD1	11	0.04
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD2	11	0.04
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD1	11	0.04
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD2	11	0.04
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	12	0.04
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	12	0.04
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	12	0.04
(1,308)	1:A:23:ALA:H	1:A:24:ASN:H	17	0.04
(1,295)	1:A:22:LEU:HD11	1:A:93:VAL:HB	11	0.04
(1,295)	1:A:22:LEU:HD12	1:A:93:VAL:HB	11	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,295)	1:A:22:LEU:HD13	1:A:93:VAL:HB	11	0.04
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD21	20	0.04
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD22	20	0.04
(1,293)	1:A:22:LEU:HD11	1:A:89:LEU:HD23	20	0.04
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD21	20	0.04
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD22	20	0.04
(1,293)	1:A:22:LEU:HD12	1:A:89:LEU:HD23	20	0.04
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD21	20	0.04
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD22	20	0.04
(1,293)	1:A:22:LEU:HD13	1:A:89:LEU:HD23	20	0.04
(1,2613)	1:B:97:ALA:H	1:B:93:VAL:O	5	0.04
(1,2593)	1:B:87:ALA:H	1:B:83:GLY:O	17	0.04
(1,2573)	1:B:66:GLY:H	1:B:63:LYS:O	20	0.04
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	1	0.04
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	10	0.04
(1,2535)	1:B:41:VAL:H	1:B:77:GLN:O	2	0.04
(1,2533)	1:B:39:ARG:H	1:B:79:TYR:O	7	0.04
(1,2533)	1:B:39:ARG:H	1:B:79:TYR:O	10	0.04
(1,2521)	1:B:21:ALA:H	1:B:17:ARG:O	1	0.04
(1,2507)	1:B:14:GLN:H	1:B:10:ALA:O	11	0.04
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	3	0.04
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	4	0.04
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	6	0.04
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	11	0.04
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	15	0.04
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	18	0.04
(1,2493)	1:A:94:GLN:H	1:A:90:PHE:O	8	0.04
(1,2469)	1:A:76:ARG:H	1:A:73:GLU:O	8	0.04
(1,2449)	1:A:61:ALA:H	1:A:57:ALA:O	16	0.04
(1,2443)	1:A:58:ASN:H	1:A:54:THR:O	4	0.04
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	2	0.04
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	3	0.04
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	7	0.04
(1,2421)	1:A:41:VAL:H	1:A:77:GLN:O	5	0.04
(1,2419)	1:A:39:ARG:H	1:A:79:TYR:O	7	0.04
(1,2407)	1:A:21:ALA:H	1:A:17:ARG:O	12	0.04
(1,2399)	1:A:17:ARG:H	1:A:13:ASP:O	18	0.04
(1,2393)	1:A:14:GLN:H	1:A:10:ALA:O	17	0.04
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	2	0.04
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	6	0.04
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	7	0.04
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	10	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD21	12	0.04
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD22	12	0.04
(1,2366)	1:B:97:ALA:HB1	1:B:101:LEU:HD23	12	0.04
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD21	12	0.04
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD22	12	0.04
(1,2366)	1:B:97:ALA:HB2	1:B:101:LEU:HD23	12	0.04
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD21	12	0.04
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD22	12	0.04
(1,2366)	1:B:97:ALA:HB3	1:B:101:LEU:HD23	12	0.04
(1,2357)	1:B:96:VAL:HG21	1:B:100:HIS:HD2	13	0.04
(1,2357)	1:B:96:VAL:HG22	1:B:100:HIS:HD2	13	0.04
(1,2357)	1:B:96:VAL:HG23	1:B:100:HIS:HD2	13	0.04
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB2	2	0.04
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB3	2	0.04
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB2	2	0.04
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB3	2	0.04
(1,231)	1:A:17:ARG:H	1:A:17:ARG:HG2	5	0.04
(1,231)	1:A:17:ARG:H	1:A:17:ARG:HG2	8	0.04
(1,231)	1:A:17:ARG:H	1:A:17:ARG:HG2	10	0.04
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA2	10	0.04
(1,2285)	1:B:90:PHE:HA	1:B:93:VAL:HG11	3	0.04
(1,2285)	1:B:90:PHE:HA	1:B:93:VAL:HG12	3	0.04
(1,2285)	1:B:90:PHE:HA	1:B:93:VAL:HG13	3	0.04
(1,2276)	1:B:89:LEU:HD21	1:B:93:VAL:HB	1	0.04
(1,2276)	1:B:89:LEU:HD22	1:B:93:VAL:HB	1	0.04
(1,2276)	1:B:89:LEU:HD23	1:B:93:VAL:HB	1	0.04
(1,2269)	1:B:89:LEU:HA	1:B:92:LEU:HD21	3	0.04
(1,2269)	1:B:89:LEU:HA	1:B:92:LEU:HD22	3	0.04
(1,2269)	1:B:89:LEU:HA	1:B:92:LEU:HD23	3	0.04
(1,2196)	1:B:81:ILE:HG21	1:B:83:GLY:H	6	0.04
(1,2196)	1:B:81:ILE:HG22	1:B:83:GLY:H	6	0.04
(1,2196)	1:B:81:ILE:HG23	1:B:83:GLY:H	6	0.04
(1,2165)	1:B:77:GLN:HG2	1:B:77:GLN:HE21	4	0.04
(1,2165)	1:B:77:GLN:HG2	1:B:77:GLN:HE21	5	0.04
(1,2126)	1:B:73:GLU:HB2	1:B:78:TYR:HD1	12	0.04
(1,2095)	1:B:70:ALA:HB1	1:B:79:TYR:HE1	20	0.04
(1,2095)	1:B:70:ALA:HB2	1:B:79:TYR:HE1	20	0.04
(1,2095)	1:B:70:ALA:HB3	1:B:79:TYR:HE1	20	0.04
(1,2031)	1:B:67:LEU:HD11	1:B:86:VAL:HA	19	0.04
(1,2031)	1:B:67:LEU:HD12	1:B:86:VAL:HA	19	0.04
(1,2031)	1:B:67:LEU:HD13	1:B:86:VAL:HA	19	0.04
(1,2023)	1:B:67:LEU:HA	1:B:86:VAL:HG11	17	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2023)	1:B:67:LEU:HA	1:B:86:VAL:HG12	17	0.04
(1,2023)	1:B:67:LEU:HA	1:B:86:VAL:HG13	17	0.04
(1,1967)	1:B:62:LEU:HA	1:B:67:LEU:HD21	3	0.04
(1,1967)	1:B:62:LEU:HA	1:B:67:LEU:HD22	3	0.04
(1,1967)	1:B:62:LEU:HA	1:B:67:LEU:HD23	3	0.04
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	14	0.04
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	14	0.04
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	14	0.04
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	14	0.04
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	14	0.04
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	14	0.04
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	15	0.04
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	15	0.04
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	15	0.04
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	15	0.04
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	15	0.04
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	15	0.04
(1,1887)	1:B:54:THR:HG21	1:B:57:ALA:H	10	0.04
(1,1887)	1:B:54:THR:HG22	1:B:57:ALA:H	10	0.04
(1,1887)	1:B:54:THR:HG23	1:B:57:ALA:H	10	0.04
(1,1881)	1:B:53:THR:HG21	1:B:54:THR:H	11	0.04
(1,1881)	1:B:53:THR:HG22	1:B:54:THR:H	11	0.04
(1,1881)	1:B:53:THR:HG23	1:B:54:THR:H	11	0.04
(1,1881)	1:B:53:THR:HG21	1:B:54:THR:H	12	0.04
(1,1881)	1:B:53:THR:HG22	1:B:54:THR:H	12	0.04
(1,1881)	1:B:53:THR:HG23	1:B:54:THR:H	12	0.04
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB1	7	0.04
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB2	7	0.04
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB3	7	0.04
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB1	7	0.04
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB2	7	0.04
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB3	7	0.04
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB1	7	0.04
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB2	7	0.04
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB3	7	0.04
(1,1750)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	14	0.04
(1,1750)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	14	0.04
(1,1750)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	14	0.04
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD11	10	0.04
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD12	10	0.04
(1,1746)	1:B:42:GLU:HG2	1:B:52:LEU:HD13	10	0.04
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB1	17	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB2	17	0.04
(1,1745)	1:B:42:GLU:HG2	1:B:45:ALA:HB3	17	0.04
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD21	10	0.04
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD22	10	0.04
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD23	10	0.04
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD21	10	0.04
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD22	10	0.04
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD23	10	0.04
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD21	10	0.04
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD22	10	0.04
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD23	10	0.04
(1,172)	1:A:11:LEU:HA	1:A:14:GLN:HG2	17	0.04
(1,1706)	1:B:41:VAL:HB	1:B:79:TYR:HE1	6	0.04
(1,1706)	1:B:41:VAL:HB	1:B:79:TYR:HE1	8	0.04
(1,1670)	1:B:39:ARG:HG2	1:B:40:ALA:H	8	0.04
(1,1662)	1:B:39:ARG:HA	1:B:39:ARG:HD2	9	0.04
(1,1648)	1:B:37:GLY:HA2	1:B:38:GLU:HB2	8	0.04
(1,1648)	1:B:37:GLY:HA2	1:B:38:GLU:HB3	8	0.04
(1,1622)	1:B:34:LEU:HD21	1:B:37:GLY:H	8	0.04
(1,1622)	1:B:34:LEU:HD22	1:B:37:GLY:H	8	0.04
(1,1622)	1:B:34:LEU:HD23	1:B:37:GLY:H	8	0.04
(1,1605)	1:B:33:LEU:HD11	1:B:47:ALA:H	14	0.04
(1,1605)	1:B:33:LEU:HD12	1:B:47:ALA:H	14	0.04
(1,1605)	1:B:33:LEU:HD13	1:B:47:ALA:H	14	0.04
(1,1592)	1:B:33:LEU:HB2	1:B:34:LEU:H	15	0.04
(1,1521)	1:B:30:ILE:HG21	1:B:33:LEU:HB2	7	0.04
(1,1521)	1:B:30:ILE:HG22	1:B:33:LEU:HB2	7	0.04
(1,1521)	1:B:30:ILE:HG23	1:B:33:LEU:HB2	7	0.04
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD11	9	0.04
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD12	9	0.04
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD13	9	0.04
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD11	9	0.04
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD12	9	0.04
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD13	9	0.04
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD11	20	0.04
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD12	20	0.04
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD13	20	0.04
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD11	20	0.04
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD12	20	0.04
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD13	20	0.04
(1,1499)	1:B:30:ILE:HA	1:B:33:LEU:HD11	7	0.04
(1,1499)	1:B:30:ILE:HA	1:B:33:LEU:HD12	7	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1499)	1:B:30:ILE:HA	1:B:33:LEU:HD13	7	0.04
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	7	0.04
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	7	0.04
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	7	0.04
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	7	0.04
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	7	0.04
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	7	0.04
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	17	0.04
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	17	0.04
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	17	0.04
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	17	0.04
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	17	0.04
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	17	0.04
(1,1431)	1:B:22:LEU:HD21	1:B:28:LEU:HD21	11	0.04
(1,1431)	1:B:22:LEU:HD21	1:B:28:LEU:HD22	11	0.04
(1,1431)	1:B:22:LEU:HD21	1:B:28:LEU:HD23	11	0.04
(1,1431)	1:B:22:LEU:HD22	1:B:28:LEU:HD21	11	0.04
(1,1431)	1:B:22:LEU:HD22	1:B:28:LEU:HD22	11	0.04
(1,1431)	1:B:22:LEU:HD22	1:B:28:LEU:HD23	11	0.04
(1,1431)	1:B:22:LEU:HD23	1:B:28:LEU:HD21	11	0.04
(1,1431)	1:B:22:LEU:HD23	1:B:28:LEU:HD22	11	0.04
(1,1431)	1:B:22:LEU:HD23	1:B:28:LEU:HD23	11	0.04
(1,1425)	1:B:22:LEU:HD11	1:B:89:LEU:HD21	11	0.04
(1,1425)	1:B:22:LEU:HD11	1:B:89:LEU:HD22	11	0.04
(1,1425)	1:B:22:LEU:HD11	1:B:89:LEU:HD23	11	0.04
(1,1425)	1:B:22:LEU:HD12	1:B:89:LEU:HD21	11	0.04
(1,1425)	1:B:22:LEU:HD12	1:B:89:LEU:HD22	11	0.04
(1,1425)	1:B:22:LEU:HD12	1:B:89:LEU:HD23	11	0.04
(1,1425)	1:B:22:LEU:HD13	1:B:89:LEU:HD21	11	0.04
(1,1425)	1:B:22:LEU:HD13	1:B:89:LEU:HD22	11	0.04
(1,1425)	1:B:22:LEU:HD13	1:B:89:LEU:HD23	11	0.04
(1,1411)	1:B:21:ALA:HB1	1:B:65:GLY:H	11	0.04
(1,1411)	1:B:21:ALA:HB2	1:B:65:GLY:H	11	0.04
(1,1411)	1:B:21:ALA:HB3	1:B:65:GLY:H	11	0.04
(1,1409)	1:B:21:ALA:HB1	1:B:65:GLY:HA2	2	0.04
(1,1409)	1:B:21:ALA:HB2	1:B:65:GLY:HA2	2	0.04
(1,1409)	1:B:21:ALA:HB3	1:B:65:GLY:HA2	2	0.04
(1,1395)	1:B:20:LYS:HB2	1:B:20:LYS:HE2	4	0.04
(1,1395)	1:B:20:LYS:HB2	1:B:20:LYS:HE3	4	0.04
(1,1395)	1:B:20:LYS:HB3	1:B:20:LYS:HE2	4	0.04
(1,1395)	1:B:20:LYS:HB3	1:B:20:LYS:HE3	4	0.04
(1,1390)	1:B:20:LYS:HA	1:B:20:LYS:HE2	11	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1390)	1:B:20:LYS:HA	1:B:20:LYS:HE3	11	0.04
(1,1367)	1:B:17:ARG:HD2	1:B:64:SER:HB2	14	0.04
(1,1367)	1:B:17:ARG:HD2	1:B:64:SER:HB3	14	0.04
(1,1367)	1:B:17:ARG:HD3	1:B:64:SER:HB2	14	0.04
(1,1367)	1:B:17:ARG:HD3	1:B:64:SER:HB3	14	0.04
(1,1363)	1:B:17:ARG:H	1:B:17:ARG:HG2	9	0.04
(1,1361)	1:B:17:ARG:HA	1:B:65:GLY:HA2	12	0.04
(1,1296)	1:B:10:ALA:HB1	1:B:13:ASP:HB2	15	0.04
(1,1296)	1:B:10:ALA:HB2	1:B:13:ASP:HB2	15	0.04
(1,1296)	1:B:10:ALA:HB3	1:B:13:ASP:HB2	15	0.04
(1,1278)	1:B:8:LYS:HA	1:B:8:LYS:HD2	1	0.04
(1,1278)	1:B:8:LYS:HA	1:B:8:LYS:HD3	1	0.04
(1,1264)	1:B:6:ASP:HA	1:B:9:ALA:HB1	13	0.04
(1,1264)	1:B:6:ASP:HA	1:B:9:ALA:HB2	13	0.04
(1,1264)	1:B:6:ASP:HA	1:B:9:ALA:HB3	13	0.04
(1,1262)	1:B:5:SER:HB2	1:B:6:ASP:H	16	0.04
(1,1258)	1:A:107:HIS:HB2	1:A:108:HIS:H	6	0.04
(1,1251)	1:A:101:LEU:HB2	1:A:102:GLU:H	7	0.04
(1,1242)	1:A:99:GLU:HG2	1:A:100:HIS:H	4	0.04
(1,121)	1:B:88:ARG:HB2	1:A:92:LEU:HD21	10	0.04
(1,121)	1:B:88:ARG:HB2	1:A:92:LEU:HD22	10	0.04
(1,121)	1:B:88:ARG:HB2	1:A:92:LEU:HD23	10	0.04
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB1	4	0.04
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB2	4	0.04
(1,118)	1:B:20:LYS:H	1:A:23:ALA:HB3	4	0.04
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB1	7	0.04
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB2	7	0.04
(1,116)	1:B:20:LYS:HG2	1:A:23:ALA:HB3	7	0.04
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD21	14	0.04
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD22	14	0.04
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD23	14	0.04
(1,1093)	1:A:84:GLU:HG2	1:A:88:ARG:HD2	14	0.04
(1,1093)	1:A:84:GLU:HG2	1:A:88:ARG:HD3	14	0.04
(1,1093)	1:A:84:GLU:HG3	1:A:88:ARG:HD2	14	0.04
(1,1093)	1:A:84:GLU:HG3	1:A:88:ARG:HD3	14	0.04
(1,1092)	1:A:84:GLU:HG2	1:A:86:VAL:H	6	0.04
(1,1092)	1:A:84:GLU:HG3	1:A:86:VAL:H	6	0.04
(1,1078)	1:A:82:ALA:HB1	1:A:86:VAL:HB	8	0.04
(1,1078)	1:A:82:ALA:HB2	1:A:86:VAL:HB	8	0.04
(1,1078)	1:A:82:ALA:HB3	1:A:86:VAL:HB	8	0.04
(1,1077)	1:A:82:ALA:HB1	1:A:83:GLY:H	17	0.04
(1,1077)	1:A:82:ALA:HB2	1:A:83:GLY:H	17	0.04

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1077)	1:A:82:ALA:HB3	1:A:83:GLY:H	17	0.04
(1,1052)	1:A:81:ILE:HD11	1:A:82:ALA:H	18	0.04
(1,1052)	1:A:81:ILE:HD12	1:A:82:ALA:H	18	0.04
(1,1052)	1:A:81:ILE:HD13	1:A:82:ALA:H	18	0.04
(1,1037)	1:A:77:GLN:H	1:A:77:GLN:HG2	7	0.04
(1,1033)	1:A:77:GLN:HG2	1:A:77:GLN:HE21	17	0.04
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB1	7	0.03
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB2	7	0.03
(1,99)	1:B:15:VAL:HG11	1:A:97:ALA:HB3	7	0.03
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB1	7	0.03
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB2	7	0.03
(1,99)	1:B:15:VAL:HG12	1:A:97:ALA:HB3	7	0.03
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB1	7	0.03
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB2	7	0.03
(1,99)	1:B:15:VAL:HG13	1:A:97:ALA:HB3	7	0.03
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB1	12	0.03
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB2	12	0.03
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB3	12	0.03
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB1	18	0.03
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB2	18	0.03
(1,96)	1:B:15:VAL:HA	1:A:97:ALA:HB3	18	0.03
(1,959)	1:A:70:ALA:HB1	1:A:77:GLN:HE22	17	0.03
(1,959)	1:A:70:ALA:HB2	1:A:77:GLN:HE22	17	0.03
(1,959)	1:A:70:ALA:HB3	1:A:77:GLN:HE22	17	0.03
(1,944)	1:A:69:GLU:HG3	1:A:82:ALA:HB1	18	0.03
(1,944)	1:A:69:GLU:HG3	1:A:82:ALA:HB2	18	0.03
(1,944)	1:A:69:GLU:HG3	1:A:82:ALA:HB3	18	0.03
(1,943)	1:A:69:GLU:HG3	1:A:82:ALA:HA	9	0.03
(1,943)	1:A:69:GLU:HG3	1:A:82:ALA:HA	16	0.03
(1,921)	1:A:68:VAL:HG11	1:A:86:VAL:HG11	13	0.03
(1,921)	1:A:68:VAL:HG11	1:A:86:VAL:HG12	13	0.03
(1,921)	1:A:68:VAL:HG11	1:A:86:VAL:HG13	13	0.03
(1,921)	1:A:68:VAL:HG12	1:A:86:VAL:HG11	13	0.03
(1,921)	1:A:68:VAL:HG12	1:A:86:VAL:HG12	13	0.03
(1,921)	1:A:68:VAL:HG12	1:A:86:VAL:HG13	13	0.03
(1,921)	1:A:68:VAL:HG13	1:A:86:VAL:HG11	13	0.03
(1,921)	1:A:68:VAL:HG13	1:A:86:VAL:HG12	13	0.03
(1,921)	1:A:68:VAL:HG13	1:A:86:VAL:HG13	13	0.03
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG21	19	0.03
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG22	19	0.03
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG23	19	0.03
(1,865)	1:A:63:LYS:HE2	1:A:70:ALA:H	3	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,865)	1:A:63:LYS:HE3	1:A:70:ALA:H	3	0.03
(1,864)	1:A:63:LYS:HE2	1:A:70:ALA:HB1	15	0.03
(1,864)	1:A:63:LYS:HE2	1:A:70:ALA:HB2	15	0.03
(1,864)	1:A:63:LYS:HE2	1:A:70:ALA:HB3	15	0.03
(1,864)	1:A:63:LYS:HE3	1:A:70:ALA:HB1	15	0.03
(1,864)	1:A:63:LYS:HE3	1:A:70:ALA:HB2	15	0.03
(1,864)	1:A:63:LYS:HE3	1:A:70:ALA:HB3	15	0.03
(1,863)	1:A:63:LYS:HE2	1:A:69:GLU:HA	4	0.03
(1,863)	1:A:63:LYS:HE3	1:A:69:GLU:HA	4	0.03
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE2	7	0.03
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE3	7	0.03
(1,842)	1:A:62:LEU:HB3	1:A:68:VAL:HG21	7	0.03
(1,842)	1:A:62:LEU:HB3	1:A:68:VAL:HG22	7	0.03
(1,842)	1:A:62:LEU:HB3	1:A:68:VAL:HG23	7	0.03
(1,824)	1:A:60:GLN:HG2	1:A:61:ALA:HA	1	0.03
(1,824)	1:A:60:GLN:HG3	1:A:61:ALA:HA	1	0.03
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	1	0.03
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	1	0.03
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	1	0.03
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	1	0.03
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	1	0.03
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	1	0.03
(1,816)	1:A:60:GLN:HA	1:A:60:GLN:HE21	10	0.03
(1,747)	1:A:53:THR:HB	1:A:54:THR:H	15	0.03
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	9	0.03
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	20	0.03
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	20	0.03
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	20	0.03
(1,70)	1:B:12:LEU:HD11	1:A:29:GLN:HB2	9	0.03
(1,70)	1:B:12:LEU:HD12	1:A:29:GLN:HB2	9	0.03
(1,70)	1:B:12:LEU:HD13	1:A:29:GLN:HB2	9	0.03
(1,691)	1:A:48:THR:HB	1:A:50:MET:HG2	12	0.03
(1,650)	1:A:44:ILE:HG21	1:A:47:ALA:HB1	6	0.03
(1,650)	1:A:44:ILE:HG21	1:A:47:ALA:HB2	6	0.03
(1,650)	1:A:44:ILE:HG21	1:A:47:ALA:HB3	6	0.03
(1,650)	1:A:44:ILE:HG22	1:A:47:ALA:HB1	6	0.03
(1,650)	1:A:44:ILE:HG22	1:A:47:ALA:HB2	6	0.03
(1,650)	1:A:44:ILE:HG22	1:A:47:ALA:HB3	6	0.03
(1,650)	1:A:44:ILE:HG23	1:A:47:ALA:HB1	6	0.03
(1,650)	1:A:44:ILE:HG23	1:A:47:ALA:HB2	6	0.03
(1,650)	1:A:44:ILE:HG23	1:A:47:ALA:HB3	6	0.03
(1,616)	1:A:42:GLU:HG3	1:A:52:LEU:HD11	3	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,616)	1:A:42:GLU:HG3	1:A:52:LEU:HD12	3	0.03
(1,616)	1:A:42:GLU:HG3	1:A:52:LEU:HD13	3	0.03
(1,60)	1:A:89:LEU:HB2	1:B:92:LEU:HD11	9	0.03
(1,60)	1:A:89:LEU:HB2	1:B:92:LEU:HD12	9	0.03
(1,60)	1:A:89:LEU:HB2	1:B:92:LEU:HD13	9	0.03
(1,60)	1:A:89:LEU:HB3	1:B:92:LEU:HD11	9	0.03
(1,60)	1:A:89:LEU:HB3	1:B:92:LEU:HD12	9	0.03
(1,60)	1:A:89:LEU:HB3	1:B:92:LEU:HD13	9	0.03
(1,592)	1:A:41:VAL:HG21	1:A:59:LEU:HD21	18	0.03
(1,592)	1:A:41:VAL:HG21	1:A:59:LEU:HD22	18	0.03
(1,592)	1:A:41:VAL:HG21	1:A:59:LEU:HD23	18	0.03
(1,592)	1:A:41:VAL:HG22	1:A:59:LEU:HD21	18	0.03
(1,592)	1:A:41:VAL:HG22	1:A:59:LEU:HD22	18	0.03
(1,592)	1:A:41:VAL:HG22	1:A:59:LEU:HD23	18	0.03
(1,592)	1:A:41:VAL:HG23	1:A:59:LEU:HD21	18	0.03
(1,592)	1:A:41:VAL:HG23	1:A:59:LEU:HD22	18	0.03
(1,592)	1:A:41:VAL:HG23	1:A:59:LEU:HD23	18	0.03
(1,574)	1:A:41:VAL:HB	1:A:79:TYR:HE1	12	0.03
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD11	7	0.03
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD12	7	0.03
(1,555)	1:A:40:ALA:HB1	1:A:52:LEU:HD13	7	0.03
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD11	7	0.03
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD12	7	0.03
(1,555)	1:A:40:ALA:HB2	1:A:52:LEU:HD13	7	0.03
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD11	7	0.03
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD12	7	0.03
(1,555)	1:A:40:ALA:HB3	1:A:52:LEU:HD13	7	0.03
(1,543)	1:A:40:ALA:HA	1:A:78:TYR:HA	18	0.03
(1,534)	1:A:39:ARG:HB2	1:A:39:ARG:HE	10	0.03
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB1	9	0.03
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB2	9	0.03
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB3	9	0.03
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB1	16	0.03
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB2	16	0.03
(1,53)	1:A:20:LYS:HG2	1:B:23:ALA:HB3	16	0.03
(1,528)	1:A:38:GLU:H	1:A:38:GLU:HG2	18	0.03
(1,528)	1:A:38:GLU:H	1:A:38:GLU:HG3	18	0.03
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	17	0.03
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	17	0.03
(1,516)	1:A:37:GLY:HA2	1:A:38:GLU:HB2	12	0.03
(1,516)	1:A:37:GLY:HA2	1:A:38:GLU:HB3	12	0.03
(1,506)	1:A:35:ALA:HB1	1:A:90:PHE:HD1	20	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,506)	1:A:35:ALA:HB1	1:A:90:PHE:HD2	20	0.03
(1,506)	1:A:35:ALA:HB2	1:A:90:PHE:HD1	20	0.03
(1,506)	1:A:35:ALA:HB2	1:A:90:PHE:HD2	20	0.03
(1,506)	1:A:35:ALA:HB3	1:A:90:PHE:HD1	20	0.03
(1,506)	1:A:35:ALA:HB3	1:A:90:PHE:HD2	20	0.03
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB1	5	0.03
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB2	5	0.03
(1,469)	1:A:33:LEU:HD11	1:A:43:ALA:HB3	5	0.03
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB1	5	0.03
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB2	5	0.03
(1,469)	1:A:33:LEU:HD12	1:A:43:ALA:HB3	5	0.03
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB1	5	0.03
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB2	5	0.03
(1,469)	1:A:33:LEU:HD13	1:A:43:ALA:HB3	5	0.03
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	2	0.03
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	2	0.03
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	2	0.03
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	2	0.03
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	2	0.03
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	2	0.03
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	4	0.03
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	4	0.03
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	4	0.03
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	4	0.03
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	4	0.03
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	4	0.03
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	9	0.03
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	9	0.03
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	9	0.03
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	9	0.03
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	9	0.03
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	9	0.03
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	14	0.03
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	14	0.03
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	14	0.03
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	14	0.03
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	14	0.03
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	14	0.03
(1,429)	1:A:31:LEU:HD21	1:A:67:LEU:HA	11	0.03
(1,429)	1:A:31:LEU:HD22	1:A:67:LEU:HA	11	0.03
(1,429)	1:A:31:LEU:HD23	1:A:67:LEU:HA	11	0.03
(1,420)	1:A:31:LEU:HD11	1:A:67:LEU:HB2	14	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,420)	1:A:31:LEU:HD11	1:A:67:LEU:HB3	14	0.03
(1,420)	1:A:31:LEU:HD12	1:A:67:LEU:HB2	14	0.03
(1,420)	1:A:31:LEU:HD12	1:A:67:LEU:HB3	14	0.03
(1,420)	1:A:31:LEU:HD13	1:A:67:LEU:HB2	14	0.03
(1,420)	1:A:31:LEU:HD13	1:A:67:LEU:HB3	14	0.03
(1,420)	1:A:31:LEU:HD11	1:A:67:LEU:HB2	15	0.03
(1,420)	1:A:31:LEU:HD11	1:A:67:LEU:HB3	15	0.03
(1,420)	1:A:31:LEU:HD12	1:A:67:LEU:HB2	15	0.03
(1,420)	1:A:31:LEU:HD12	1:A:67:LEU:HB3	15	0.03
(1,420)	1:A:31:LEU:HD13	1:A:67:LEU:HB2	15	0.03
(1,420)	1:A:31:LEU:HD13	1:A:67:LEU:HB3	15	0.03
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD1	7	0.03
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD2	7	0.03
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD1	7	0.03
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD2	7	0.03
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD1	7	0.03
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD2	7	0.03
(1,330)	1:A:27:ARG:HD2	1:A:62:LEU:H	4	0.03
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	9	0.03
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	9	0.03
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	9	0.03
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	15	0.03
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	15	0.03
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	15	0.03
(1,308)	1:A:23:ALA:H	1:A:24:ASN:H	18	0.03
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD21	13	0.03
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD22	13	0.03
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD23	13	0.03
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD21	13	0.03
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD22	13	0.03
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD23	13	0.03
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD21	13	0.03
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD22	13	0.03
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD23	13	0.03
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD21	12	0.03
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD22	12	0.03
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD23	12	0.03
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	5	0.03
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	5	0.03
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	5	0.03
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	13	0.03
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	13	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	13	0.03
(1,2613)	1:B:97:ALA:H	1:B:93:VAL:O	10	0.03
(1,2589)	1:B:80:ARG:H	1:B:69:GLU:O	9	0.03
(1,2583)	1:B:76:ARG:H	1:B:73:GLU:O	12	0.03
(1,2583)	1:B:76:ARG:H	1:B:73:GLU:O	18	0.03
(1,258)	1:A:20:LYS:HA	1:A:20:LYS:HE2	8	0.03
(1,258)	1:A:20:LYS:HA	1:A:20:LYS:HE3	8	0.03
(1,2575)	1:B:67:LEU:H	1:B:62:LEU:O	6	0.03
(1,2571)	1:B:65:GLY:H	1:B:61:ALA:O	7	0.03
(1,2571)	1:B:65:GLY:H	1:B:61:ALA:O	15	0.03
(1,2563)	1:B:61:ALA:H	1:B:57:ALA:O	7	0.03
(1,2557)	1:B:58:ASN:H	1:B:54:THR:O	11	0.03
(1,2555)	1:B:57:ALA:H	1:B:53:THR:O	7	0.03
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	4	0.03
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	6	0.03
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	8	0.03
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	12	0.03
(1,2535)	1:B:41:VAL:H	1:B:77:GLN:O	9	0.03
(1,2527)	1:B:33:LEU:H	1:B:29:GLN:O	11	0.03
(1,2525)	1:B:32:ASP:H	1:B:28:LEU:O	8	0.03
(1,2523)	1:B:22:LEU:H	1:B:18:VAL:O	10	0.03
(1,2523)	1:B:22:LEU:H	1:B:18:VAL:O	16	0.03
(1,2521)	1:B:21:ALA:H	1:B:17:ARG:O	2	0.03
(1,2521)	1:B:21:ALA:H	1:B:17:ARG:O	3	0.03
(1,2521)	1:B:21:ALA:H	1:B:17:ARG:O	6	0.03
(1,2521)	1:B:21:ALA:H	1:B:17:ARG:O	9	0.03
(1,2521)	1:B:21:ALA:H	1:B:17:ARG:O	14	0.03
(1,2521)	1:B:21:ALA:H	1:B:17:ARG:O	16	0.03
(1,2521)	1:B:21:ALA:H	1:B:17:ARG:O	18	0.03
(1,2515)	1:B:18:VAL:H	1:B:14:GLN:O	3	0.03
(1,2515)	1:B:18:VAL:H	1:B:14:GLN:O	5	0.03
(1,2515)	1:B:18:VAL:H	1:B:14:GLN:O	7	0.03
(1,2515)	1:B:18:VAL:H	1:B:14:GLN:O	8	0.03
(1,2515)	1:B:18:VAL:H	1:B:14:GLN:O	10	0.03
(1,2513)	1:B:17:ARG:H	1:B:13:ASP:O	11	0.03
(1,2507)	1:B:14:GLN:H	1:B:10:ALA:O	12	0.03
(1,2507)	1:B:14:GLN:H	1:B:10:ALA:O	15	0.03
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	1	0.03
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	7	0.03
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	9	0.03
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	12	0.03
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	14	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	20	0.03
(1,2499)	1:A:97:ALA:H	1:A:93:VAL:O	3	0.03
(1,2499)	1:A:97:ALA:H	1:A:93:VAL:O	11	0.03
(1,2495)	1:A:95:VAL:H	1:A:91:ALA:O	16	0.03
(1,2483)	1:A:89:LEU:H	1:A:85:ASP:O	7	0.03
(1,2475)	1:A:80:ARG:H	1:A:69:GLU:O	4	0.03
(1,2469)	1:A:76:ARG:H	1:A:73:GLU:O	16	0.03
(1,2461)	1:A:67:LEU:H	1:A:62:LEU:O	12	0.03
(1,2461)	1:A:67:LEU:H	1:A:62:LEU:O	15	0.03
(1,2449)	1:A:61:ALA:H	1:A:57:ALA:O	1	0.03
(1,2449)	1:A:61:ALA:H	1:A:57:ALA:O	8	0.03
(1,2443)	1:A:58:ASN:H	1:A:54:THR:O	11	0.03
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	1	0.03
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	11	0.03
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	13	0.03
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	16	0.03
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	17	0.03
(1,2419)	1:A:39:ARG:H	1:A:79:TYR:O	15	0.03
(1,2417)	1:A:35:ALA:H	1:A:31:LEU:O	9	0.03
(1,2417)	1:A:35:ALA:H	1:A:31:LEU:O	20	0.03
(1,2413)	1:A:33:LEU:H	1:A:29:GLN:O	16	0.03
(1,2409)	1:A:22:LEU:H	1:A:18:VAL:O	3	0.03
(1,2409)	1:A:22:LEU:H	1:A:18:VAL:O	16	0.03
(1,2407)	1:A:21:ALA:H	1:A:17:ARG:O	4	0.03
(1,2407)	1:A:21:ALA:H	1:A:17:ARG:O	15	0.03
(1,2401)	1:A:18:VAL:H	1:A:14:GLN:O	8	0.03
(1,2401)	1:A:18:VAL:H	1:A:14:GLN:O	14	0.03
(1,2401)	1:A:18:VAL:H	1:A:14:GLN:O	15	0.03
(1,2393)	1:A:14:GLN:H	1:A:10:ALA:O	16	0.03
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	3	0.03
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	15	0.03
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	16	0.03
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	18	0.03
(1,2384)	1:B:101:LEU:HD21	1:B:102:GLU:H	5	0.03
(1,2384)	1:B:101:LEU:HD22	1:B:102:GLU:H	5	0.03
(1,2384)	1:B:101:LEU:HD23	1:B:102:GLU:H	5	0.03
(1,2375)	1:B:99:GLU:H	1:B:99:GLU:HB2	17	0.03
(1,2362)	1:B:97:ALA:HA	1:B:101:LEU:HD21	5	0.03
(1,2362)	1:B:97:ALA:HA	1:B:101:LEU:HD22	5	0.03
(1,2362)	1:B:97:ALA:HA	1:B:101:LEU:HD23	5	0.03
(1,2362)	1:B:97:ALA:HA	1:B:101:LEU:HD21	14	0.03
(1,2362)	1:B:97:ALA:HA	1:B:101:LEU:HD22	14	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2362)	1:B:97:ALA:HA	1:B:101:LEU:HD23	14	0.03
(1,2333)	1:B:95:VAL:HA	1:B:98:ASP:HB2	8	0.03
(1,231)	1:A:17:ARG:H	1:A:17:ARG:HG2	4	0.03
(1,230)	1:A:17:ARG:H	1:A:17:ARG:HD2	14	0.03
(1,230)	1:A:17:ARG:H	1:A:17:ARG:HD3	14	0.03
(1,2269)	1:B:89:LEU:HA	1:B:92:LEU:HD21	15	0.03
(1,2269)	1:B:89:LEU:HA	1:B:92:LEU:HD22	15	0.03
(1,2269)	1:B:89:LEU:HA	1:B:92:LEU:HD23	15	0.03
(1,2213)	1:B:82:ALA:H	1:B:86:VAL:HG21	2	0.03
(1,2213)	1:B:82:ALA:H	1:B:86:VAL:HG22	2	0.03
(1,2213)	1:B:82:ALA:H	1:B:86:VAL:HG23	2	0.03
(1,22)	1:A:12:LEU:HG	1:B:29:GLN:HG2	7	0.03
(1,2196)	1:B:81:ILE:HG21	1:B:83:GLY:H	3	0.03
(1,2196)	1:B:81:ILE:HG22	1:B:83:GLY:H	3	0.03
(1,2196)	1:B:81:ILE:HG23	1:B:83:GLY:H	3	0.03
(1,2162)	1:B:77:GLN:HB2	1:B:77:GLN:HE21	12	0.03
(1,2162)	1:B:77:GLN:HB3	1:B:77:GLN:HE21	12	0.03
(1,2162)	1:B:77:GLN:HB2	1:B:77:GLN:HE21	16	0.03
(1,2162)	1:B:77:GLN:HB3	1:B:77:GLN:HE21	16	0.03
(1,2135)	1:B:74:GLY:HA2	1:B:76:ARG:H	18	0.03
(1,2095)	1:B:70:ALA:HB1	1:B:79:TYR:HE1	4	0.03
(1,2095)	1:B:70:ALA:HB2	1:B:79:TYR:HE1	4	0.03
(1,2095)	1:B:70:ALA:HB3	1:B:79:TYR:HE1	4	0.03
(1,2035)	1:B:67:LEU:H	1:B:67:LEU:HD21	6	0.03
(1,2035)	1:B:67:LEU:H	1:B:67:LEU:HD22	6	0.03
(1,2035)	1:B:67:LEU:H	1:B:67:LEU:HD23	6	0.03
(1,2024)	1:B:67:LEU:HA	1:B:86:VAL:HG21	8	0.03
(1,2024)	1:B:67:LEU:HA	1:B:86:VAL:HG22	8	0.03
(1,2024)	1:B:67:LEU:HA	1:B:86:VAL:HG23	8	0.03
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE2	20	0.03
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE3	20	0.03
(1,1967)	1:B:62:LEU:HA	1:B:67:LEU:HD21	14	0.03
(1,1967)	1:B:62:LEU:HA	1:B:67:LEU:HD22	14	0.03
(1,1967)	1:B:62:LEU:HA	1:B:67:LEU:HD23	14	0.03
(1,1956)	1:B:60:GLN:HG2	1:B:61:ALA:HA	17	0.03
(1,1956)	1:B:60:GLN:HG3	1:B:61:ALA:HA	17	0.03
(1,1951)	1:B:60:GLN:HA	1:B:63:LYS:HG2	8	0.03
(1,1951)	1:B:60:GLN:HA	1:B:63:LYS:HG3	8	0.03
(1,1934)	1:B:59:LEU:HB2	1:B:79:TYR:HE1	10	0.03
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	12	0.03
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	12	0.03
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	12	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	12	0.03
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	12	0.03
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	12	0.03
(1,1889)	1:B:54:THR:HG21	1:B:58:ASN:HD22	10	0.03
(1,1889)	1:B:54:THR:HG22	1:B:58:ASN:HD22	10	0.03
(1,1889)	1:B:54:THR:HG23	1:B:58:ASN:HD22	10	0.03
(1,1877)	1:B:52:LEU:H	1:B:52:LEU:HG	3	0.03
(1,1782)	1:B:44:ILE:HG21	1:B:47:ALA:HB1	13	0.03
(1,1782)	1:B:44:ILE:HG21	1:B:47:ALA:HB2	13	0.03
(1,1782)	1:B:44:ILE:HG21	1:B:47:ALA:HB3	13	0.03
(1,1782)	1:B:44:ILE:HG22	1:B:47:ALA:HB1	13	0.03
(1,1782)	1:B:44:ILE:HG22	1:B:47:ALA:HB2	13	0.03
(1,1782)	1:B:44:ILE:HG22	1:B:47:ALA:HB3	13	0.03
(1,1782)	1:B:44:ILE:HG23	1:B:47:ALA:HB1	13	0.03
(1,1782)	1:B:44:ILE:HG23	1:B:47:ALA:HB2	13	0.03
(1,1782)	1:B:44:ILE:HG23	1:B:47:ALA:HB3	13	0.03
(1,1749)	1:B:42:GLU:HG3	1:B:52:LEU:HD21	15	0.03
(1,1749)	1:B:42:GLU:HG3	1:B:52:LEU:HD22	15	0.03
(1,1749)	1:B:42:GLU:HG3	1:B:52:LEU:HD23	15	0.03
(1,1748)	1:B:42:GLU:HG3	1:B:52:LEU:HD11	18	0.03
(1,1748)	1:B:42:GLU:HG3	1:B:52:LEU:HD12	18	0.03
(1,1748)	1:B:42:GLU:HG3	1:B:52:LEU:HD13	18	0.03
(1,1744)	1:B:42:GLU:HG2	1:B:43:ALA:H	17	0.03
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD21	2	0.03
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD22	2	0.03
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD23	2	0.03
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD21	2	0.03
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD22	2	0.03
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD23	2	0.03
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD21	2	0.03
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD22	2	0.03
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD23	2	0.03
(1,172)	1:A:11:LEU:HA	1:A:14:GLN:HG2	19	0.03
(1,1706)	1:B:41:VAL:HB	1:B:79:TYR:HE1	9	0.03
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD11	1	0.03
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD12	1	0.03
(1,170)	1:A:11:LEU:HA	1:A:11:LEU:HD13	1	0.03
(1,1691)	1:B:40:ALA:HB1	1:B:78:TYR:HE1	12	0.03
(1,1691)	1:B:40:ALA:HB2	1:B:78:TYR:HE1	12	0.03
(1,1691)	1:B:40:ALA:HB3	1:B:78:TYR:HE1	12	0.03
(1,1675)	1:B:40:ALA:HA	1:B:78:TYR:HA	10	0.03
(1,1647)	1:B:36:GLN:H	1:B:36:GLN:HG2	18	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1643)	1:B:36:GLN:HB2	1:B:37:GLY:H	5	0.03
(1,1621)	1:B:34:LEU:HD11	1:B:80:ARG:HA	7	0.03
(1,1621)	1:B:34:LEU:HD12	1:B:80:ARG:HA	7	0.03
(1,1621)	1:B:34:LEU:HD13	1:B:80:ARG:HA	7	0.03
(1,1592)	1:B:33:LEU:HB2	1:B:34:LEU:H	5	0.03
(1,1592)	1:B:33:LEU:HB2	1:B:34:LEU:H	6	0.03
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	1	0.03
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	1	0.03
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	1	0.03
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	1	0.03
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	1	0.03
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	1	0.03
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	3	0.03
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	3	0.03
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	3	0.03
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	3	0.03
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	3	0.03
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	3	0.03
(1,1537)	1:B:31:LEU:HA	1:B:34:LEU:HD11	4	0.03
(1,1537)	1:B:31:LEU:HA	1:B:34:LEU:HD12	4	0.03
(1,1537)	1:B:31:LEU:HA	1:B:34:LEU:HD13	4	0.03
(1,1521)	1:B:30:ILE:HG21	1:B:33:LEU:HB2	4	0.03
(1,1521)	1:B:30:ILE:HG22	1:B:33:LEU:HB2	4	0.03
(1,1521)	1:B:30:ILE:HG23	1:B:33:LEU:HB2	4	0.03
(1,150)	1:A:8:LYS:HB2	1:A:9:ALA:H	11	0.03
(1,150)	1:A:8:LYS:HB3	1:A:9:ALA:H	11	0.03
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG21	4	0.03
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG22	4	0.03
(1,1493)	1:B:29:GLN:HG2	1:B:48:THR:HG23	4	0.03
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG21	19	0.03
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG22	19	0.03
(1,1487)	1:B:29:GLN:HB2	1:B:48:THR:HG23	19	0.03
(1,1462)	1:B:27:ARG:HD2	1:B:62:LEU:H	13	0.03
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD2	8	0.03
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD3	8	0.03
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD2	11	0.03
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD3	11	0.03
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD2	17	0.03
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD3	17	0.03
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD21	7	0.03
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD22	7	0.03
(1,1447)	1:B:25:GLY:HA2	1:B:28:LEU:HD23	7	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1440)	1:B:23:ALA:H	1:B:24:ASN:H	14	0.03
(1,1411)	1:B:21:ALA:HB1	1:B:65:GLY:H	1	0.03
(1,1411)	1:B:21:ALA:HB2	1:B:65:GLY:H	1	0.03
(1,1411)	1:B:21:ALA:HB3	1:B:65:GLY:H	1	0.03
(1,1395)	1:B:20:LYS:HB2	1:B:20:LYS:HE2	2	0.03
(1,1395)	1:B:20:LYS:HB2	1:B:20:LYS:HE3	2	0.03
(1,1395)	1:B:20:LYS:HB3	1:B:20:LYS:HE2	2	0.03
(1,1395)	1:B:20:LYS:HB3	1:B:20:LYS:HE3	2	0.03
(1,1390)	1:B:20:LYS:HA	1:B:20:LYS:HE2	6	0.03
(1,1390)	1:B:20:LYS:HA	1:B:20:LYS:HE3	6	0.03
(1,1367)	1:B:17:ARG:HD2	1:B:64:SER:HB2	1	0.03
(1,1367)	1:B:17:ARG:HD2	1:B:64:SER:HB3	1	0.03
(1,1367)	1:B:17:ARG:HD3	1:B:64:SER:HB2	1	0.03
(1,1367)	1:B:17:ARG:HD3	1:B:64:SER:HB3	1	0.03
(1,1367)	1:B:17:ARG:HD2	1:B:64:SER:HB2	10	0.03
(1,1367)	1:B:17:ARG:HD2	1:B:64:SER:HB3	10	0.03
(1,1367)	1:B:17:ARG:HD3	1:B:64:SER:HB2	10	0.03
(1,1367)	1:B:17:ARG:HD3	1:B:64:SER:HB3	10	0.03
(1,1304)	1:B:11:LEU:HA	1:B:14:GLN:HG2	17	0.03
(1,130)	1:A:5:SER:HB2	1:A:6:ASP:H	19	0.03
(1,1282)	1:B:8:LYS:HB2	1:B:9:ALA:H	1	0.03
(1,1282)	1:B:8:LYS:HB3	1:B:9:ALA:H	1	0.03
(1,1282)	1:B:8:LYS:HB2	1:B:9:ALA:H	17	0.03
(1,1282)	1:B:8:LYS:HB3	1:B:9:ALA:H	17	0.03
(1,1234)	1:A:97:ALA:HB1	1:A:101:LEU:HD21	6	0.03
(1,1234)	1:A:97:ALA:HB1	1:A:101:LEU:HD22	6	0.03
(1,1234)	1:A:97:ALA:HB1	1:A:101:LEU:HD23	6	0.03
(1,1234)	1:A:97:ALA:HB2	1:A:101:LEU:HD21	6	0.03
(1,1234)	1:A:97:ALA:HB2	1:A:101:LEU:HD22	6	0.03
(1,1234)	1:A:97:ALA:HB2	1:A:101:LEU:HD23	6	0.03
(1,1234)	1:A:97:ALA:HB3	1:A:101:LEU:HD21	6	0.03
(1,1234)	1:A:97:ALA:HB3	1:A:101:LEU:HD22	6	0.03
(1,1234)	1:A:97:ALA:HB3	1:A:101:LEU:HD23	6	0.03
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD11	19	0.03
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD12	19	0.03
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD13	19	0.03
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD11	19	0.03
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD12	19	0.03
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD13	19	0.03
(1,1220)	1:A:96:VAL:HA	1:A:100:HIS:HD2	14	0.03
(1,120)	1:B:88:ARG:HB2	1:A:92:LEU:HD11	15	0.03
(1,120)	1:B:88:ARG:HB2	1:A:92:LEU:HD12	15	0.03

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,120)	1:B:88:ARG:HB2	1:A:92:LEU:HD13	15	0.03
(1,1183)	1:A:93:VAL:HG11	1:A:94:GLN:H	1	0.03
(1,1183)	1:A:93:VAL:HG12	1:A:94:GLN:H	1	0.03
(1,1183)	1:A:93:VAL:HG13	1:A:94:GLN:H	1	0.03
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG11	5	0.03
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG12	5	0.03
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG13	5	0.03
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG11	5	0.03
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG12	5	0.03
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG13	5	0.03
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG11	18	0.03
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG12	18	0.03
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG13	18	0.03
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG11	18	0.03
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG12	18	0.03
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG13	18	0.03
(1,114)	1:B:20:LYS:HB2	1:A:23:ALA:HB1	4	0.03
(1,114)	1:B:20:LYS:HB2	1:A:23:ALA:HB2	4	0.03
(1,114)	1:B:20:LYS:HB2	1:A:23:ALA:HB3	4	0.03
(1,114)	1:B:20:LYS:HB3	1:A:23:ALA:HB1	4	0.03
(1,114)	1:B:20:LYS:HB3	1:A:23:ALA:HB2	4	0.03
(1,114)	1:B:20:LYS:HB3	1:A:23:ALA:HB3	4	0.03
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD21	7	0.03
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD22	7	0.03
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD23	7	0.03
(1,11)	1:A:12:LEU:HD11	1:B:32:ASP:HB2	17	0.03
(1,11)	1:A:12:LEU:HD11	1:B:32:ASP:HB3	17	0.03
(1,11)	1:A:12:LEU:HD12	1:B:32:ASP:HB2	17	0.03
(1,11)	1:A:12:LEU:HD12	1:B:32:ASP:HB3	17	0.03
(1,11)	1:A:12:LEU:HD13	1:B:32:ASP:HB2	17	0.03
(1,11)	1:A:12:LEU:HD13	1:B:32:ASP:HB3	17	0.03
(1,1046)	1:A:80:ARG:H	1:A:80:ARG:HD2	19	0.03
(1,1046)	1:A:80:ARG:H	1:A:80:ARG:HD3	19	0.03
(1,1019)	1:A:76:ARG:HD2	1:A:77:GLN:H	10	0.03
(1,1019)	1:A:76:ARG:HD3	1:A:77:GLN:H	10	0.03
(1,1019)	1:A:76:ARG:HD2	1:A:77:GLN:H	20	0.03
(1,1019)	1:A:76:ARG:HD3	1:A:77:GLN:H	20	0.03
(1,100)	1:B:15:VAL:HG11	1:A:94:GLN:HA	13	0.03
(1,100)	1:B:15:VAL:HG12	1:A:94:GLN:HA	13	0.03
(1,100)	1:B:15:VAL:HG13	1:A:94:GLN:HA	13	0.03
(1,968)	1:A:71:ARG:HB2	1:A:72:ARG:H	2	0.02
(1,968)	1:A:71:ARG:HB2	1:A:72:ARG:H	12	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,968)	1:A:71:ARG:HB2	1:A:72:ARG:H	20	0.02
(1,958)	1:A:70:ALA:HB1	1:A:77:GLN:HE21	16	0.02
(1,958)	1:A:70:ALA:HB2	1:A:77:GLN:HE21	16	0.02
(1,958)	1:A:70:ALA:HB3	1:A:77:GLN:HE21	16	0.02
(1,943)	1:A:69:GLU:HG3	1:A:82:ALA:HA	5	0.02
(1,899)	1:A:67:LEU:HD11	1:A:86:VAL:HA	12	0.02
(1,899)	1:A:67:LEU:HD12	1:A:86:VAL:HA	12	0.02
(1,899)	1:A:67:LEU:HD13	1:A:86:VAL:HA	12	0.02
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG21	9	0.02
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG22	9	0.02
(1,892)	1:A:67:LEU:HA	1:A:86:VAL:HG23	9	0.02
(1,88)	1:B:14:GLN:HB2	1:A:101:LEU:HD11	8	0.02
(1,88)	1:B:14:GLN:HB2	1:A:101:LEU:HD12	8	0.02
(1,88)	1:B:14:GLN:HB2	1:A:101:LEU:HD13	8	0.02
(1,88)	1:B:14:GLN:HB3	1:A:101:LEU:HD11	8	0.02
(1,88)	1:B:14:GLN:HB3	1:A:101:LEU:HD12	8	0.02
(1,88)	1:B:14:GLN:HB3	1:A:101:LEU:HD13	8	0.02
(1,864)	1:A:63:LYS:HE2	1:A:70:ALA:HB1	12	0.02
(1,864)	1:A:63:LYS:HE2	1:A:70:ALA:HB2	12	0.02
(1,864)	1:A:63:LYS:HE2	1:A:70:ALA:HB3	12	0.02
(1,864)	1:A:63:LYS:HE3	1:A:70:ALA:HB1	12	0.02
(1,864)	1:A:63:LYS:HE3	1:A:70:ALA:HB2	12	0.02
(1,864)	1:A:63:LYS:HE3	1:A:70:ALA:HB3	12	0.02
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE2	9	0.02
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE3	9	0.02
(1,749)	1:A:53:THR:HG21	1:A:54:THR:H	3	0.02
(1,749)	1:A:53:THR:HG22	1:A:54:THR:H	3	0.02
(1,749)	1:A:53:THR:HG23	1:A:54:THR:H	3	0.02
(1,715)	1:A:50:MET:H	1:A:50:MET:HB2	16	0.02
(1,68)	1:B:12:LEU:HB2	1:A:28:LEU:HB2	7	0.02
(1,66)	1:B:11:LEU:HD11	1:A:98:ASP:HB2	18	0.02
(1,66)	1:B:11:LEU:HD12	1:A:98:ASP:HB2	18	0.02
(1,66)	1:B:11:LEU:HD13	1:A:98:ASP:HB2	18	0.02
(1,650)	1:A:44:ILE:HG21	1:A:47:ALA:HB1	17	0.02
(1,650)	1:A:44:ILE:HG21	1:A:47:ALA:HB2	17	0.02
(1,650)	1:A:44:ILE:HG21	1:A:47:ALA:HB3	17	0.02
(1,650)	1:A:44:ILE:HG22	1:A:47:ALA:HB1	17	0.02
(1,650)	1:A:44:ILE:HG22	1:A:47:ALA:HB2	17	0.02
(1,650)	1:A:44:ILE:HG22	1:A:47:ALA:HB3	17	0.02
(1,650)	1:A:44:ILE:HG23	1:A:47:ALA:HB1	17	0.02
(1,650)	1:A:44:ILE:HG23	1:A:47:ALA:HB2	17	0.02
(1,650)	1:A:44:ILE:HG23	1:A:47:ALA:HB3	17	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,645)	1:A:44:ILE:HD11	1:A:59:LEU:HD21	9	0.02
(1,645)	1:A:44:ILE:HD11	1:A:59:LEU:HD22	9	0.02
(1,645)	1:A:44:ILE:HD11	1:A:59:LEU:HD23	9	0.02
(1,645)	1:A:44:ILE:HD12	1:A:59:LEU:HD21	9	0.02
(1,645)	1:A:44:ILE:HD12	1:A:59:LEU:HD22	9	0.02
(1,645)	1:A:44:ILE:HD12	1:A:59:LEU:HD23	9	0.02
(1,645)	1:A:44:ILE:HD13	1:A:59:LEU:HD21	9	0.02
(1,645)	1:A:44:ILE:HD13	1:A:59:LEU:HD22	9	0.02
(1,645)	1:A:44:ILE:HD13	1:A:59:LEU:HD23	9	0.02
(1,618)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	9	0.02
(1,618)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	9	0.02
(1,618)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	9	0.02
(1,618)	1:A:42:GLU:HG2	1:A:52:LEU:HD11	17	0.02
(1,618)	1:A:42:GLU:HG2	1:A:52:LEU:HD12	17	0.02
(1,618)	1:A:42:GLU:HG2	1:A:52:LEU:HD13	17	0.02
(1,616)	1:A:42:GLU:HG3	1:A:52:LEU:HD11	1	0.02
(1,616)	1:A:42:GLU:HG3	1:A:52:LEU:HD12	1	0.02
(1,616)	1:A:42:GLU:HG3	1:A:52:LEU:HD13	1	0.02
(1,616)	1:A:42:GLU:HG3	1:A:52:LEU:HD11	5	0.02
(1,616)	1:A:42:GLU:HG3	1:A:52:LEU:HD12	5	0.02
(1,616)	1:A:42:GLU:HG3	1:A:52:LEU:HD13	5	0.02
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD11	4	0.02
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD12	4	0.02
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD13	4	0.02
(1,592)	1:A:41:VAL:HG21	1:A:59:LEU:HD21	20	0.02
(1,592)	1:A:41:VAL:HG21	1:A:59:LEU:HD22	20	0.02
(1,592)	1:A:41:VAL:HG21	1:A:59:LEU:HD23	20	0.02
(1,592)	1:A:41:VAL:HG22	1:A:59:LEU:HD21	20	0.02
(1,592)	1:A:41:VAL:HG22	1:A:59:LEU:HD22	20	0.02
(1,592)	1:A:41:VAL:HG22	1:A:59:LEU:HD23	20	0.02
(1,592)	1:A:41:VAL:HG23	1:A:59:LEU:HD21	20	0.02
(1,592)	1:A:41:VAL:HG23	1:A:59:LEU:HD22	20	0.02
(1,592)	1:A:41:VAL:HG23	1:A:59:LEU:HD23	20	0.02
(1,528)	1:A:38:GLU:H	1:A:38:GLU:HG2	1	0.02
(1,528)	1:A:38:GLU:H	1:A:38:GLU:HG3	1	0.02
(1,528)	1:A:38:GLU:H	1:A:38:GLU:HG2	5	0.02
(1,528)	1:A:38:GLU:H	1:A:38:GLU:HG3	5	0.02
(1,511)	1:A:36:GLN:HB2	1:A:37:GLY:H	14	0.02
(1,476)	1:A:33:LEU:HG	1:A:39:ARG:HE	3	0.02
(1,460)	1:A:33:LEU:HB2	1:A:34:LEU:H	13	0.02
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	11	0.02
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	11	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	11	0.02
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	11	0.02
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	11	0.02
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	11	0.02
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	15	0.02
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	15	0.02
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	15	0.02
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	15	0.02
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	15	0.02
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	15	0.02
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD1	20	0.02
(1,439)	1:A:31:LEU:HD21	1:A:90:PHE:HD2	20	0.02
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD1	20	0.02
(1,439)	1:A:31:LEU:HD22	1:A:90:PHE:HD2	20	0.02
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD1	20	0.02
(1,439)	1:A:31:LEU:HD23	1:A:90:PHE:HD2	20	0.02
(1,438)	1:A:31:LEU:HD21	1:A:86:VAL:HG11	17	0.02
(1,438)	1:A:31:LEU:HD21	1:A:86:VAL:HG12	17	0.02
(1,438)	1:A:31:LEU:HD21	1:A:86:VAL:HG13	17	0.02
(1,438)	1:A:31:LEU:HD22	1:A:86:VAL:HG11	17	0.02
(1,438)	1:A:31:LEU:HD22	1:A:86:VAL:HG12	17	0.02
(1,438)	1:A:31:LEU:HD22	1:A:86:VAL:HG13	17	0.02
(1,438)	1:A:31:LEU:HD23	1:A:86:VAL:HG11	17	0.02
(1,438)	1:A:31:LEU:HD23	1:A:86:VAL:HG12	17	0.02
(1,438)	1:A:31:LEU:HD23	1:A:86:VAL:HG13	17	0.02
(1,435)	1:A:31:LEU:HD21	1:A:81:ILE:HD11	16	0.02
(1,435)	1:A:31:LEU:HD21	1:A:81:ILE:HD12	16	0.02
(1,435)	1:A:31:LEU:HD21	1:A:81:ILE:HD13	16	0.02
(1,435)	1:A:31:LEU:HD22	1:A:81:ILE:HD11	16	0.02
(1,435)	1:A:31:LEU:HD22	1:A:81:ILE:HD12	16	0.02
(1,435)	1:A:31:LEU:HD22	1:A:81:ILE:HD13	16	0.02
(1,435)	1:A:31:LEU:HD23	1:A:81:ILE:HD11	16	0.02
(1,435)	1:A:31:LEU:HD23	1:A:81:ILE:HD12	16	0.02
(1,435)	1:A:31:LEU:HD23	1:A:81:ILE:HD13	16	0.02
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD21	5	0.02
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD22	5	0.02
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD23	5	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD21	5	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD22	5	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD23	5	0.02
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD21	5	0.02
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD22	5	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD23	5	0.02
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD21	8	0.02
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD22	8	0.02
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD23	8	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD21	8	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD22	8	0.02
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD23	8	0.02
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD21	8	0.02
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD22	8	0.02
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD23	8	0.02
(1,381)	1:A:30:ILE:HD11	1:A:59:LEU:HA	3	0.02
(1,381)	1:A:30:ILE:HD12	1:A:59:LEU:HA	3	0.02
(1,381)	1:A:30:ILE:HD13	1:A:59:LEU:HA	3	0.02
(1,338)	1:A:28:LEU:HD11	1:A:90:PHE:HE1	8	0.02
(1,338)	1:A:28:LEU:HD12	1:A:90:PHE:HE1	8	0.02
(1,338)	1:A:28:LEU:HD13	1:A:90:PHE:HE1	8	0.02
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD1	2	0.02
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD2	2	0.02
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD1	2	0.02
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD2	2	0.02
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD1	2	0.02
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD2	2	0.02
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD1	5	0.02
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD2	5	0.02
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD1	5	0.02
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD2	5	0.02
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD1	5	0.02
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD2	5	0.02
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD1	14	0.02
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD2	14	0.02
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD1	14	0.02
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD2	14	0.02
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD1	14	0.02
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD2	14	0.02
(1,314)	1:A:25:GLY:HA3	1:A:28:LEU:HD11	2	0.02
(1,314)	1:A:25:GLY:HA3	1:A:28:LEU:HD12	2	0.02
(1,314)	1:A:25:GLY:HA3	1:A:28:LEU:HD13	2	0.02
(1,30)	1:A:14:GLN:HG2	1:B:97:ALA:HA	8	0.02
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD21	17	0.02
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD22	17	0.02
(1,299)	1:A:22:LEU:HD21	1:A:28:LEU:HD23	17	0.02
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD21	17	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD22	17	0.02
(1,299)	1:A:22:LEU:HD22	1:A:28:LEU:HD23	17	0.02
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD21	17	0.02
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD22	17	0.02
(1,299)	1:A:22:LEU:HD23	1:A:28:LEU:HD23	17	0.02
(1,296)	1:A:22:LEU:HD11	1:A:93:VAL:HG11	4	0.02
(1,296)	1:A:22:LEU:HD11	1:A:93:VAL:HG12	4	0.02
(1,296)	1:A:22:LEU:HD11	1:A:93:VAL:HG13	4	0.02
(1,296)	1:A:22:LEU:HD12	1:A:93:VAL:HG11	4	0.02
(1,296)	1:A:22:LEU:HD12	1:A:93:VAL:HG12	4	0.02
(1,296)	1:A:22:LEU:HD12	1:A:93:VAL:HG13	4	0.02
(1,296)	1:A:22:LEU:HD13	1:A:93:VAL:HG11	4	0.02
(1,296)	1:A:22:LEU:HD13	1:A:93:VAL:HG12	4	0.02
(1,296)	1:A:22:LEU:HD13	1:A:93:VAL:HG13	4	0.02
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	1	0.02
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	1	0.02
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	1	0.02
(1,270)	1:A:20:LYS:H	1:A:20:LYS:HD2	16	0.02
(1,270)	1:A:20:LYS:H	1:A:20:LYS:HD3	16	0.02
(1,2617)	1:B:99:GLU:H	1:B:95:VAL:O	4	0.02
(1,2613)	1:B:97:ALA:H	1:B:93:VAL:O	16	0.02
(1,2607)	1:B:94:GLN:H	1:B:90:PHE:O	12	0.02
(1,2601)	1:B:91:ALA:H	1:B:87:ALA:O	12	0.02
(1,2601)	1:B:91:ALA:H	1:B:87:ALA:O	14	0.02
(1,2593)	1:B:87:ALA:H	1:B:83:GLY:O	15	0.02
(1,2589)	1:B:80:ARG:H	1:B:69:GLU:O	3	0.02
(1,2585)	1:B:78:TYR:H	1:B:71:ARG:O	9	0.02
(1,2585)	1:B:78:TYR:H	1:B:71:ARG:O	19	0.02
(1,2581)	1:B:73:GLU:H	1:B:76:ARG:O	11	0.02
(1,2581)	1:B:73:GLU:H	1:B:76:ARG:O	15	0.02
(1,2579)	1:B:71:ARG:H	1:B:78:TYR:O	8	0.02
(1,2575)	1:B:67:LEU:H	1:B:62:LEU:O	3	0.02
(1,2573)	1:B:66:GLY:H	1:B:63:LYS:O	8	0.02
(1,2573)	1:B:66:GLY:H	1:B:63:LYS:O	12	0.02
(1,2573)	1:B:66:GLY:H	1:B:63:LYS:O	14	0.02
(1,2571)	1:B:65:GLY:H	1:B:61:ALA:O	18	0.02
(1,2563)	1:B:61:ALA:H	1:B:57:ALA:O	6	0.02
(1,2563)	1:B:61:ALA:H	1:B:57:ALA:O	13	0.02
(1,2563)	1:B:61:ALA:H	1:B:57:ALA:O	17	0.02
(1,2563)	1:B:61:ALA:H	1:B:57:ALA:O	20	0.02
(1,2561)	1:B:60:GLN:H	1:B:56:SER:O	12	0.02
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	3	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	5	0.02
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	7	0.02
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	9	0.02
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	16	0.02
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	17	0.02
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	19	0.02
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	20	0.02
(1,2535)	1:B:41:VAL:H	1:B:77:GLN:O	11	0.02
(1,2535)	1:B:41:VAL:H	1:B:77:GLN:O	16	0.02
(1,2533)	1:B:39:ARG:H	1:B:79:TYR:O	1	0.02
(1,2533)	1:B:39:ARG:H	1:B:79:TYR:O	2	0.02
(1,2533)	1:B:39:ARG:H	1:B:79:TYR:O	9	0.02
(1,2527)	1:B:33:LEU:H	1:B:29:GLN:O	15	0.02
(1,2525)	1:B:32:ASP:H	1:B:28:LEU:O	17	0.02
(1,2523)	1:B:22:LEU:H	1:B:18:VAL:O	8	0.02
(1,2523)	1:B:22:LEU:H	1:B:18:VAL:O	12	0.02
(1,2521)	1:B:21:ALA:H	1:B:17:ARG:O	11	0.02
(1,2521)	1:B:21:ALA:H	1:B:17:ARG:O	15	0.02
(1,2516)	1:B:18:VAL:N	1:B:14:GLN:O	4	0.02
(1,2515)	1:B:18:VAL:H	1:B:14:GLN:O	11	0.02
(1,2515)	1:B:18:VAL:H	1:B:14:GLN:O	12	0.02
(1,2513)	1:B:17:ARG:H	1:B:13:ASP:O	4	0.02
(1,2513)	1:B:17:ARG:H	1:B:13:ASP:O	18	0.02
(1,2511)	1:B:16:ALA:H	1:B:12:LEU:O	7	0.02
(1,2511)	1:B:16:ALA:H	1:B:12:LEU:O	14	0.02
(1,2507)	1:B:14:GLN:H	1:B:10:ALA:O	19	0.02
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	8	0.02
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	10	0.02
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	16	0.02
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	17	0.02
(1,2505)	1:B:11:LEU:H	1:B:8:LYS:O	19	0.02
(1,2499)	1:A:97:ALA:H	1:A:93:VAL:O	13	0.02
(1,2493)	1:A:94:GLN:H	1:A:90:PHE:O	4	0.02
(1,2493)	1:A:94:GLN:H	1:A:90:PHE:O	5	0.02
(1,2483)	1:A:89:LEU:H	1:A:85:ASP:O	5	0.02
(1,2479)	1:A:87:ALA:H	1:A:83:GLY:O	4	0.02
(1,2475)	1:A:80:ARG:H	1:A:69:GLU:O	2	0.02
(1,2469)	1:A:76:ARG:H	1:A:73:GLU:O	2	0.02
(1,2469)	1:A:76:ARG:H	1:A:73:GLU:O	7	0.02
(1,2465)	1:A:71:ARG:H	1:A:78:TYR:O	12	0.02
(1,2461)	1:A:67:LEU:H	1:A:62:LEU:O	14	0.02
(1,2459)	1:A:66:GLY:H	1:A:63:LYS:O	10	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2459)	1:A:66:GLY:H	1:A:63:LYS:O	12	0.02
(1,2457)	1:A:65:GLY:H	1:A:61:ALA:O	4	0.02
(1,2449)	1:A:61:ALA:H	1:A:57:ALA:O	5	0.02
(1,2449)	1:A:61:ALA:H	1:A:57:ALA:O	11	0.02
(1,2443)	1:A:58:ASN:H	1:A:54:THR:O	17	0.02
(1,2441)	1:A:57:ALA:H	1:A:53:THR:O	1	0.02
(1,2441)	1:A:57:ALA:H	1:A:53:THR:O	11	0.02
(1,2441)	1:A:57:ALA:H	1:A:53:THR:O	15	0.02
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	4	0.02
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	5	0.02
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	9	0.02
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	10	0.02
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	12	0.02
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	14	0.02
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	15	0.02
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	18	0.02
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	19	0.02
(1,2421)	1:A:41:VAL:H	1:A:77:GLN:O	3	0.02
(1,2421)	1:A:41:VAL:H	1:A:77:GLN:O	11	0.02
(1,2421)	1:A:41:VAL:H	1:A:77:GLN:O	18	0.02
(1,2421)	1:A:41:VAL:H	1:A:77:GLN:O	20	0.02
(1,2419)	1:A:39:ARG:H	1:A:79:TYR:O	1	0.02
(1,2419)	1:A:39:ARG:H	1:A:79:TYR:O	6	0.02
(1,2417)	1:A:35:ALA:H	1:A:31:LEU:O	2	0.02
(1,2417)	1:A:35:ALA:H	1:A:31:LEU:O	8	0.02
(1,2413)	1:A:33:LEU:H	1:A:29:GLN:O	11	0.02
(1,2411)	1:A:32:ASP:H	1:A:28:LEU:O	2	0.02
(1,2407)	1:A:21:ALA:H	1:A:17:ARG:O	1	0.02
(1,2407)	1:A:21:ALA:H	1:A:17:ARG:O	8	0.02
(1,2403)	1:A:19:GLY:H	1:A:15:VAL:O	16	0.02
(1,2401)	1:A:18:VAL:H	1:A:14:GLN:O	9	0.02
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB1	18	0.02
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB2	18	0.02
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB3	18	0.02
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB1	18	0.02
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB2	18	0.02
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB3	18	0.02
(1,2393)	1:A:14:GLN:H	1:A:10:ALA:O	3	0.02
(1,2393)	1:A:14:GLN:H	1:A:10:ALA:O	6	0.02
(1,2393)	1:A:14:GLN:H	1:A:10:ALA:O	8	0.02
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	1	0.02
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	5	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	9	0.02
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	11	0.02
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	20	0.02
(1,2390)	1:B:107:HIS:HB2	1:B:108:HIS:H	1	0.02
(1,2389)	1:B:102:GLU:H	1:B:102:GLU:HG2	7	0.02
(1,2389)	1:B:102:GLU:H	1:B:102:GLU:HG3	7	0.02
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB2	6	0.02
(1,235)	1:A:17:ARG:HD2	1:A:64:SER:HB3	6	0.02
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB2	6	0.02
(1,235)	1:A:17:ARG:HD3	1:A:64:SER:HB3	6	0.02
(1,231)	1:A:17:ARG:H	1:A:17:ARG:HG2	19	0.02
(1,2291)	1:B:90:PHE:HD1	1:B:93:VAL:HG11	7	0.02
(1,2291)	1:B:90:PHE:HD1	1:B:93:VAL:HG12	7	0.02
(1,2291)	1:B:90:PHE:HD1	1:B:93:VAL:HG13	7	0.02
(1,2291)	1:B:90:PHE:HD2	1:B:93:VAL:HG11	7	0.02
(1,2291)	1:B:90:PHE:HD2	1:B:93:VAL:HG12	7	0.02
(1,2291)	1:B:90:PHE:HD2	1:B:93:VAL:HG13	7	0.02
(1,229)	1:A:17:ARG:HA	1:A:65:GLY:HA2	18	0.02
(1,2276)	1:B:89:LEU:HD21	1:B:93:VAL:HB	17	0.02
(1,2276)	1:B:89:LEU:HD22	1:B:93:VAL:HB	17	0.02
(1,2276)	1:B:89:LEU:HD23	1:B:93:VAL:HB	17	0.02
(1,2225)	1:B:84:GLU:HG2	1:B:88:ARG:HD2	5	0.02
(1,2225)	1:B:84:GLU:HG2	1:B:88:ARG:HD3	5	0.02
(1,2225)	1:B:84:GLU:HG3	1:B:88:ARG:HD2	5	0.02
(1,2225)	1:B:84:GLU:HG3	1:B:88:ARG:HD3	5	0.02
(1,2201)	1:B:81:ILE:HG21	1:B:87:ALA:HB1	7	0.02
(1,2201)	1:B:81:ILE:HG21	1:B:87:ALA:HB2	7	0.02
(1,2201)	1:B:81:ILE:HG21	1:B:87:ALA:HB3	7	0.02
(1,2201)	1:B:81:ILE:HG22	1:B:87:ALA:HB1	7	0.02
(1,2201)	1:B:81:ILE:HG22	1:B:87:ALA:HB2	7	0.02
(1,2201)	1:B:81:ILE:HG22	1:B:87:ALA:HB3	7	0.02
(1,2201)	1:B:81:ILE:HG23	1:B:87:ALA:HB1	7	0.02
(1,2201)	1:B:81:ILE:HG23	1:B:87:ALA:HB2	7	0.02
(1,2201)	1:B:81:ILE:HG23	1:B:87:ALA:HB3	7	0.02
(1,2184)	1:B:81:ILE:HD11	1:B:82:ALA:H	11	0.02
(1,2184)	1:B:81:ILE:HD12	1:B:82:ALA:H	11	0.02
(1,2184)	1:B:81:ILE:HD13	1:B:82:ALA:H	11	0.02
(1,2184)	1:B:81:ILE:HD11	1:B:82:ALA:H	15	0.02
(1,2184)	1:B:81:ILE:HD12	1:B:82:ALA:H	15	0.02
(1,2184)	1:B:81:ILE:HD13	1:B:82:ALA:H	15	0.02
(1,2152)	1:B:76:ARG:HD2	1:B:78:TYR:HE1	9	0.02
(1,2152)	1:B:76:ARG:HD3	1:B:78:TYR:HE1	9	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2152)	1:B:76:ARG:HD2	1:B:78:TYR:HE1	10	0.02
(1,2152)	1:B:76:ARG:HD3	1:B:78:TYR:HE1	10	0.02
(1,2151)	1:B:76:ARG:HD2	1:B:77:GLN:H	6	0.02
(1,2151)	1:B:76:ARG:HD3	1:B:77:GLN:H	6	0.02
(1,2151)	1:B:76:ARG:HD2	1:B:77:GLN:H	16	0.02
(1,2151)	1:B:76:ARG:HD3	1:B:77:GLN:H	16	0.02
(1,2151)	1:B:76:ARG:HD2	1:B:77:GLN:H	20	0.02
(1,2151)	1:B:76:ARG:HD3	1:B:77:GLN:H	20	0.02
(1,2135)	1:B:74:GLY:HA2	1:B:76:ARG:H	16	0.02
(1,2100)	1:B:71:ARG:HB2	1:B:72:ARG:H	9	0.02
(1,2100)	1:B:71:ARG:HB2	1:B:72:ARG:H	15	0.02
(1,210)	1:A:15:VAL:HA	1:A:18:VAL:HB	10	0.02
(1,2099)	1:B:71:ARG:HB2	1:B:71:ARG:HE	4	0.02
(1,2091)	1:B:70:ALA:HB1	1:B:77:GLN:HE22	11	0.02
(1,2091)	1:B:70:ALA:HB2	1:B:77:GLN:HE22	11	0.02
(1,2091)	1:B:70:ALA:HB3	1:B:77:GLN:HE22	11	0.02
(1,2078)	1:B:69:GLU:HG2	1:B:82:ALA:HB1	10	0.02
(1,2078)	1:B:69:GLU:HG2	1:B:82:ALA:HB2	10	0.02
(1,2078)	1:B:69:GLU:HG2	1:B:82:ALA:HB3	10	0.02
(1,203)	1:A:14:GLN:HB2	1:A:14:GLN:HE21	9	0.02
(1,203)	1:A:14:GLN:HB3	1:A:14:GLN:HE21	9	0.02
(1,2029)	1:B:67:LEU:HB2	1:B:68:VAL:HG21	6	0.02
(1,2029)	1:B:67:LEU:HB2	1:B:68:VAL:HG22	6	0.02
(1,2029)	1:B:67:LEU:HB2	1:B:68:VAL:HG23	6	0.02
(1,2029)	1:B:67:LEU:HB3	1:B:68:VAL:HG21	6	0.02
(1,2029)	1:B:67:LEU:HB3	1:B:68:VAL:HG22	6	0.02
(1,2029)	1:B:67:LEU:HB3	1:B:68:VAL:HG23	6	0.02
(1,2024)	1:B:67:LEU:HA	1:B:86:VAL:HG21	3	0.02
(1,2024)	1:B:67:LEU:HA	1:B:86:VAL:HG22	3	0.02
(1,2024)	1:B:67:LEU:HA	1:B:86:VAL:HG23	3	0.02
(1,2024)	1:B:67:LEU:HA	1:B:86:VAL:HG21	16	0.02
(1,2024)	1:B:67:LEU:HA	1:B:86:VAL:HG22	16	0.02
(1,2024)	1:B:67:LEU:HA	1:B:86:VAL:HG23	16	0.02
(1,2024)	1:B:67:LEU:HA	1:B:86:VAL:HG21	19	0.02
(1,2024)	1:B:67:LEU:HA	1:B:86:VAL:HG22	19	0.02
(1,2024)	1:B:67:LEU:HA	1:B:86:VAL:HG23	19	0.02
(1,1997)	1:B:63:LYS:HE2	1:B:70:ALA:H	8	0.02
(1,1997)	1:B:63:LYS:HE3	1:B:70:ALA:H	8	0.02
(1,1996)	1:B:63:LYS:HE2	1:B:70:ALA:HB1	2	0.02
(1,1996)	1:B:63:LYS:HE2	1:B:70:ALA:HB2	2	0.02
(1,1996)	1:B:63:LYS:HE2	1:B:70:ALA:HB3	2	0.02
(1,1996)	1:B:63:LYS:HE3	1:B:70:ALA:HB1	2	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1996)	1:B:63:LYS:HE3	1:B:70:ALA:HB2	2	0.02
(1,1996)	1:B:63:LYS:HE3	1:B:70:ALA:HB3	2	0.02
(1,1996)	1:B:63:LYS:HE2	1:B:70:ALA:HB1	15	0.02
(1,1996)	1:B:63:LYS:HE2	1:B:70:ALA:HB2	15	0.02
(1,1996)	1:B:63:LYS:HE2	1:B:70:ALA:HB3	15	0.02
(1,1996)	1:B:63:LYS:HE3	1:B:70:ALA:HB1	15	0.02
(1,1996)	1:B:63:LYS:HE3	1:B:70:ALA:HB2	15	0.02
(1,1996)	1:B:63:LYS:HE3	1:B:70:ALA:HB3	15	0.02
(1,1956)	1:B:60:GLN:HG2	1:B:61:ALA:HA	7	0.02
(1,1956)	1:B:60:GLN:HG3	1:B:61:ALA:HA	7	0.02
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	1	0.02
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	1	0.02
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	1	0.02
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	1	0.02
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	1	0.02
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	1	0.02
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	2	0.02
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	2	0.02
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	2	0.02
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	2	0.02
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	2	0.02
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	2	0.02
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	7	0.02
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	7	0.02
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	7	0.02
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	7	0.02
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	7	0.02
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	7	0.02
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD1	19	0.02
(1,19)	1:A:12:LEU:HD21	1:B:90:PHE:HD2	19	0.02
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD1	19	0.02
(1,19)	1:A:12:LEU:HD22	1:B:90:PHE:HD2	19	0.02
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD1	19	0.02
(1,19)	1:A:12:LEU:HD23	1:B:90:PHE:HD2	19	0.02
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB1	1	0.02
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB2	1	0.02
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB3	1	0.02
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB1	1	0.02
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB2	1	0.02
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB3	1	0.02
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB1	1	0.02
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB2	1	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB3	1	0.02
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB1	5	0.02
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB2	5	0.02
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB3	5	0.02
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB1	5	0.02
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB2	5	0.02
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB3	5	0.02
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB1	5	0.02
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB2	5	0.02
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB3	5	0.02
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB1	16	0.02
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB2	16	0.02
(1,1872)	1:B:52:LEU:HD11	1:B:55:ALA:HB3	16	0.02
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB1	16	0.02
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB2	16	0.02
(1,1872)	1:B:52:LEU:HD12	1:B:55:ALA:HB3	16	0.02
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB1	16	0.02
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB2	16	0.02
(1,1872)	1:B:52:LEU:HD13	1:B:55:ALA:HB3	16	0.02
(1,1854)	1:B:51:ASN:HB2	1:B:53:THR:H	10	0.02
(1,1849)	1:B:50:MET:H	1:B:50:MET:HG2	11	0.02
(1,1849)	1:B:50:MET:H	1:B:50:MET:HG2	12	0.02
(1,1847)	1:B:50:MET:H	1:B:50:MET:HB2	5	0.02
(1,1847)	1:B:50:MET:H	1:B:50:MET:HB2	9	0.02
(1,1823)	1:B:48:THR:HB	1:B:50:MET:HG2	4	0.02
(1,1782)	1:B:44:ILE:HG21	1:B:47:ALA:HB1	7	0.02
(1,1782)	1:B:44:ILE:HG21	1:B:47:ALA:HB2	7	0.02
(1,1782)	1:B:44:ILE:HG21	1:B:47:ALA:HB3	7	0.02
(1,1782)	1:B:44:ILE:HG22	1:B:47:ALA:HB1	7	0.02
(1,1782)	1:B:44:ILE:HG22	1:B:47:ALA:HB2	7	0.02
(1,1782)	1:B:44:ILE:HG22	1:B:47:ALA:HB3	7	0.02
(1,1782)	1:B:44:ILE:HG23	1:B:47:ALA:HB1	7	0.02
(1,1782)	1:B:44:ILE:HG23	1:B:47:ALA:HB2	7	0.02
(1,1782)	1:B:44:ILE:HG23	1:B:47:ALA:HB3	7	0.02
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD21	7	0.02
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD22	7	0.02
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD23	7	0.02
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD21	7	0.02
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD22	7	0.02
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD23	7	0.02
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD21	7	0.02
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD22	7	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD23	7	0.02
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD21	18	0.02
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD22	18	0.02
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD23	18	0.02
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD21	18	0.02
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD22	18	0.02
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD23	18	0.02
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD21	18	0.02
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD22	18	0.02
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD23	18	0.02
(1,1690)	1:B:40:ALA:HB1	1:B:78:TYR:HD1	6	0.02
(1,1690)	1:B:40:ALA:HB2	1:B:78:TYR:HD1	6	0.02
(1,1690)	1:B:40:ALA:HB3	1:B:78:TYR:HD1	6	0.02
(1,1681)	1:B:40:ALA:HB1	1:B:42:GLU:HG2	3	0.02
(1,1681)	1:B:40:ALA:HB2	1:B:42:GLU:HG2	3	0.02
(1,1681)	1:B:40:ALA:HB3	1:B:42:GLU:HG2	3	0.02
(1,1675)	1:B:40:ALA:HA	1:B:78:TYR:HA	6	0.02
(1,1675)	1:B:40:ALA:HA	1:B:78:TYR:HA	20	0.02
(1,1660)	1:B:38:GLU:H	1:B:38:GLU:HG2	2	0.02
(1,1660)	1:B:38:GLU:H	1:B:38:GLU:HG3	2	0.02
(1,1660)	1:B:38:GLU:H	1:B:38:GLU:HG2	13	0.02
(1,1660)	1:B:38:GLU:H	1:B:38:GLU:HG3	13	0.02
(1,1625)	1:B:34:LEU:HD21	1:B:80:ARG:HA	8	0.02
(1,1625)	1:B:34:LEU:HD22	1:B:80:ARG:HA	8	0.02
(1,1625)	1:B:34:LEU:HD23	1:B:80:ARG:HA	8	0.02
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB1	12	0.02
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB2	12	0.02
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB3	12	0.02
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB1	12	0.02
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB2	12	0.02
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB3	12	0.02
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB1	12	0.02
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB2	12	0.02
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB3	12	0.02
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	4	0.02
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	4	0.02
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	4	0.02
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	5	0.02
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	5	0.02
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	5	0.02
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	5	0.02
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	5	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	5	0.02
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	6	0.02
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	6	0.02
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	6	0.02
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	6	0.02
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	6	0.02
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	6	0.02
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	9	0.02
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	9	0.02
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	9	0.02
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	9	0.02
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	9	0.02
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	9	0.02
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	11	0.02
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	11	0.02
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	11	0.02
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	11	0.02
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	11	0.02
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	11	0.02
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	16	0.02
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	16	0.02
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	16	0.02
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	16	0.02
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	16	0.02
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	16	0.02
(1,1552)	1:B:31:LEU:HD11	1:B:67:LEU:HB2	3	0.02
(1,1552)	1:B:31:LEU:HD11	1:B:67:LEU:HB3	3	0.02
(1,1552)	1:B:31:LEU:HD12	1:B:67:LEU:HB2	3	0.02
(1,1552)	1:B:31:LEU:HD12	1:B:67:LEU:HB3	3	0.02
(1,1552)	1:B:31:LEU:HD13	1:B:67:LEU:HB2	3	0.02
(1,1552)	1:B:31:LEU:HD13	1:B:67:LEU:HB3	3	0.02
(1,1541)	1:B:31:LEU:HA	1:B:81:ILE:HD11	20	0.02
(1,1541)	1:B:31:LEU:HA	1:B:81:ILE:HD12	20	0.02
(1,1541)	1:B:31:LEU:HA	1:B:81:ILE:HD13	20	0.02
(1,1527)	1:B:30:ILE:HG21	1:B:59:LEU:HD21	11	0.02
(1,1527)	1:B:30:ILE:HG21	1:B:59:LEU:HD22	11	0.02
(1,1527)	1:B:30:ILE:HG21	1:B:59:LEU:HD23	11	0.02
(1,1527)	1:B:30:ILE:HG22	1:B:59:LEU:HD21	11	0.02
(1,1527)	1:B:30:ILE:HG22	1:B:59:LEU:HD22	11	0.02
(1,1527)	1:B:30:ILE:HG22	1:B:59:LEU:HD23	11	0.02
(1,1527)	1:B:30:ILE:HG23	1:B:59:LEU:HD21	11	0.02
(1,1527)	1:B:30:ILE:HG23	1:B:59:LEU:HD22	11	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1527)	1:B:30:ILE:HG23	1:B:59:LEU:HD23	11	0.02
(1,1527)	1:B:30:ILE:HG21	1:B:59:LEU:HD21	12	0.02
(1,1527)	1:B:30:ILE:HG21	1:B:59:LEU:HD22	12	0.02
(1,1527)	1:B:30:ILE:HG21	1:B:59:LEU:HD23	12	0.02
(1,1527)	1:B:30:ILE:HG22	1:B:59:LEU:HD21	12	0.02
(1,1527)	1:B:30:ILE:HG22	1:B:59:LEU:HD22	12	0.02
(1,1527)	1:B:30:ILE:HG22	1:B:59:LEU:HD23	12	0.02
(1,1527)	1:B:30:ILE:HG23	1:B:59:LEU:HD21	12	0.02
(1,1527)	1:B:30:ILE:HG23	1:B:59:LEU:HD22	12	0.02
(1,1527)	1:B:30:ILE:HG23	1:B:59:LEU:HD23	12	0.02
(1,1527)	1:B:30:ILE:HG21	1:B:59:LEU:HD21	19	0.02
(1,1527)	1:B:30:ILE:HG21	1:B:59:LEU:HD22	19	0.02
(1,1527)	1:B:30:ILE:HG21	1:B:59:LEU:HD23	19	0.02
(1,1527)	1:B:30:ILE:HG22	1:B:59:LEU:HD21	19	0.02
(1,1527)	1:B:30:ILE:HG22	1:B:59:LEU:HD22	19	0.02
(1,1527)	1:B:30:ILE:HG22	1:B:59:LEU:HD23	19	0.02
(1,1527)	1:B:30:ILE:HG23	1:B:59:LEU:HD21	19	0.02
(1,1527)	1:B:30:ILE:HG23	1:B:59:LEU:HD22	19	0.02
(1,1527)	1:B:30:ILE:HG23	1:B:59:LEU:HD23	19	0.02
(1,1512)	1:B:30:ILE:HD11	1:B:58:ASN:H	18	0.02
(1,1512)	1:B:30:ILE:HD12	1:B:58:ASN:H	18	0.02
(1,1512)	1:B:30:ILE:HD13	1:B:58:ASN:H	18	0.02
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD11	3	0.02
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD12	3	0.02
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD13	3	0.02
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD11	3	0.02
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD12	3	0.02
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD13	3	0.02
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD11	14	0.02
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD12	14	0.02
(1,151)	1:A:8:LYS:HE2	1:A:12:LEU:HD13	14	0.02
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD11	14	0.02
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD12	14	0.02
(1,151)	1:A:8:LYS:HE3	1:A:12:LEU:HD13	14	0.02
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	3	0.02
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	3	0.02
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	3	0.02
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	3	0.02
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	3	0.02
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	3	0.02
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	4	0.02
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	4	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	4	0.02
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	4	0.02
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	4	0.02
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	4	0.02
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	11	0.02
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	11	0.02
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	11	0.02
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	11	0.02
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	11	0.02
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	11	0.02
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	20	0.02
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	20	0.02
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	20	0.02
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	20	0.02
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	20	0.02
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	20	0.02
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB1	5	0.02
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB2	5	0.02
(1,1461)	1:B:27:ARG:HD2	1:B:61:ALA:HB3	5	0.02
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD2	4	0.02
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD3	4	0.02
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD11	8	0.02
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD12	8	0.02
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD13	8	0.02
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD11	17	0.02
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD12	17	0.02
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD13	17	0.02
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD11	18	0.02
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD12	18	0.02
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD13	18	0.02
(1,144)	1:A:7:ARG:H	1:A:7:ARG:HG2	20	0.02
(1,1431)	1:B:22:LEU:HD21	1:B:28:LEU:HD21	19	0.02
(1,1431)	1:B:22:LEU:HD21	1:B:28:LEU:HD22	19	0.02
(1,1431)	1:B:22:LEU:HD21	1:B:28:LEU:HD23	19	0.02
(1,1431)	1:B:22:LEU:HD22	1:B:28:LEU:HD21	19	0.02
(1,1431)	1:B:22:LEU:HD22	1:B:28:LEU:HD22	19	0.02
(1,1431)	1:B:22:LEU:HD22	1:B:28:LEU:HD23	19	0.02
(1,1431)	1:B:22:LEU:HD23	1:B:28:LEU:HD21	19	0.02
(1,1431)	1:B:22:LEU:HD23	1:B:28:LEU:HD22	19	0.02
(1,1431)	1:B:22:LEU:HD23	1:B:28:LEU:HD23	19	0.02
(1,1428)	1:B:22:LEU:HD11	1:B:93:VAL:HG11	4	0.02
(1,1428)	1:B:22:LEU:HD11	1:B:93:VAL:HG12	4	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1428)	1:B:22:LEU:HD11	1:B:93:VAL:HG13	4	0.02
(1,1428)	1:B:22:LEU:HD12	1:B:93:VAL:HG11	4	0.02
(1,1428)	1:B:22:LEU:HD12	1:B:93:VAL:HG12	4	0.02
(1,1428)	1:B:22:LEU:HD12	1:B:93:VAL:HG13	4	0.02
(1,1428)	1:B:22:LEU:HD13	1:B:93:VAL:HG11	4	0.02
(1,1428)	1:B:22:LEU:HD13	1:B:93:VAL:HG12	4	0.02
(1,1428)	1:B:22:LEU:HD13	1:B:93:VAL:HG13	4	0.02
(1,1427)	1:B:22:LEU:HD11	1:B:93:VAL:HB	15	0.02
(1,1427)	1:B:22:LEU:HD12	1:B:93:VAL:HB	15	0.02
(1,1427)	1:B:22:LEU:HD13	1:B:93:VAL:HB	15	0.02
(1,1425)	1:B:22:LEU:HD11	1:B:89:LEU:HD21	17	0.02
(1,1425)	1:B:22:LEU:HD11	1:B:89:LEU:HD22	17	0.02
(1,1425)	1:B:22:LEU:HD11	1:B:89:LEU:HD23	17	0.02
(1,1425)	1:B:22:LEU:HD12	1:B:89:LEU:HD21	17	0.02
(1,1425)	1:B:22:LEU:HD12	1:B:89:LEU:HD22	17	0.02
(1,1425)	1:B:22:LEU:HD12	1:B:89:LEU:HD23	17	0.02
(1,1425)	1:B:22:LEU:HD13	1:B:89:LEU:HD21	17	0.02
(1,1425)	1:B:22:LEU:HD13	1:B:89:LEU:HD22	17	0.02
(1,1425)	1:B:22:LEU:HD13	1:B:89:LEU:HD23	17	0.02
(1,1425)	1:B:22:LEU:HD11	1:B:89:LEU:HD21	20	0.02
(1,1425)	1:B:22:LEU:HD11	1:B:89:LEU:HD22	20	0.02
(1,1425)	1:B:22:LEU:HD11	1:B:89:LEU:HD23	20	0.02
(1,1425)	1:B:22:LEU:HD12	1:B:89:LEU:HD21	20	0.02
(1,1425)	1:B:22:LEU:HD12	1:B:89:LEU:HD22	20	0.02
(1,1425)	1:B:22:LEU:HD12	1:B:89:LEU:HD23	20	0.02
(1,1425)	1:B:22:LEU:HD13	1:B:89:LEU:HD21	20	0.02
(1,1425)	1:B:22:LEU:HD13	1:B:89:LEU:HD22	20	0.02
(1,1425)	1:B:22:LEU:HD13	1:B:89:LEU:HD23	20	0.02
(1,1418)	1:B:22:LEU:HA	1:B:28:LEU:HD21	1	0.02
(1,1418)	1:B:22:LEU:HA	1:B:28:LEU:HD22	1	0.02
(1,1418)	1:B:22:LEU:HA	1:B:28:LEU:HD23	1	0.02
(1,14)	1:A:12:LEU:HD21	1:B:28:LEU:H	19	0.02
(1,14)	1:A:12:LEU:HD22	1:B:28:LEU:H	19	0.02
(1,14)	1:A:12:LEU:HD23	1:B:28:LEU:H	19	0.02
(1,1363)	1:B:17:ARG:H	1:B:17:ARG:HG2	18	0.02
(1,1362)	1:B:17:ARG:H	1:B:17:ARG:HD2	2	0.02
(1,1362)	1:B:17:ARG:H	1:B:17:ARG:HD3	2	0.02
(1,1333)	1:B:14:GLN:HA	1:B:17:ARG:HD2	11	0.02
(1,1333)	1:B:14:GLN:HA	1:B:17:ARG:HD3	11	0.02
(1,130)	1:A:5:SER:HB2	1:A:6:ASP:H	1	0.02
(1,1282)	1:B:8:LYS:HB2	1:B:9:ALA:H	2	0.02
(1,1282)	1:B:8:LYS:HB3	1:B:9:ALA:H	2	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1278)	1:B:8:LYS:HA	1:B:8:LYS:HD2	11	0.02
(1,1278)	1:B:8:LYS:HA	1:B:8:LYS:HD3	11	0.02
(1,1278)	1:B:8:LYS:HA	1:B:8:LYS:HD2	14	0.02
(1,1278)	1:B:8:LYS:HA	1:B:8:LYS:HD3	14	0.02
(1,1273)	1:B:7:ARG:HB2	1:B:8:LYS:H	20	0.02
(1,1252)	1:A:101:LEU:HD21	1:A:102:GLU:H	7	0.02
(1,1252)	1:A:101:LEU:HD22	1:A:102:GLU:H	7	0.02
(1,1252)	1:A:101:LEU:HD23	1:A:102:GLU:H	7	0.02
(1,1252)	1:A:101:LEU:HD21	1:A:102:GLU:H	11	0.02
(1,1252)	1:A:101:LEU:HD22	1:A:102:GLU:H	11	0.02
(1,1252)	1:A:101:LEU:HD23	1:A:102:GLU:H	11	0.02
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD11	2	0.02
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD12	2	0.02
(1,123)	1:B:89:LEU:HB2	1:A:92:LEU:HD13	2	0.02
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD11	2	0.02
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD12	2	0.02
(1,123)	1:B:89:LEU:HB3	1:A:92:LEU:HD13	2	0.02
(1,121)	1:B:88:ARG:HB2	1:A:92:LEU:HD21	14	0.02
(1,121)	1:B:88:ARG:HB2	1:A:92:LEU:HD22	14	0.02
(1,121)	1:B:88:ARG:HB2	1:A:92:LEU:HD23	14	0.02
(1,1166)	1:A:91:ALA:HA	1:A:94:GLN:HG2	20	0.02
(1,1164)	1:A:91:ALA:HA	1:A:94:GLN:HE21	17	0.02
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG11	12	0.02
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG12	12	0.02
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG13	12	0.02
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG11	12	0.02
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG12	12	0.02
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG13	12	0.02
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG11	13	0.02
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG12	13	0.02
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG13	13	0.02
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG11	13	0.02
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG12	13	0.02
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG13	13	0.02
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG11	15	0.02
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG12	15	0.02
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG13	15	0.02
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG11	15	0.02
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG12	15	0.02
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG13	15	0.02
(1,1144)	1:A:89:LEU:HD21	1:A:93:VAL:HB	12	0.02
(1,1144)	1:A:89:LEU:HD22	1:A:93:VAL:HB	12	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1144)	1:A:89:LEU:HD23	1:A:93:VAL:HB	12	0.02
(1,1144)	1:A:89:LEU:HD21	1:A:93:VAL:HB	20	0.02
(1,1144)	1:A:89:LEU:HD22	1:A:93:VAL:HB	20	0.02
(1,1144)	1:A:89:LEU:HD23	1:A:93:VAL:HB	20	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD21	1	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD22	1	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD23	1	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD21	3	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD22	3	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD23	3	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD21	6	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD22	6	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD23	6	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD21	8	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD22	8	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD23	8	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD21	12	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD22	12	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD23	12	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD21	17	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD22	17	0.02
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD23	17	0.02
(1,1093)	1:A:84:GLU:HG2	1:A:88:ARG:HD2	9	0.02
(1,1093)	1:A:84:GLU:HG2	1:A:88:ARG:HD3	9	0.02
(1,1093)	1:A:84:GLU:HG3	1:A:88:ARG:HD2	9	0.02
(1,1093)	1:A:84:GLU:HG3	1:A:88:ARG:HD3	9	0.02
(1,107)	1:B:16:ALA:H	1:A:28:LEU:HD11	7	0.02
(1,107)	1:B:16:ALA:H	1:A:28:LEU:HD12	7	0.02
(1,107)	1:B:16:ALA:H	1:A:28:LEU:HD13	7	0.02
(1,1064)	1:A:81:ILE:HG21	1:A:83:GLY:H	3	0.02
(1,1064)	1:A:81:ILE:HG22	1:A:83:GLY:H	3	0.02
(1,1064)	1:A:81:ILE:HG23	1:A:83:GLY:H	3	0.02
(1,1052)	1:A:81:ILE:HD11	1:A:82:ALA:H	4	0.02
(1,1052)	1:A:81:ILE:HD12	1:A:82:ALA:H	4	0.02
(1,1052)	1:A:81:ILE:HD13	1:A:82:ALA:H	4	0.02
(1,1052)	1:A:81:ILE:HD11	1:A:82:ALA:H	10	0.02
(1,1052)	1:A:81:ILE:HD12	1:A:82:ALA:H	10	0.02
(1,1052)	1:A:81:ILE:HD13	1:A:82:ALA:H	10	0.02
(1,1046)	1:A:80:ARG:H	1:A:80:ARG:HD2	20	0.02
(1,1046)	1:A:80:ARG:H	1:A:80:ARG:HD3	20	0.02
(1,1033)	1:A:77:GLN:HG2	1:A:77:GLN:HE21	14	0.02
(1,1030)	1:A:77:GLN:HB2	1:A:77:GLN:HE21	11	0.02

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1030)	1:A:77:GLN:HB3	1:A:77:GLN:HE21	11	0.02
(1,1030)	1:A:77:GLN:HB2	1:A:77:GLN:HE21	12	0.02
(1,1030)	1:A:77:GLN:HB3	1:A:77:GLN:HE21	12	0.02
(1,1019)	1:A:76:ARG:HD2	1:A:77:GLN:H	5	0.02
(1,1019)	1:A:76:ARG:HD3	1:A:77:GLN:H	5	0.02
(1,1019)	1:A:76:ARG:HD2	1:A:77:GLN:H	8	0.02
(1,1019)	1:A:76:ARG:HD3	1:A:77:GLN:H	8	0.02
(1,1019)	1:A:76:ARG:HD2	1:A:77:GLN:H	13	0.02
(1,1019)	1:A:76:ARG:HD3	1:A:77:GLN:H	13	0.02
(1,1003)	1:A:74:GLY:HA2	1:A:76:ARG:H	8	0.02
(1,100)	1:B:15:VAL:HG11	1:A:94:GLN:HA	15	0.02
(1,100)	1:B:15:VAL:HG12	1:A:94:GLN:HA	15	0.02
(1,100)	1:B:15:VAL:HG13	1:A:94:GLN:HA	15	0.02
(1,996)	1:A:73:GLU:HG2	1:A:78:TYR:HD1	15	0.01
(1,996)	1:A:73:GLU:HG3	1:A:78:TYR:HD1	15	0.01
(1,980)	1:A:72:ARG:HA	1:A:77:GLN:HA	4	0.01
(1,97)	1:B:15:VAL:HB	1:A:28:LEU:HD11	6	0.01
(1,97)	1:B:15:VAL:HB	1:A:28:LEU:HD12	6	0.01
(1,97)	1:B:15:VAL:HB	1:A:28:LEU:HD13	6	0.01
(1,944)	1:A:69:GLU:HG3	1:A:82:ALA:HB1	7	0.01
(1,944)	1:A:69:GLU:HG3	1:A:82:ALA:HB2	7	0.01
(1,944)	1:A:69:GLU:HG3	1:A:82:ALA:HB3	7	0.01
(1,91)	1:B:14:GLN:HG2	1:A:101:LEU:HD21	20	0.01
(1,91)	1:B:14:GLN:HG2	1:A:101:LEU:HD22	20	0.01
(1,91)	1:B:14:GLN:HG2	1:A:101:LEU:HD23	20	0.01
(1,897)	1:A:67:LEU:HB2	1:A:68:VAL:HG21	11	0.01
(1,897)	1:A:67:LEU:HB2	1:A:68:VAL:HG22	11	0.01
(1,897)	1:A:67:LEU:HB2	1:A:68:VAL:HG23	11	0.01
(1,897)	1:A:67:LEU:HB3	1:A:68:VAL:HG21	11	0.01
(1,897)	1:A:67:LEU:HB3	1:A:68:VAL:HG22	11	0.01
(1,897)	1:A:67:LEU:HB3	1:A:68:VAL:HG23	11	0.01
(1,891)	1:A:67:LEU:HA	1:A:86:VAL:HG11	2	0.01
(1,891)	1:A:67:LEU:HA	1:A:86:VAL:HG12	2	0.01
(1,891)	1:A:67:LEU:HA	1:A:86:VAL:HG13	2	0.01
(1,891)	1:A:67:LEU:HA	1:A:86:VAL:HG11	5	0.01
(1,891)	1:A:67:LEU:HA	1:A:86:VAL:HG12	5	0.01
(1,891)	1:A:67:LEU:HA	1:A:86:VAL:HG13	5	0.01
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB2	17	0.01
(1,881)	1:A:65:GLY:HA2	1:A:67:LEU:HB3	17	0.01
(1,864)	1:A:63:LYS:HE2	1:A:70:ALA:HB1	9	0.01
(1,864)	1:A:63:LYS:HE2	1:A:70:ALA:HB2	9	0.01
(1,864)	1:A:63:LYS:HE2	1:A:70:ALA:HB3	9	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,864)	1:A:63:LYS:HE3	1:A:70:ALA:HB1	9	0.01
(1,864)	1:A:63:LYS:HE3	1:A:70:ALA:HB2	9	0.01
(1,864)	1:A:63:LYS:HE3	1:A:70:ALA:HB3	9	0.01
(1,855)	1:A:63:LYS:HB2	1:A:64:SER:H	18	0.01
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE2	5	0.01
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE3	5	0.01
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE2	10	0.01
(1,854)	1:A:63:LYS:HB2	1:A:63:LYS:HE3	10	0.01
(1,85)	1:B:12:LEU:HG	1:A:29:GLN:HG2	11	0.01
(1,845)	1:A:62:LEU:HD11	1:A:63:LYS:H	14	0.01
(1,845)	1:A:62:LEU:HD12	1:A:63:LYS:H	14	0.01
(1,845)	1:A:62:LEU:HD13	1:A:63:LYS:H	14	0.01
(1,845)	1:A:62:LEU:HD11	1:A:63:LYS:H	15	0.01
(1,845)	1:A:62:LEU:HD12	1:A:63:LYS:H	15	0.01
(1,845)	1:A:62:LEU:HD13	1:A:63:LYS:H	15	0.01
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD1	9	0.01
(1,82)	1:B:12:LEU:HD21	1:A:90:PHE:HD2	9	0.01
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD1	9	0.01
(1,82)	1:B:12:LEU:HD22	1:A:90:PHE:HD2	9	0.01
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD1	9	0.01
(1,82)	1:B:12:LEU:HD23	1:A:90:PHE:HD2	9	0.01
(1,819)	1:A:60:GLN:HA	1:A:63:LYS:HG2	5	0.01
(1,819)	1:A:60:GLN:HA	1:A:63:LYS:HG3	5	0.01
(1,802)	1:A:59:LEU:HB2	1:A:79:TYR:HE1	1	0.01
(1,78)	1:B:12:LEU:HD21	1:A:29:GLN:H	4	0.01
(1,78)	1:B:12:LEU:HD22	1:A:29:GLN:H	4	0.01
(1,78)	1:B:12:LEU:HD23	1:A:29:GLN:H	4	0.01
(1,78)	1:B:12:LEU:HD21	1:A:29:GLN:H	7	0.01
(1,78)	1:B:12:LEU:HD22	1:A:29:GLN:H	7	0.01
(1,78)	1:B:12:LEU:HD23	1:A:29:GLN:H	7	0.01
(1,775)	1:A:56:SER:HA	1:A:59:LEU:HD11	3	0.01
(1,775)	1:A:56:SER:HA	1:A:59:LEU:HD12	3	0.01
(1,775)	1:A:56:SER:HA	1:A:59:LEU:HD13	3	0.01
(1,750)	1:A:53:THR:H	1:A:53:THR:HB	12	0.01
(1,749)	1:A:53:THR:HG21	1:A:54:THR:H	8	0.01
(1,749)	1:A:53:THR:HG22	1:A:54:THR:H	8	0.01
(1,749)	1:A:53:THR:HG23	1:A:54:THR:H	8	0.01
(1,748)	1:A:53:THR:HB	1:A:55:ALA:H	15	0.01
(1,722)	1:A:51:ASN:HB2	1:A:53:THR:H	5	0.01
(1,717)	1:A:50:MET:H	1:A:50:MET:HG2	18	0.01
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB1	10	0.01
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB2	10	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,714)	1:A:50:MET:HG2	1:A:55:ALA:HB3	10	0.01
(1,705)	1:A:50:MET:HB2	1:A:55:ALA:H	2	0.01
(1,7)	1:A:12:LEU:HD11	1:B:29:GLN:HB2	5	0.01
(1,7)	1:A:12:LEU:HD12	1:B:29:GLN:HB2	5	0.01
(1,7)	1:A:12:LEU:HD13	1:B:29:GLN:HB2	5	0.01
(1,619)	1:A:42:GLU:HG2	1:A:52:LEU:HD21	6	0.01
(1,619)	1:A:42:GLU:HG2	1:A:52:LEU:HD22	6	0.01
(1,619)	1:A:42:GLU:HG2	1:A:52:LEU:HD23	6	0.01
(1,616)	1:A:42:GLU:HG3	1:A:52:LEU:HD11	19	0.01
(1,616)	1:A:42:GLU:HG3	1:A:52:LEU:HD12	19	0.01
(1,616)	1:A:42:GLU:HG3	1:A:52:LEU:HD13	19	0.01
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD11	20	0.01
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD12	20	0.01
(1,606)	1:A:42:GLU:HA	1:A:52:LEU:HD13	20	0.01
(1,592)	1:A:41:VAL:HG21	1:A:59:LEU:HD21	5	0.01
(1,592)	1:A:41:VAL:HG21	1:A:59:LEU:HD22	5	0.01
(1,592)	1:A:41:VAL:HG21	1:A:59:LEU:HD23	5	0.01
(1,592)	1:A:41:VAL:HG22	1:A:59:LEU:HD21	5	0.01
(1,592)	1:A:41:VAL:HG22	1:A:59:LEU:HD22	5	0.01
(1,592)	1:A:41:VAL:HG22	1:A:59:LEU:HD23	5	0.01
(1,592)	1:A:41:VAL:HG23	1:A:59:LEU:HD21	5	0.01
(1,592)	1:A:41:VAL:HG23	1:A:59:LEU:HD22	5	0.01
(1,592)	1:A:41:VAL:HG23	1:A:59:LEU:HD23	5	0.01
(1,592)	1:A:41:VAL:HG21	1:A:59:LEU:HD21	17	0.01
(1,592)	1:A:41:VAL:HG21	1:A:59:LEU:HD22	17	0.01
(1,592)	1:A:41:VAL:HG21	1:A:59:LEU:HD23	17	0.01
(1,592)	1:A:41:VAL:HG22	1:A:59:LEU:HD21	17	0.01
(1,592)	1:A:41:VAL:HG22	1:A:59:LEU:HD22	17	0.01
(1,592)	1:A:41:VAL:HG22	1:A:59:LEU:HD23	17	0.01
(1,592)	1:A:41:VAL:HG23	1:A:59:LEU:HD21	17	0.01
(1,592)	1:A:41:VAL:HG23	1:A:59:LEU:HD22	17	0.01
(1,592)	1:A:41:VAL:HG23	1:A:59:LEU:HD23	17	0.01
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD21	15	0.01
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD22	15	0.01
(1,58)	1:A:88:ARG:HB2	1:B:92:LEU:HD23	15	0.01
(1,543)	1:A:40:ALA:HA	1:A:78:TYR:HA	1	0.01
(1,543)	1:A:40:ALA:HA	1:A:78:TYR:HA	7	0.01
(1,538)	1:A:39:ARG:HG2	1:A:40:ALA:H	6	0.01
(1,538)	1:A:39:ARG:HG2	1:A:40:ALA:H	16	0.01
(1,526)	1:A:38:GLU:HG2	1:A:78:TYR:HD1	6	0.01
(1,526)	1:A:38:GLU:HG3	1:A:78:TYR:HD1	6	0.01
(1,516)	1:A:37:GLY:HA2	1:A:38:GLU:HB2	15	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,516)	1:A:37:GLY:HA2	1:A:38:GLU:HB3	15	0.01
(1,516)	1:A:37:GLY:HA2	1:A:38:GLU:HB2	16	0.01
(1,516)	1:A:37:GLY:HA2	1:A:38:GLU:HB3	16	0.01
(1,512)	1:A:36:GLN:HG2	1:A:36:GLN:HE21	13	0.01
(1,500)	1:A:35:ALA:HA	1:A:81:ILE:HD11	5	0.01
(1,500)	1:A:35:ALA:HA	1:A:81:ILE:HD12	5	0.01
(1,500)	1:A:35:ALA:HA	1:A:81:ILE:HD13	5	0.01
(1,490)	1:A:34:LEU:HD21	1:A:37:GLY:H	9	0.01
(1,490)	1:A:34:LEU:HD22	1:A:37:GLY:H	9	0.01
(1,490)	1:A:34:LEU:HD23	1:A:37:GLY:H	9	0.01
(1,476)	1:A:33:LEU:HG	1:A:39:ARG:HE	17	0.01
(1,467)	1:A:33:LEU:HD11	1:A:39:ARG:HD2	2	0.01
(1,467)	1:A:33:LEU:HD12	1:A:39:ARG:HD2	2	0.01
(1,467)	1:A:33:LEU:HD13	1:A:39:ARG:HD2	2	0.01
(1,446)	1:A:31:LEU:H	1:A:62:LEU:HD11	7	0.01
(1,446)	1:A:31:LEU:H	1:A:62:LEU:HD12	7	0.01
(1,446)	1:A:31:LEU:H	1:A:62:LEU:HD13	7	0.01
(1,434)	1:A:31:LEU:HD21	1:A:81:ILE:HA	16	0.01
(1,434)	1:A:31:LEU:HD22	1:A:81:ILE:HA	16	0.01
(1,434)	1:A:31:LEU:HD23	1:A:81:ILE:HA	16	0.01
(1,422)	1:A:31:LEU:HD11	1:A:86:VAL:HG11	5	0.01
(1,422)	1:A:31:LEU:HD11	1:A:86:VAL:HG12	5	0.01
(1,422)	1:A:31:LEU:HD11	1:A:86:VAL:HG13	5	0.01
(1,422)	1:A:31:LEU:HD12	1:A:86:VAL:HG11	5	0.01
(1,422)	1:A:31:LEU:HD12	1:A:86:VAL:HG12	5	0.01
(1,422)	1:A:31:LEU:HD12	1:A:86:VAL:HG13	5	0.01
(1,422)	1:A:31:LEU:HD13	1:A:86:VAL:HG11	5	0.01
(1,422)	1:A:31:LEU:HD13	1:A:86:VAL:HG12	5	0.01
(1,422)	1:A:31:LEU:HD13	1:A:86:VAL:HG13	5	0.01
(1,42)	1:A:16:ALA:HB1	1:B:25:GLY:HA2	19	0.01
(1,42)	1:A:16:ALA:HB2	1:B:25:GLY:HA2	19	0.01
(1,42)	1:A:16:ALA:HB3	1:B:25:GLY:HA2	19	0.01
(1,419)	1:A:31:LEU:HD11	1:A:62:LEU:HB2	17	0.01
(1,419)	1:A:31:LEU:HD12	1:A:62:LEU:HB2	17	0.01
(1,419)	1:A:31:LEU:HD13	1:A:62:LEU:HB2	17	0.01
(1,412)	1:A:31:LEU:HB2	1:A:62:LEU:HD11	12	0.01
(1,412)	1:A:31:LEU:HB2	1:A:62:LEU:HD12	12	0.01
(1,412)	1:A:31:LEU:HB2	1:A:62:LEU:HD13	12	0.01
(1,4)	1:A:11:LEU:HD11	1:B:98:ASP:H	13	0.01
(1,4)	1:A:11:LEU:HD12	1:B:98:ASP:H	13	0.01
(1,4)	1:A:11:LEU:HD13	1:B:98:ASP:H	13	0.01
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD21	2	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD22	2	0.01
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD23	2	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD21	2	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD22	2	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD23	2	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD21	2	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD22	2	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD23	2	0.01
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD21	10	0.01
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD22	10	0.01
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD23	10	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD21	10	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD22	10	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD23	10	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD21	10	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD22	10	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD23	10	0.01
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD21	13	0.01
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD22	13	0.01
(1,395)	1:A:30:ILE:HG21	1:A:59:LEU:HD23	13	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD21	13	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD22	13	0.01
(1,395)	1:A:30:ILE:HG22	1:A:59:LEU:HD23	13	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD21	13	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD22	13	0.01
(1,395)	1:A:30:ILE:HG23	1:A:59:LEU:HD23	13	0.01
(1,375)	1:A:30:ILE:HB	1:A:62:LEU:HD11	5	0.01
(1,375)	1:A:30:ILE:HB	1:A:62:LEU:HD12	5	0.01
(1,375)	1:A:30:ILE:HB	1:A:62:LEU:HD13	5	0.01
(1,360)	1:A:29:GLN:HG2	1:A:48:THR:HB	3	0.01
(1,342)	1:A:28:LEU:HD21	1:A:90:PHE:HE1	4	0.01
(1,342)	1:A:28:LEU:HD22	1:A:90:PHE:HE1	4	0.01
(1,342)	1:A:28:LEU:HD23	1:A:90:PHE:HE1	4	0.01
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD1	19	0.01
(1,337)	1:A:28:LEU:HD11	1:A:90:PHE:HD2	19	0.01
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD1	19	0.01
(1,337)	1:A:28:LEU:HD12	1:A:90:PHE:HD2	19	0.01
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD1	19	0.01
(1,337)	1:A:28:LEU:HD13	1:A:90:PHE:HD2	19	0.01
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB1	8	0.01
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB2	8	0.01
(1,329)	1:A:27:ARG:HD2	1:A:61:ALA:HB3	8	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,314)	1:A:25:GLY:HA3	1:A:28:LEU:HD11	11	0.01
(1,314)	1:A:25:GLY:HA3	1:A:28:LEU:HD12	11	0.01
(1,314)	1:A:25:GLY:HA3	1:A:28:LEU:HD13	11	0.01
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	10	0.01
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	10	0.01
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	10	0.01
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD11	14	0.01
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD12	14	0.01
(1,310)	1:A:24:ASN:H	1:A:28:LEU:HD13	14	0.01
(1,295)	1:A:22:LEU:HD11	1:A:93:VAL:HB	7	0.01
(1,295)	1:A:22:LEU:HD12	1:A:93:VAL:HB	7	0.01
(1,295)	1:A:22:LEU:HD13	1:A:93:VAL:HB	7	0.01
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD21	8	0.01
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD22	8	0.01
(1,286)	1:A:22:LEU:HA	1:A:28:LEU:HD23	8	0.01
(1,279)	1:A:21:ALA:HB1	1:A:65:GLY:H	8	0.01
(1,279)	1:A:21:ALA:HB2	1:A:65:GLY:H	8	0.01
(1,279)	1:A:21:ALA:HB3	1:A:65:GLY:H	8	0.01
(1,278)	1:A:21:ALA:HB1	1:A:65:GLY:HA3	2	0.01
(1,278)	1:A:21:ALA:HB2	1:A:65:GLY:HA3	2	0.01
(1,278)	1:A:21:ALA:HB3	1:A:65:GLY:HA3	2	0.01
(1,277)	1:A:21:ALA:HB1	1:A:65:GLY:HA2	15	0.01
(1,277)	1:A:21:ALA:HB2	1:A:65:GLY:HA2	15	0.01
(1,277)	1:A:21:ALA:HB3	1:A:65:GLY:HA2	15	0.01
(1,2613)	1:B:97:ALA:H	1:B:93:VAL:O	4	0.01
(1,2613)	1:B:97:ALA:H	1:B:93:VAL:O	9	0.01
(1,2613)	1:B:97:ALA:H	1:B:93:VAL:O	14	0.01
(1,2613)	1:B:97:ALA:H	1:B:93:VAL:O	17	0.01
(1,2607)	1:B:94:GLN:H	1:B:90:PHE:O	5	0.01
(1,2607)	1:B:94:GLN:H	1:B:90:PHE:O	9	0.01
(1,2607)	1:B:94:GLN:H	1:B:90:PHE:O	14	0.01
(1,2597)	1:B:89:LEU:H	1:B:85:ASP:O	1	0.01
(1,2597)	1:B:89:LEU:H	1:B:85:ASP:O	3	0.01
(1,2597)	1:B:89:LEU:H	1:B:85:ASP:O	6	0.01
(1,2593)	1:B:87:ALA:H	1:B:83:GLY:O	13	0.01
(1,2589)	1:B:80:ARG:H	1:B:69:GLU:O	1	0.01
(1,2589)	1:B:80:ARG:H	1:B:69:GLU:O	5	0.01
(1,2583)	1:B:76:ARG:H	1:B:73:GLU:O	2	0.01
(1,2583)	1:B:76:ARG:H	1:B:73:GLU:O	7	0.01
(1,2583)	1:B:76:ARG:H	1:B:73:GLU:O	15	0.01
(1,2579)	1:B:71:ARG:H	1:B:78:TYR:O	4	0.01
(1,2579)	1:B:71:ARG:H	1:B:78:TYR:O	6	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2579)	1:B:71:ARG:H	1:B:78:TYR:O	11	0.01
(1,2579)	1:B:71:ARG:H	1:B:78:TYR:O	12	0.01
(1,2573)	1:B:66:GLY:H	1:B:63:LYS:O	1	0.01
(1,2573)	1:B:66:GLY:H	1:B:63:LYS:O	6	0.01
(1,2573)	1:B:66:GLY:H	1:B:63:LYS:O	16	0.01
(1,2571)	1:B:65:GLY:H	1:B:61:ALA:O	4	0.01
(1,2571)	1:B:65:GLY:H	1:B:61:ALA:O	10	0.01
(1,2571)	1:B:65:GLY:H	1:B:61:ALA:O	17	0.01
(1,2567)	1:B:63:LYS:H	1:B:59:LEU:O	3	0.01
(1,2565)	1:B:62:LEU:H	1:B:58:ASN:O	7	0.01
(1,2563)	1:B:61:ALA:H	1:B:57:ALA:O	5	0.01
(1,2563)	1:B:61:ALA:H	1:B:57:ALA:O	9	0.01
(1,2563)	1:B:61:ALA:H	1:B:57:ALA:O	10	0.01
(1,2563)	1:B:61:ALA:H	1:B:57:ALA:O	16	0.01
(1,2561)	1:B:60:GLN:H	1:B:56:SER:O	3	0.01
(1,2557)	1:B:58:ASN:H	1:B:54:THR:O	6	0.01
(1,2557)	1:B:58:ASN:H	1:B:54:THR:O	14	0.01
(1,2555)	1:B:57:ALA:H	1:B:53:THR:O	8	0.01
(1,2555)	1:B:57:ALA:H	1:B:53:THR:O	9	0.01
(1,2555)	1:B:57:ALA:H	1:B:53:THR:O	16	0.01
(1,2549)	1:B:50:MET:H	1:B:45:ALA:O	18	0.01
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	2	0.01
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	11	0.01
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	14	0.01
(1,2547)	1:B:49:GLY:H	1:B:46:THR:O	15	0.01
(1,2545)	1:B:48:THR:H	1:B:44:ILE:O	4	0.01
(1,2545)	1:B:48:THR:H	1:B:44:ILE:O	7	0.01
(1,2541)	1:B:46:THR:H	1:B:42:GLU:O	16	0.01
(1,2535)	1:B:41:VAL:H	1:B:77:GLN:O	1	0.01
(1,2535)	1:B:41:VAL:H	1:B:77:GLN:O	18	0.01
(1,2534)	1:B:39:ARG:N	1:B:79:TYR:O	19	0.01
(1,2533)	1:B:39:ARG:H	1:B:79:TYR:O	3	0.01
(1,2533)	1:B:39:ARG:H	1:B:79:TYR:O	4	0.01
(1,2533)	1:B:39:ARG:H	1:B:79:TYR:O	13	0.01
(1,2533)	1:B:39:ARG:H	1:B:79:TYR:O	20	0.01
(1,2531)	1:B:35:ALA:H	1:B:31:LEU:O	3	0.01
(1,2531)	1:B:35:ALA:H	1:B:31:LEU:O	6	0.01
(1,2531)	1:B:35:ALA:H	1:B:31:LEU:O	12	0.01
(1,2531)	1:B:35:ALA:H	1:B:31:LEU:O	13	0.01
(1,2531)	1:B:35:ALA:H	1:B:31:LEU:O	15	0.01
(1,2527)	1:B:33:LEU:H	1:B:29:GLN:O	5	0.01
(1,2527)	1:B:33:LEU:H	1:B:29:GLN:O	8	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2527)	1:B:33:LEU:H	1:B:29:GLN:O	14	0.01
(1,2527)	1:B:33:LEU:H	1:B:29:GLN:O	16	0.01
(1,2527)	1:B:33:LEU:H	1:B:29:GLN:O	19	0.01
(1,2527)	1:B:33:LEU:H	1:B:29:GLN:O	20	0.01
(1,2523)	1:B:22:LEU:H	1:B:18:VAL:O	6	0.01
(1,2523)	1:B:22:LEU:H	1:B:18:VAL:O	14	0.01
(1,2523)	1:B:22:LEU:H	1:B:18:VAL:O	15	0.01
(1,2521)	1:B:21:ALA:H	1:B:17:ARG:O	17	0.01
(1,2517)	1:B:19:GLY:H	1:B:15:VAL:O	5	0.01
(1,2517)	1:B:19:GLY:H	1:B:15:VAL:O	7	0.01
(1,2515)	1:B:18:VAL:H	1:B:14:GLN:O	13	0.01
(1,2515)	1:B:18:VAL:H	1:B:14:GLN:O	16	0.01
(1,2513)	1:B:17:ARG:H	1:B:13:ASP:O	15	0.01
(1,2511)	1:B:16:ALA:H	1:B:12:LEU:O	6	0.01
(1,2511)	1:B:16:ALA:H	1:B:12:LEU:O	8	0.01
(1,2508)	1:B:14:GLN:N	1:B:10:ALA:O	9	0.01
(1,2507)	1:B:14:GLN:H	1:B:10:ALA:O	3	0.01
(1,2507)	1:B:14:GLN:H	1:B:10:ALA:O	4	0.01
(1,2507)	1:B:14:GLN:H	1:B:10:ALA:O	20	0.01
(1,2501)	1:A:98:ASP:H	1:A:94:GLN:O	12	0.01
(1,2499)	1:A:97:ALA:H	1:A:93:VAL:O	20	0.01
(1,2493)	1:A:94:GLN:H	1:A:90:PHE:O	13	0.01
(1,2493)	1:A:94:GLN:H	1:A:90:PHE:O	14	0.01
(1,2493)	1:A:94:GLN:H	1:A:90:PHE:O	16	0.01
(1,2485)	1:A:90:PHE:H	1:A:86:VAL:O	17	0.01
(1,2483)	1:A:89:LEU:H	1:A:85:ASP:O	1	0.01
(1,2483)	1:A:89:LEU:H	1:A:85:ASP:O	6	0.01
(1,2483)	1:A:89:LEU:H	1:A:85:ASP:O	13	0.01
(1,2479)	1:A:87:ALA:H	1:A:83:GLY:O	3	0.01
(1,2479)	1:A:87:ALA:H	1:A:83:GLY:O	8	0.01
(1,2475)	1:A:80:ARG:H	1:A:69:GLU:O	16	0.01
(1,2475)	1:A:80:ARG:H	1:A:69:GLU:O	20	0.01
(1,2471)	1:A:78:TYR:H	1:A:71:ARG:O	16	0.01
(1,2469)	1:A:76:ARG:H	1:A:73:GLU:O	6	0.01
(1,2469)	1:A:76:ARG:H	1:A:73:GLU:O	10	0.01
(1,2465)	1:A:71:ARG:H	1:A:78:TYR:O	18	0.01
(1,2465)	1:A:71:ARG:H	1:A:78:TYR:O	19	0.01
(1,2462)	1:A:67:LEU:N	1:A:62:LEU:O	12	0.01
(1,2459)	1:A:66:GLY:H	1:A:63:LYS:O	1	0.01
(1,2459)	1:A:66:GLY:H	1:A:63:LYS:O	3	0.01
(1,2459)	1:A:66:GLY:H	1:A:63:LYS:O	11	0.01
(1,2459)	1:A:66:GLY:H	1:A:63:LYS:O	16	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2459)	1:A:66:GLY:H	1:A:63:LYS:O	17	0.01
(1,2457)	1:A:65:GLY:H	1:A:61:ALA:O	2	0.01
(1,2457)	1:A:65:GLY:H	1:A:61:ALA:O	6	0.01
(1,2457)	1:A:65:GLY:H	1:A:61:ALA:O	13	0.01
(1,2457)	1:A:65:GLY:H	1:A:61:ALA:O	18	0.01
(1,2451)	1:A:62:LEU:H	1:A:58:ASN:O	13	0.01
(1,2449)	1:A:61:ALA:H	1:A:57:ALA:O	4	0.01
(1,2449)	1:A:61:ALA:H	1:A:57:ALA:O	7	0.01
(1,2449)	1:A:61:ALA:H	1:A:57:ALA:O	14	0.01
(1,2449)	1:A:61:ALA:H	1:A:57:ALA:O	15	0.01
(1,2449)	1:A:61:ALA:H	1:A:57:ALA:O	17	0.01
(1,2443)	1:A:58:ASN:H	1:A:54:THR:O	3	0.01
(1,2443)	1:A:58:ASN:H	1:A:54:THR:O	5	0.01
(1,2441)	1:A:57:ALA:H	1:A:53:THR:O	3	0.01
(1,2441)	1:A:57:ALA:H	1:A:53:THR:O	12	0.01
(1,2441)	1:A:57:ALA:H	1:A:53:THR:O	16	0.01
(1,2435)	1:A:50:MET:H	1:A:45:ALA:O	11	0.01
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	6	0.01
(1,2433)	1:A:49:GLY:H	1:A:46:THR:O	8	0.01
(1,2431)	1:A:48:THR:H	1:A:44:ILE:O	5	0.01
(1,2431)	1:A:48:THR:H	1:A:44:ILE:O	8	0.01
(1,2427)	1:A:46:THR:H	1:A:42:GLU:O	2	0.01
(1,2427)	1:A:46:THR:H	1:A:42:GLU:O	14	0.01
(1,2427)	1:A:46:THR:H	1:A:42:GLU:O	19	0.01
(1,2421)	1:A:41:VAL:H	1:A:77:GLN:O	9	0.01
(1,2421)	1:A:41:VAL:H	1:A:77:GLN:O	12	0.01
(1,2419)	1:A:39:ARG:H	1:A:79:TYR:O	2	0.01
(1,2419)	1:A:39:ARG:H	1:A:79:TYR:O	3	0.01
(1,2417)	1:A:35:ALA:H	1:A:31:LEU:O	12	0.01
(1,2417)	1:A:35:ALA:H	1:A:31:LEU:O	14	0.01
(1,2413)	1:A:33:LEU:H	1:A:29:GLN:O	2	0.01
(1,2413)	1:A:33:LEU:H	1:A:29:GLN:O	8	0.01
(1,2413)	1:A:33:LEU:H	1:A:29:GLN:O	12	0.01
(1,2413)	1:A:33:LEU:H	1:A:29:GLN:O	14	0.01
(1,2409)	1:A:22:LEU:H	1:A:18:VAL:O	8	0.01
(1,2407)	1:A:21:ALA:H	1:A:17:ARG:O	6	0.01
(1,2407)	1:A:21:ALA:H	1:A:17:ARG:O	10	0.01
(1,2407)	1:A:21:ALA:H	1:A:17:ARG:O	11	0.01
(1,2407)	1:A:21:ALA:H	1:A:17:ARG:O	19	0.01
(1,2407)	1:A:21:ALA:H	1:A:17:ARG:O	20	0.01
(1,2405)	1:A:20:LYS:H	1:A:16:ALA:O	11	0.01
(1,2401)	1:A:18:VAL:H	1:A:14:GLN:O	3	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2401)	1:A:18:VAL:H	1:A:14:GLN:O	20	0.01
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB1	12	0.01
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB2	12	0.01
(1,24)	1:A:14:GLN:HB2	1:B:97:ALA:HB3	12	0.01
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB1	12	0.01
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB2	12	0.01
(1,24)	1:A:14:GLN:HB3	1:B:97:ALA:HB3	12	0.01
(1,2399)	1:A:17:ARG:H	1:A:13:ASP:O	3	0.01
(1,2399)	1:A:17:ARG:H	1:A:13:ASP:O	6	0.01
(1,2399)	1:A:17:ARG:H	1:A:13:ASP:O	8	0.01
(1,2399)	1:A:17:ARG:H	1:A:13:ASP:O	11	0.01
(1,2397)	1:A:16:ALA:H	1:A:12:LEU:O	8	0.01
(1,2397)	1:A:16:ALA:H	1:A:12:LEU:O	20	0.01
(1,2393)	1:A:14:GLN:H	1:A:10:ALA:O	1	0.01
(1,2393)	1:A:14:GLN:H	1:A:10:ALA:O	4	0.01
(1,2393)	1:A:14:GLN:H	1:A:10:ALA:O	18	0.01
(1,2393)	1:A:14:GLN:H	1:A:10:ALA:O	19	0.01
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	4	0.01
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	8	0.01
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	12	0.01
(1,2391)	1:A:11:LEU:H	1:A:8:LYS:O	14	0.01
(1,2379)	1:B:100:HIS:H	1:B:100:HIS:HD2	18	0.01
(1,2357)	1:B:96:VAL:HG21	1:B:100:HIS:HD2	4	0.01
(1,2357)	1:B:96:VAL:HG22	1:B:100:HIS:HD2	4	0.01
(1,2357)	1:B:96:VAL:HG23	1:B:100:HIS:HD2	4	0.01
(1,2356)	1:B:96:VAL:HG21	1:B:97:ALA:H	17	0.01
(1,2356)	1:B:96:VAL:HG22	1:B:97:ALA:H	17	0.01
(1,2356)	1:B:96:VAL:HG23	1:B:97:ALA:H	17	0.01
(1,231)	1:A:17:ARG:H	1:A:17:ARG:HG2	9	0.01
(1,2277)	1:B:89:LEU:HD21	1:B:93:VAL:HG11	18	0.01
(1,2277)	1:B:89:LEU:HD21	1:B:93:VAL:HG12	18	0.01
(1,2277)	1:B:89:LEU:HD21	1:B:93:VAL:HG13	18	0.01
(1,2277)	1:B:89:LEU:HD22	1:B:93:VAL:HG11	18	0.01
(1,2277)	1:B:89:LEU:HD22	1:B:93:VAL:HG12	18	0.01
(1,2277)	1:B:89:LEU:HD22	1:B:93:VAL:HG13	18	0.01
(1,2277)	1:B:89:LEU:HD23	1:B:93:VAL:HG11	18	0.01
(1,2277)	1:B:89:LEU:HD23	1:B:93:VAL:HG12	18	0.01
(1,2277)	1:B:89:LEU:HD23	1:B:93:VAL:HG13	18	0.01
(1,2269)	1:B:89:LEU:HA	1:B:92:LEU:HD21	6	0.01
(1,2269)	1:B:89:LEU:HA	1:B:92:LEU:HD22	6	0.01
(1,2269)	1:B:89:LEU:HA	1:B:92:LEU:HD23	6	0.01
(1,2269)	1:B:89:LEU:HA	1:B:92:LEU:HD21	10	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2269)	1:B:89:LEU:HA	1:B:92:LEU:HD22	10	0.01
(1,2269)	1:B:89:LEU:HA	1:B:92:LEU:HD23	10	0.01
(1,2179)	1:B:80:ARG:H	1:B:80:ARG:HG2	1	0.01
(1,2162)	1:B:77:GLN:HB2	1:B:77:GLN:HE21	7	0.01
(1,2162)	1:B:77:GLN:HB3	1:B:77:GLN:HE21	7	0.01
(1,2162)	1:B:77:GLN:HB2	1:B:77:GLN:HE21	13	0.01
(1,2162)	1:B:77:GLN:HB3	1:B:77:GLN:HE21	13	0.01
(1,2151)	1:B:76:ARG:HD2	1:B:77:GLN:H	14	0.01
(1,2151)	1:B:76:ARG:HD3	1:B:77:GLN:H	14	0.01
(1,2127)	1:B:73:GLU:HB2	1:B:78:TYR:HE1	1	0.01
(1,2115)	1:B:72:ARG:HB2	1:B:73:GLU:H	10	0.01
(1,2090)	1:B:70:ALA:HB1	1:B:77:GLN:HE21	13	0.01
(1,2090)	1:B:70:ALA:HB2	1:B:77:GLN:HE21	13	0.01
(1,2090)	1:B:70:ALA:HB3	1:B:77:GLN:HE21	13	0.01
(1,2076)	1:B:69:GLU:HG3	1:B:82:ALA:HB1	1	0.01
(1,2076)	1:B:69:GLU:HG3	1:B:82:ALA:HB2	1	0.01
(1,2076)	1:B:69:GLU:HG3	1:B:82:ALA:HB3	1	0.01
(1,2076)	1:B:69:GLU:HG3	1:B:82:ALA:HB1	4	0.01
(1,2076)	1:B:69:GLU:HG3	1:B:82:ALA:HB2	4	0.01
(1,2076)	1:B:69:GLU:HG3	1:B:82:ALA:HB3	4	0.01
(1,2053)	1:B:68:VAL:HG11	1:B:86:VAL:HG11	9	0.01
(1,2053)	1:B:68:VAL:HG11	1:B:86:VAL:HG12	9	0.01
(1,2053)	1:B:68:VAL:HG11	1:B:86:VAL:HG13	9	0.01
(1,2053)	1:B:68:VAL:HG12	1:B:86:VAL:HG11	9	0.01
(1,2053)	1:B:68:VAL:HG12	1:B:86:VAL:HG12	9	0.01
(1,2053)	1:B:68:VAL:HG12	1:B:86:VAL:HG13	9	0.01
(1,2053)	1:B:68:VAL:HG13	1:B:86:VAL:HG11	9	0.01
(1,2053)	1:B:68:VAL:HG13	1:B:86:VAL:HG12	9	0.01
(1,2053)	1:B:68:VAL:HG13	1:B:86:VAL:HG13	9	0.01
(1,2032)	1:B:67:LEU:HD11	1:B:86:VAL:HG11	5	0.01
(1,2032)	1:B:67:LEU:HD11	1:B:86:VAL:HG12	5	0.01
(1,2032)	1:B:67:LEU:HD11	1:B:86:VAL:HG13	5	0.01
(1,2032)	1:B:67:LEU:HD12	1:B:86:VAL:HG11	5	0.01
(1,2032)	1:B:67:LEU:HD12	1:B:86:VAL:HG12	5	0.01
(1,2032)	1:B:67:LEU:HD12	1:B:86:VAL:HG13	5	0.01
(1,2032)	1:B:67:LEU:HD13	1:B:86:VAL:HG11	5	0.01
(1,2032)	1:B:67:LEU:HD13	1:B:86:VAL:HG12	5	0.01
(1,2032)	1:B:67:LEU:HD13	1:B:86:VAL:HG13	5	0.01
(1,2031)	1:B:67:LEU:HD11	1:B:86:VAL:HA	10	0.01
(1,2031)	1:B:67:LEU:HD12	1:B:86:VAL:HA	10	0.01
(1,2031)	1:B:67:LEU:HD13	1:B:86:VAL:HA	10	0.01
(1,2023)	1:B:67:LEU:HA	1:B:86:VAL:HG11	7	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,2023)	1:B:67:LEU:HA	1:B:86:VAL:HG12	7	0.01
(1,2023)	1:B:67:LEU:HA	1:B:86:VAL:HG13	7	0.01
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD2	2	0.01
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD3	2	0.01
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD2	12	0.01
(1,201)	1:A:14:GLN:HA	1:A:17:ARG:HD3	12	0.01
(1,1995)	1:B:63:LYS:HE2	1:B:69:GLU:HA	20	0.01
(1,1995)	1:B:63:LYS:HE3	1:B:69:GLU:HA	20	0.01
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE2	9	0.01
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE3	9	0.01
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE2	11	0.01
(1,1986)	1:B:63:LYS:HB2	1:B:63:LYS:HE3	11	0.01
(1,1951)	1:B:60:GLN:HA	1:B:63:LYS:HG2	11	0.01
(1,1951)	1:B:60:GLN:HA	1:B:63:LYS:HG3	11	0.01
(1,1934)	1:B:59:LEU:HB2	1:B:79:TYR:HE1	6	0.01
(1,1907)	1:B:56:SER:HA	1:B:59:LEU:HD11	18	0.01
(1,1907)	1:B:56:SER:HA	1:B:59:LEU:HD12	18	0.01
(1,1907)	1:B:56:SER:HA	1:B:59:LEU:HD13	18	0.01
(1,1882)	1:B:53:THR:H	1:B:53:THR:HB	17	0.01
(1,1879)	1:B:53:THR:HB	1:B:54:THR:H	14	0.01
(1,1854)	1:B:51:ASN:HB2	1:B:53:THR:H	6	0.01
(1,1854)	1:B:51:ASN:HB2	1:B:53:THR:H	19	0.01
(1,1847)	1:B:50:MET:H	1:B:50:MET:HB2	16	0.01
(1,1751)	1:B:42:GLU:HG2	1:B:52:LEU:HD21	11	0.01
(1,1751)	1:B:42:GLU:HG2	1:B:52:LEU:HD22	11	0.01
(1,1751)	1:B:42:GLU:HG2	1:B:52:LEU:HD23	11	0.01
(1,1748)	1:B:42:GLU:HG3	1:B:52:LEU:HD11	1	0.01
(1,1748)	1:B:42:GLU:HG3	1:B:52:LEU:HD12	1	0.01
(1,1748)	1:B:42:GLU:HG3	1:B:52:LEU:HD13	1	0.01
(1,1748)	1:B:42:GLU:HG3	1:B:52:LEU:HD11	5	0.01
(1,1748)	1:B:42:GLU:HG3	1:B:52:LEU:HD12	5	0.01
(1,1748)	1:B:42:GLU:HG3	1:B:52:LEU:HD13	5	0.01
(1,1748)	1:B:42:GLU:HG3	1:B:52:LEU:HD11	7	0.01
(1,1748)	1:B:42:GLU:HG3	1:B:52:LEU:HD12	7	0.01
(1,1748)	1:B:42:GLU:HG3	1:B:52:LEU:HD13	7	0.01
(1,1728)	1:B:41:VAL:HG21	1:B:79:TYR:HE1	2	0.01
(1,1728)	1:B:41:VAL:HG22	1:B:79:TYR:HE1	2	0.01
(1,1728)	1:B:41:VAL:HG23	1:B:79:TYR:HE1	2	0.01
(1,1727)	1:B:41:VAL:HG21	1:B:79:TYR:HD1	15	0.01
(1,1727)	1:B:41:VAL:HG22	1:B:79:TYR:HD1	15	0.01
(1,1727)	1:B:41:VAL:HG23	1:B:79:TYR:HD1	15	0.01
(1,1726)	1:B:41:VAL:HG21	1:B:77:GLN:HG2	11	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1726)	1:B:41:VAL:HG22	1:B:77:GLN:HG2	11	0.01
(1,1726)	1:B:41:VAL:HG23	1:B:77:GLN:HG2	11	0.01
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD21	14	0.01
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD22	14	0.01
(1,1724)	1:B:41:VAL:HG21	1:B:59:LEU:HD23	14	0.01
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD21	14	0.01
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD22	14	0.01
(1,1724)	1:B:41:VAL:HG22	1:B:59:LEU:HD23	14	0.01
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD21	14	0.01
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD22	14	0.01
(1,1724)	1:B:41:VAL:HG23	1:B:59:LEU:HD23	14	0.01
(1,1675)	1:B:40:ALA:HA	1:B:78:TYR:HA	8	0.01
(1,1662)	1:B:39:ARG:HA	1:B:39:ARG:HD2	11	0.01
(1,1625)	1:B:34:LEU:HD21	1:B:80:ARG:HA	4	0.01
(1,1625)	1:B:34:LEU:HD22	1:B:80:ARG:HA	4	0.01
(1,1625)	1:B:34:LEU:HD23	1:B:80:ARG:HA	4	0.01
(1,1621)	1:B:34:LEU:HD11	1:B:80:ARG:HA	8	0.01
(1,1621)	1:B:34:LEU:HD12	1:B:80:ARG:HA	8	0.01
(1,1621)	1:B:34:LEU:HD13	1:B:80:ARG:HA	8	0.01
(1,1607)	1:B:33:LEU:HG	1:B:36:GLN:HE21	17	0.01
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB1	4	0.01
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB2	4	0.01
(1,1604)	1:B:33:LEU:HD11	1:B:47:ALA:HB3	4	0.01
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB1	4	0.01
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB2	4	0.01
(1,1604)	1:B:33:LEU:HD12	1:B:47:ALA:HB3	4	0.01
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB1	4	0.01
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB2	4	0.01
(1,1604)	1:B:33:LEU:HD13	1:B:47:ALA:HB3	4	0.01
(1,1572)	1:B:31:LEU:HD21	1:B:90:PHE:HE1	13	0.01
(1,1572)	1:B:31:LEU:HD22	1:B:90:PHE:HE1	13	0.01
(1,1572)	1:B:31:LEU:HD23	1:B:90:PHE:HE1	13	0.01
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	4	0.01
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	4	0.01
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	4	0.01
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	4	0.01
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	4	0.01
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	4	0.01
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	10	0.01
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	10	0.01
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	10	0.01
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	10	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	10	0.01
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	10	0.01
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	15	0.01
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	15	0.01
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	15	0.01
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	15	0.01
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	15	0.01
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	15	0.01
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD1	20	0.01
(1,1571)	1:B:31:LEU:HD21	1:B:90:PHE:HD2	20	0.01
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD1	20	0.01
(1,1571)	1:B:31:LEU:HD22	1:B:90:PHE:HD2	20	0.01
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD1	20	0.01
(1,1571)	1:B:31:LEU:HD23	1:B:90:PHE:HD2	20	0.01
(1,1567)	1:B:31:LEU:HD21	1:B:81:ILE:HD11	10	0.01
(1,1567)	1:B:31:LEU:HD21	1:B:81:ILE:HD12	10	0.01
(1,1567)	1:B:31:LEU:HD21	1:B:81:ILE:HD13	10	0.01
(1,1567)	1:B:31:LEU:HD22	1:B:81:ILE:HD11	10	0.01
(1,1567)	1:B:31:LEU:HD22	1:B:81:ILE:HD12	10	0.01
(1,1567)	1:B:31:LEU:HD22	1:B:81:ILE:HD13	10	0.01
(1,1567)	1:B:31:LEU:HD23	1:B:81:ILE:HD11	10	0.01
(1,1567)	1:B:31:LEU:HD23	1:B:81:ILE:HD12	10	0.01
(1,1567)	1:B:31:LEU:HD23	1:B:81:ILE:HD13	10	0.01
(1,1567)	1:B:31:LEU:HD21	1:B:81:ILE:HD11	20	0.01
(1,1567)	1:B:31:LEU:HD21	1:B:81:ILE:HD12	20	0.01
(1,1567)	1:B:31:LEU:HD21	1:B:81:ILE:HD13	20	0.01
(1,1567)	1:B:31:LEU:HD22	1:B:81:ILE:HD11	20	0.01
(1,1567)	1:B:31:LEU:HD22	1:B:81:ILE:HD12	20	0.01
(1,1567)	1:B:31:LEU:HD22	1:B:81:ILE:HD13	20	0.01
(1,1567)	1:B:31:LEU:HD23	1:B:81:ILE:HD11	20	0.01
(1,1567)	1:B:31:LEU:HD23	1:B:81:ILE:HD12	20	0.01
(1,1567)	1:B:31:LEU:HD23	1:B:81:ILE:HD13	20	0.01
(1,1553)	1:B:31:LEU:HD11	1:B:67:LEU:HG	14	0.01
(1,1553)	1:B:31:LEU:HD12	1:B:67:LEU:HG	14	0.01
(1,1553)	1:B:31:LEU:HD13	1:B:67:LEU:HG	14	0.01
(1,1492)	1:B:29:GLN:HG2	1:B:48:THR:HB	3	0.01
(1,1484)	1:B:29:GLN:HB2	1:B:29:GLN:HE21	7	0.01
(1,1484)	1:B:29:GLN:HB2	1:B:29:GLN:HE21	12	0.01
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	2	0.01
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	2	0.01
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	2	0.01
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	2	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	2	0.01
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	2	0.01
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD1	12	0.01
(1,1469)	1:B:28:LEU:HD11	1:B:90:PHE:HD2	12	0.01
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD1	12	0.01
(1,1469)	1:B:28:LEU:HD12	1:B:90:PHE:HD2	12	0.01
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD1	12	0.01
(1,1469)	1:B:28:LEU:HD13	1:B:90:PHE:HD2	12	0.01
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD2	6	0.01
(1,146)	1:A:8:LYS:HA	1:A:8:LYS:HD3	6	0.01
(1,1448)	1:B:25:GLY:HA2	1:B:28:LEU:H	11	0.01
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD11	7	0.01
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD12	7	0.01
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD13	7	0.01
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD11	15	0.01
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD12	15	0.01
(1,1442)	1:B:24:ASN:H	1:B:28:LEU:HD13	15	0.01
(1,1432)	1:B:22:LEU:HD21	1:B:90:PHE:HD1	10	0.01
(1,1432)	1:B:22:LEU:HD21	1:B:90:PHE:HD2	10	0.01
(1,1432)	1:B:22:LEU:HD22	1:B:90:PHE:HD1	10	0.01
(1,1432)	1:B:22:LEU:HD22	1:B:90:PHE:HD2	10	0.01
(1,1432)	1:B:22:LEU:HD23	1:B:90:PHE:HD1	10	0.01
(1,1432)	1:B:22:LEU:HD23	1:B:90:PHE:HD2	10	0.01
(1,1432)	1:B:22:LEU:HD21	1:B:90:PHE:HD1	19	0.01
(1,1432)	1:B:22:LEU:HD21	1:B:90:PHE:HD2	19	0.01
(1,1432)	1:B:22:LEU:HD22	1:B:90:PHE:HD1	19	0.01
(1,1432)	1:B:22:LEU:HD22	1:B:90:PHE:HD2	19	0.01
(1,1432)	1:B:22:LEU:HD23	1:B:90:PHE:HD1	19	0.01
(1,1432)	1:B:22:LEU:HD23	1:B:90:PHE:HD2	19	0.01
(1,1421)	1:B:22:LEU:HB2	1:B:23:ALA:H	11	0.01
(1,1411)	1:B:21:ALA:HB1	1:B:65:GLY:H	19	0.01
(1,1411)	1:B:21:ALA:HB2	1:B:65:GLY:H	19	0.01
(1,1411)	1:B:21:ALA:HB3	1:B:65:GLY:H	19	0.01
(1,1409)	1:B:21:ALA:HB1	1:B:65:GLY:HA2	3	0.01
(1,1409)	1:B:21:ALA:HB2	1:B:65:GLY:HA2	3	0.01
(1,1409)	1:B:21:ALA:HB3	1:B:65:GLY:HA2	3	0.01
(1,1367)	1:B:17:ARG:HD2	1:B:64:SER:HB2	19	0.01
(1,1367)	1:B:17:ARG:HD2	1:B:64:SER:HB3	19	0.01
(1,1367)	1:B:17:ARG:HD3	1:B:64:SER:HB2	19	0.01
(1,1367)	1:B:17:ARG:HD3	1:B:64:SER:HB3	19	0.01
(1,1363)	1:B:17:ARG:H	1:B:17:ARG:HG2	5	0.01
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB1	2	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB2	2	0.01
(1,132)	1:A:6:ASP:HA	1:A:9:ALA:HB3	2	0.01
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD11	7	0.01
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD12	7	0.01
(1,1302)	1:B:11:LEU:HA	1:B:11:LEU:HD13	7	0.01
(1,1287)	1:B:8:LYS:H	1:B:8:LYS:HG2	18	0.01
(1,1287)	1:B:8:LYS:H	1:B:8:LYS:HG3	18	0.01
(1,1282)	1:B:8:LYS:HB2	1:B:9:ALA:H	11	0.01
(1,1282)	1:B:8:LYS:HB3	1:B:9:ALA:H	11	0.01
(1,1276)	1:B:7:ARG:H	1:B:7:ARG:HG2	6	0.01
(1,1252)	1:A:101:LEU:HD21	1:A:102:GLU:H	15	0.01
(1,1252)	1:A:101:LEU:HD22	1:A:102:GLU:H	15	0.01
(1,1252)	1:A:101:LEU:HD23	1:A:102:GLU:H	15	0.01
(1,1251)	1:A:101:LEU:HB2	1:A:102:GLU:H	8	0.01
(1,1243)	1:A:99:GLU:H	1:A:99:GLU:HB2	12	0.01
(1,1223)	1:A:96:VAL:HG11	1:A:100:HIS:HD2	2	0.01
(1,1223)	1:A:96:VAL:HG12	1:A:100:HIS:HD2	2	0.01
(1,1223)	1:A:96:VAL:HG13	1:A:100:HIS:HD2	2	0.01
(1,1219)	1:A:96:VAL:HA	1:A:99:GLU:HB2	14	0.01
(1,1183)	1:A:93:VAL:HG11	1:A:94:GLN:H	13	0.01
(1,1183)	1:A:93:VAL:HG12	1:A:94:GLN:H	13	0.01
(1,1183)	1:A:93:VAL:HG13	1:A:94:GLN:H	13	0.01
(1,1183)	1:A:93:VAL:HG11	1:A:94:GLN:H	18	0.01
(1,1183)	1:A:93:VAL:HG12	1:A:94:GLN:H	18	0.01
(1,1183)	1:A:93:VAL:HG13	1:A:94:GLN:H	18	0.01
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG11	1	0.01
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG12	1	0.01
(1,1159)	1:A:90:PHE:HD1	1:A:93:VAL:HG13	1	0.01
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG11	1	0.01
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG12	1	0.01
(1,1159)	1:A:90:PHE:HD2	1:A:93:VAL:HG13	1	0.01
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD21	13	0.01
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD22	13	0.01
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD23	13	0.01
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD21	18	0.01
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD22	18	0.01
(1,1137)	1:A:89:LEU:HA	1:A:92:LEU:HD23	18	0.01
(1,112)	1:B:19:GLY:HA2	1:A:23:ALA:HB1	11	0.01
(1,112)	1:B:19:GLY:HA2	1:A:23:ALA:HB2	11	0.01
(1,112)	1:B:19:GLY:HA2	1:A:23:ALA:HB3	11	0.01
(1,112)	1:B:19:GLY:HA3	1:A:23:ALA:HB1	11	0.01
(1,112)	1:B:19:GLY:HA3	1:A:23:ALA:HB2	11	0.01

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Key	Atom-1	Atom-2	Model	Violation (Å)
(1,112)	1:B:19:GLY:HA3	1:A:23:ALA:HB3	11	0.01
(1,1064)	1:A:81:ILE:HG21	1:A:83:GLY:H	7	0.01
(1,1064)	1:A:81:ILE:HG22	1:A:83:GLY:H	7	0.01
(1,1064)	1:A:81:ILE:HG23	1:A:83:GLY:H	7	0.01
(1,1064)	1:A:81:ILE:HG21	1:A:83:GLY:H	8	0.01
(1,1064)	1:A:81:ILE:HG22	1:A:83:GLY:H	8	0.01
(1,1064)	1:A:81:ILE:HG23	1:A:83:GLY:H	8	0.01
(1,1052)	1:A:81:ILE:HD11	1:A:82:ALA:H	20	0.01
(1,1052)	1:A:81:ILE:HD12	1:A:82:ALA:H	20	0.01
(1,1052)	1:A:81:ILE:HD13	1:A:82:ALA:H	20	0.01
(1,1030)	1:A:77:GLN:HB2	1:A:77:GLN:HE21	4	0.01
(1,1030)	1:A:77:GLN:HB3	1:A:77:GLN:HE21	4	0.01
(1,1021)	1:A:76:ARG:HG2	1:A:77:GLN:H	16	0.01
(1,1019)	1:A:76:ARG:HD2	1:A:77:GLN:H	7	0.01
(1,1019)	1:A:76:ARG:HD3	1:A:77:GLN:H	7	0.01
(1,1019)	1:A:76:ARG:HD2	1:A:77:GLN:H	16	0.01
(1,1019)	1:A:76:ARG:HD3	1:A:77:GLN:H	16	0.01
(1,100)	1:B:15:VAL:HG11	1:A:94:GLN:HA	9	0.01
(1,100)	1:B:15:VAL:HG12	1:A:94:GLN:HA	9	0.01
(1,100)	1:B:15:VAL:HG13	1:A:94:GLN:HA	9	0.01

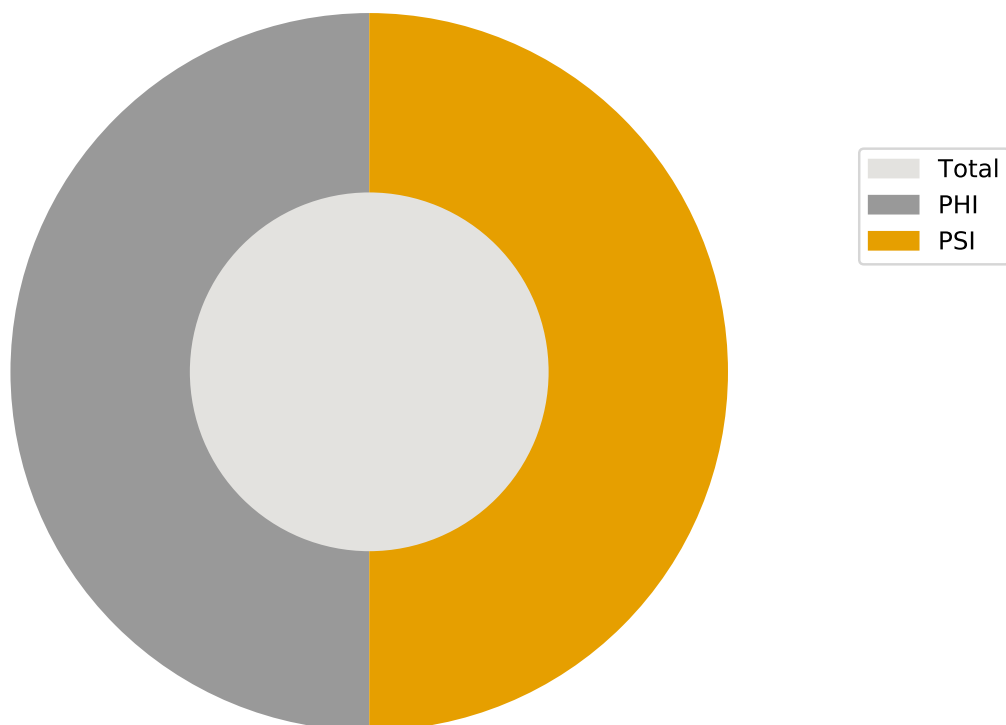
## 9 Dihedral angle restraints analysis

### 9.1 Dihedral angle restraints summary

Angle name	Count	%
PHI	168	50.0
PSI	168	50.0
Total	336	100.0

#### 9.1.1 Pie chart : Dihedral angle restraints

There are 0 unmapped restraints



### 9.2 Dihedral angle violations

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

Angle name	Count	% <sup>1</sup>	% <sup>2</sup>
PHI	21	12.5	33.3
PSI	42	25.0	66.7

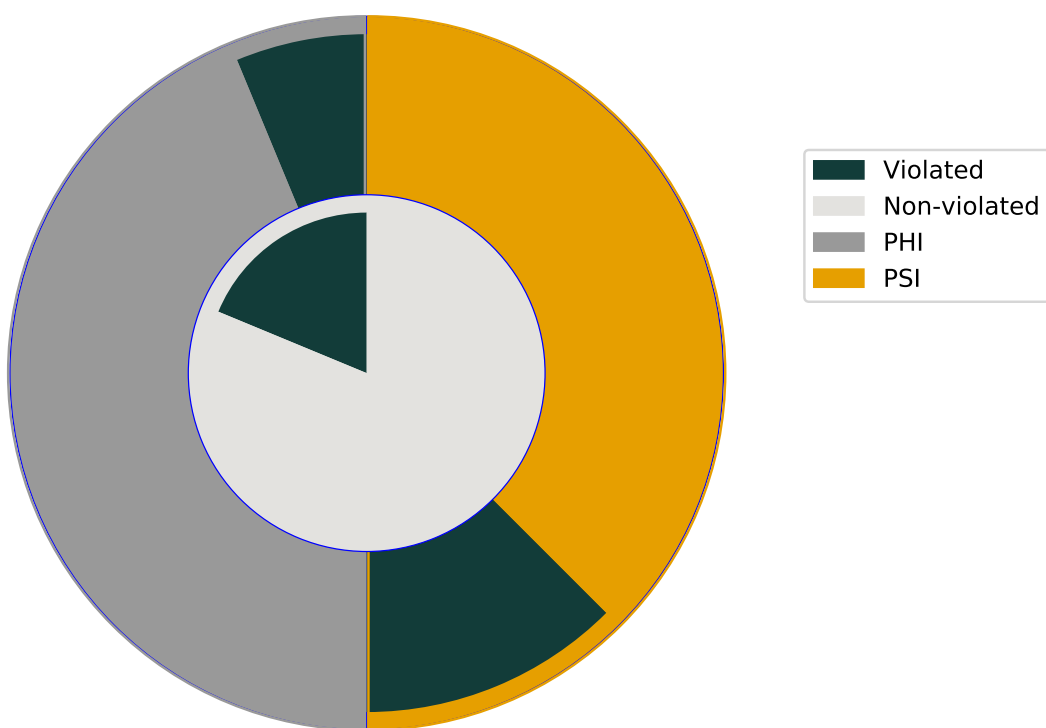
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Angle name	Count	% <sup>1</sup>	% <sup>2</sup>
Total	63	18.8	100.0

<sup>1</sup>percentage of violated restraints in that particular angle type, <sup>2</sup>percentage of violation in total violations.

### 9.2.1 Pie chart : Dihedral angle violations



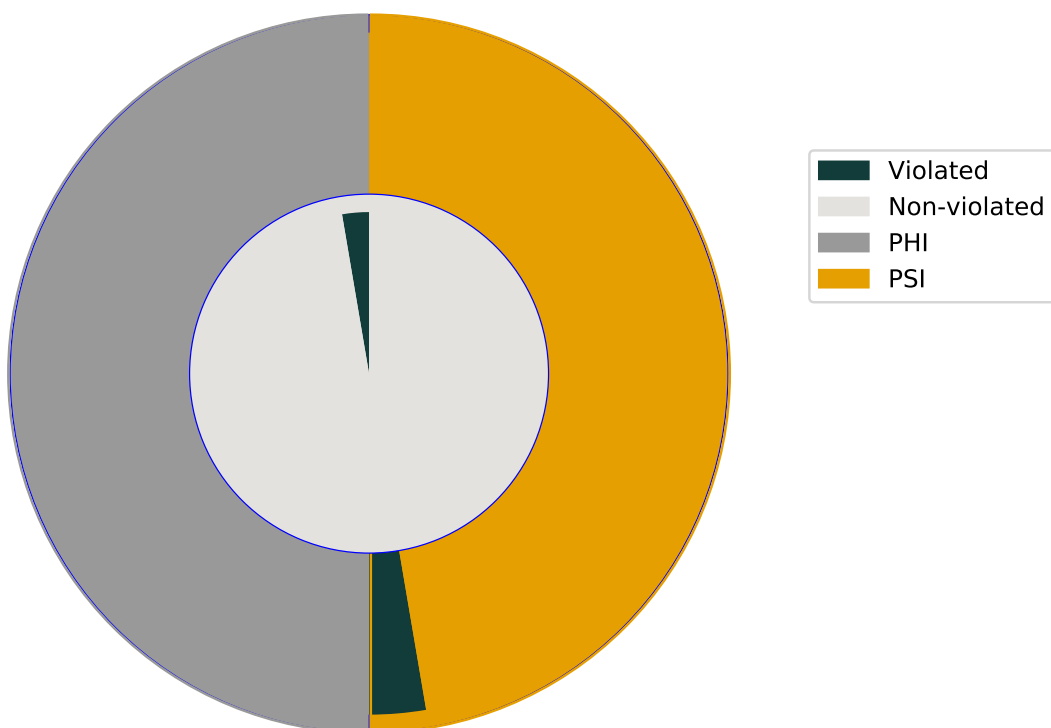
## 9.3 Consistent dihedral angle violations

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

Angle name	Count	% <sup>1</sup>	% <sup>2</sup>
PHI	0	0.0	0.0
PSI	9	5.4	100.0
Total	9	2.7	100.0

<sup>1</sup>percentage of violated restraints in that particular angle type, <sup>2</sup>percentage of violation in total violations.

### 9.3.1 Pie chart : Consistent dihedral angle violations



## 9.4 Residual dihedral angle violations

Violation are counted in different bin sizes and listed below

Range ( ° )	No. of violated restraints per model	Max violation ( ° )
0.0-5.0	6.8	3.82
5.0-10.0	1.1	9.85
10.0-20.0	3.8	20.0
20.0-40.0	5.8	39.96
40.0-80.0	None	None
80.0<	None	None

## 9.5 Dihedral angle violations in the ensemble

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

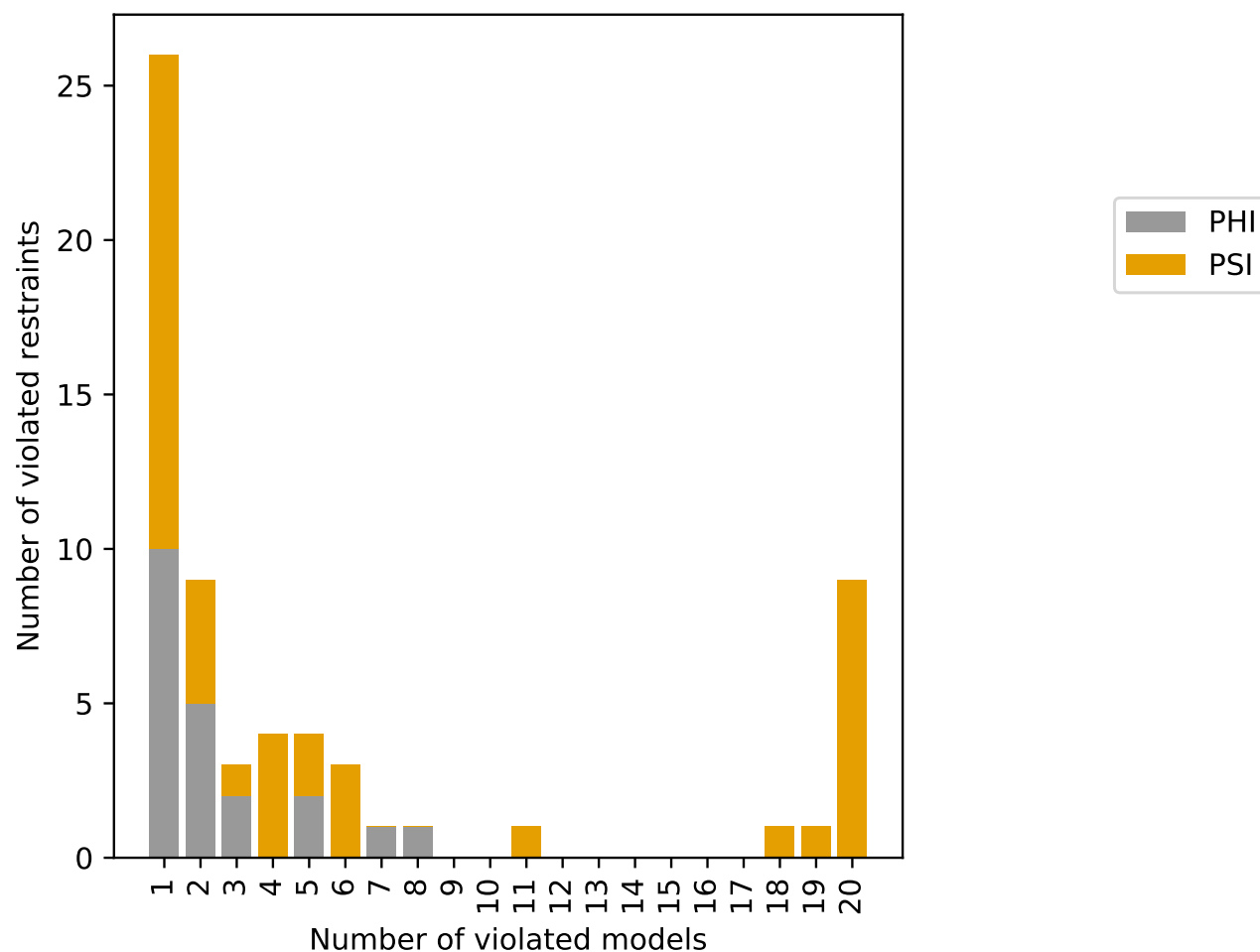
No. of violated restraints			No. of violated models
PHI	PSI	Total	
10	16	26	1

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

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



## 9.6 Violations in each model

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

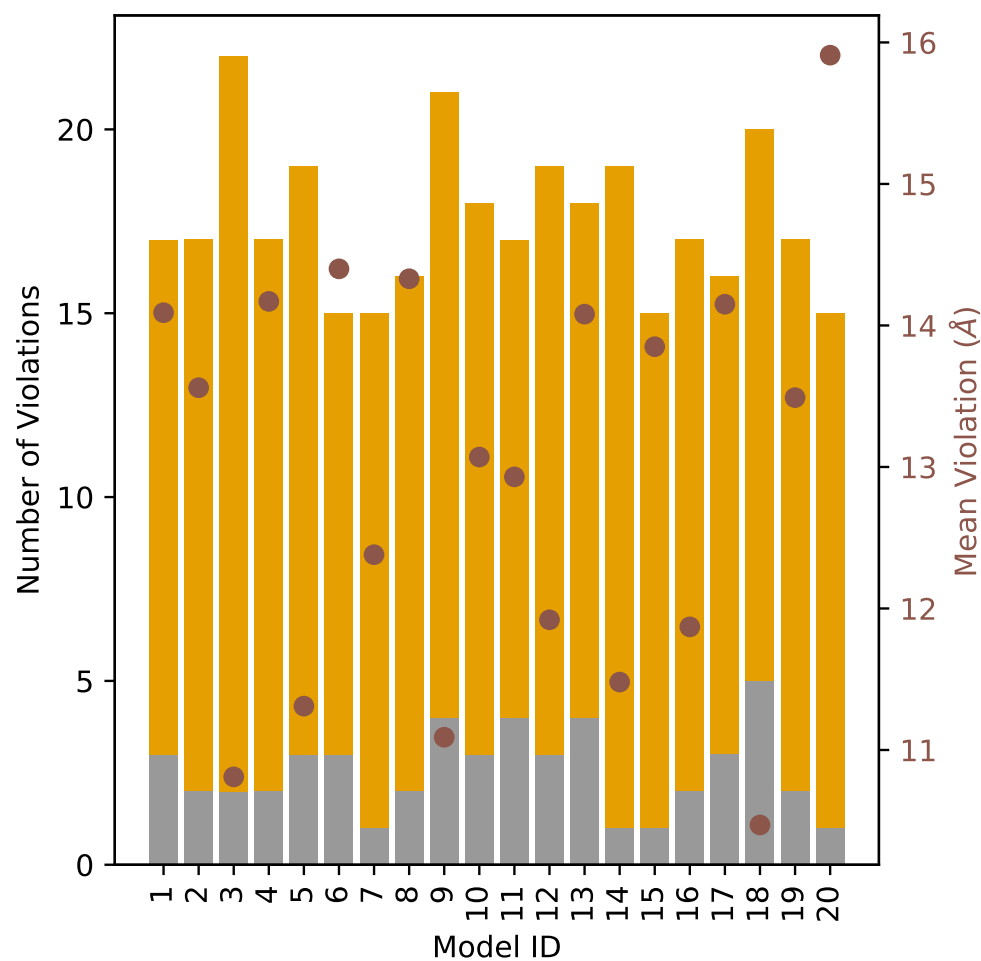
Model ID	No. of violations			Mean (Å)	Max (Å)
	PHI	PSI	Total		
1	3	14	17	14.09	37.8
2	2	15	17	13.56	29.26
3	2	20	22	10.81	28.38
4	2	15	17	14.17	36.89
5	3	16	19	11.31	32.67
6	3	12	15	14.4	36.22
7	1	14	15	12.38	26.32
8	2	14	16	14.33	37.57
9	4	17	21	11.09	32.31

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Model ID	No. of violations			Mean (Å)	Max (Å)
	PHI	PSI	Total		
10	3	15	18	13.07	29.69
11	4	13	17	12.93	37.74
12	3	16	19	11.92	38.81
13	4	14	18	14.08	30.17
14	1	18	19	11.48	39.96
15	1	14	15	13.85	26.41
16	2	15	17	11.87	34.79
17	3	13	16	14.15	35.48
18	5	15	20	10.47	29.69
19	2	15	17	13.49	29.54
20	1	14	15	15.91	29.18

### 9.6.1 Bar graph : Violations in each model

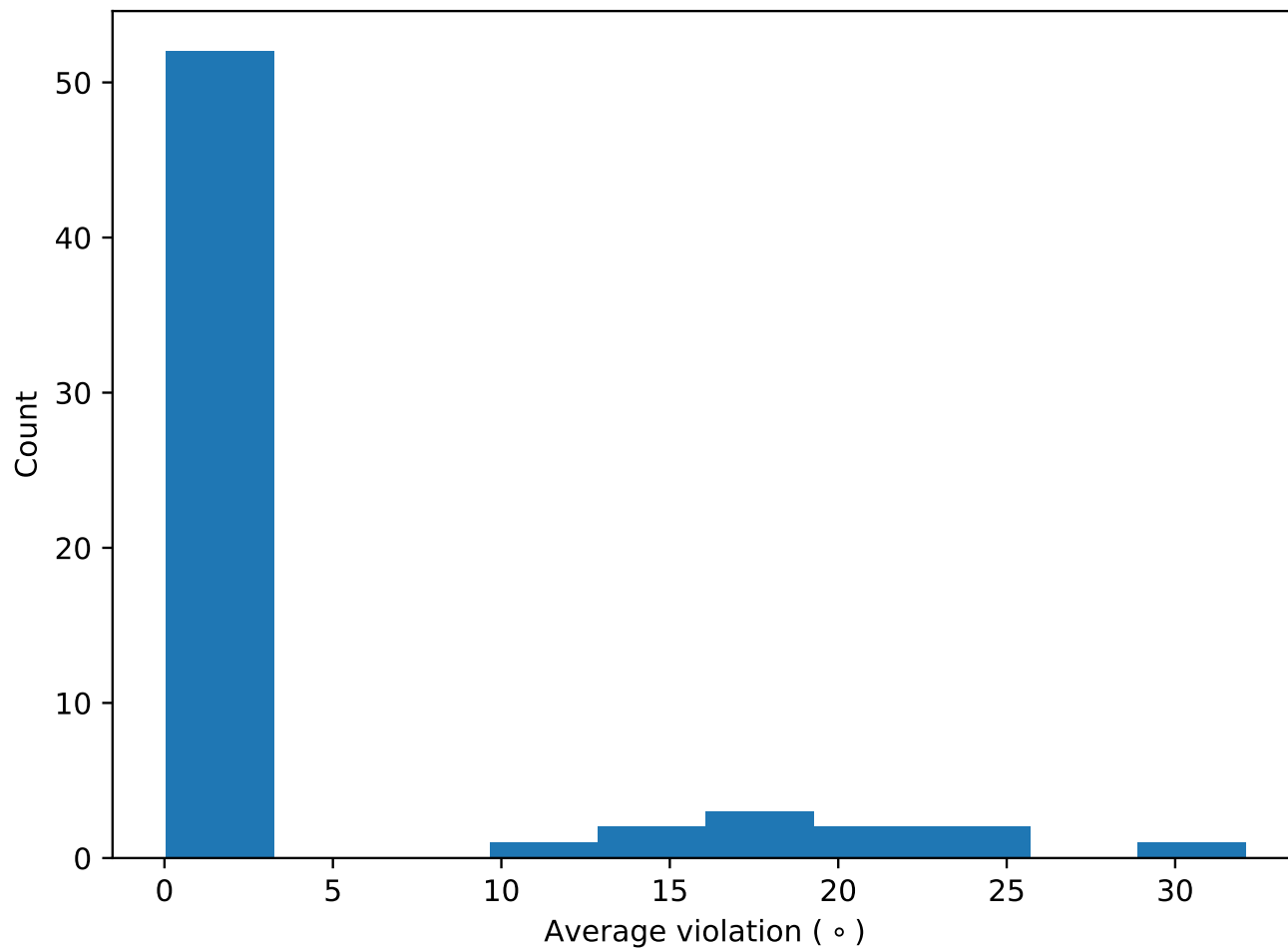




## 9.7 Most violated dihedral angle restraints

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

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



### 9.7.2 Table: Most violated dihedral angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models	Mean ( ° )	Max ( ° )
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	20	32.09	39.96
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	20	17.11	29.8
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	20	25.29	29.69
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	20	24.32	29.34
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	19	12.65	28.94
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	20	19.46	28.56
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	20	22.03	28.38
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	18	14.83	28.25
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	20	19.2	27.57
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	20	19.22	25.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models	Mean ( ° )	Max ( ° )
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	20	15.63	21.87
(1,272)	1:B:62:LEU:N	1:B:62:LEU:CA	1:B:62:LEU:C	1:B:63:LYS:N	1	3.16	3.16
(1,168)	1:A:100:HIS:N	1:A:100:HIS:CA	1:A:100:HIS:C	1:A:101:LEU:N	5	1.3	2.88
(1,104)	1:A:62:LEU:N	1:A:62:LEU:CA	1:A:62:LEU:C	1:A:63:LYS:N	2	1.93	2.15
(1,274)	1:B:63:LYS:N	1:B:63:LYS:CA	1:B:63:LYS:C	1:B:64:SER:N	1	2.11	2.11
(1,118)	1:A:72:ARG:N	1:A:72:ARG:CA	1:A:72:ARG:C	1:A:73:GLU:N	4	0.78	1.95
(1,116)	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	1:A:72:ARG:N	5	0.97	1.82
(1,222)	1:B:36:GLN:N	1:B:36:GLN:CA	1:B:36:GLN:C	1:B:37:GLY:N	1	1.75	1.75
(1,204)	1:B:27:ARG:N	1:B:27:ARG:CA	1:B:27:ARG:C	1:B:28:LEU:N	3	0.96	1.65
(1,36)	1:A:27:ARG:N	1:A:27:ARG:CA	1:A:27:ARG:C	1:A:28:LEU:N	4	0.77	1.63
(1,206)	1:B:28:LEU:N	1:B:28:LEU:CA	1:B:28:LEU:C	1:B:29:GLN:N	1	1.54	1.54
(1,202)	1:B:26:ARG:N	1:B:26:ARG:CA	1:B:26:ARG:C	1:B:27:ARG:N	1	1.5	1.5
(1,106)	1:A:63:LYS:N	1:A:63:LYS:CA	1:A:63:LYS:C	1:A:64:SER:N	2	1.39	1.42
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	11	0.59	1.37
(1,166)	1:A:99:GLU:N	1:A:99:GLU:CA	1:A:99:GLU:C	1:A:100:HIS:N	1	1.34	1.34
(1,284)	1:B:71:ARG:N	1:B:71:ARG:CA	1:B:71:ARG:C	1:B:72:ARG:N	1	1.29	1.29
(1,336)	1:B:100:HIS:N	1:B:100:HIS:CA	1:B:100:HIS:C	1:B:101:LEU:N	6	0.77	1.25
(1,200)	1:B:22:LEU:N	1:B:22:LEU:CA	1:B:22:LEU:C	1:B:23:ALA:N	4	0.88	1.22
(1,34)	1:A:26:ARG:N	1:A:26:ARG:CA	1:A:26:ARG:C	1:A:27:ARG:N	2	0.66	1.14
(1,32)	1:A:22:LEU:N	1:A:22:LEU:CA	1:A:22:LEU:C	1:A:23:ALA:N	6	0.67	1.08
(1,78)	1:A:49:GLY:N	1:A:49:GLY:CA	1:A:49:GLY:C	1:A:50:MET:N	6	0.32	1.01
(1,296)	1:B:77:GLN:N	1:B:77:GLN:CA	1:B:77:GLN:C	1:B:78:TYR:N	4	0.7	0.84
(1,170)	1:B:7:ARG:N	1:B:7:ARG:CA	1:B:7:ARG:C	1:B:8:LYS:N	1	0.77	0.77
(1,286)	1:B:72:ARG:N	1:B:72:ARG:CA	1:B:72:ARG:C	1:B:73:GLU:N	1	0.74	0.74
(1,282)	1:B:70:ALA:N	1:B:70:ALA:CA	1:B:70:ALA:C	1:B:71:ARG:N	1	0.44	0.44
(1,164)	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	1:A:99:GLU:N	1	0.44	0.44
(1,332)	1:B:98:ASP:N	1:B:98:ASP:CA	1:B:98:ASP:C	1:B:99:GLU:N	1	0.37	0.37
(1,162)	1:A:97:ALA:N	1:A:97:ALA:CA	1:A:97:ALA:C	1:A:98:ASP:N	1	0.32	0.32
(1,288)	1:B:73:GLU:N	1:B:73:GLU:CA	1:B:73:GLU:C	1:B:74:GLY:N	1	0.31	0.31
(1,114)	1:A:70:ALA:N	1:A:70:ALA:CA	1:A:70:ALA:C	1:A:71:ARG:N	2	0.19	0.21
(1,112)	1:A:69:GLU:N	1:A:69:GLU:CA	1:A:69:GLU:C	1:A:70:ALA:N	1	0.19	0.19
(1,334)	1:B:99:GLU:N	1:B:99:GLU:CA	1:B:99:GLU:C	1:B:100:HIS:N	1	0.18	0.18
(1,131)	1:A:78:TYR:C	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	7	0.79	1.81
(1,169)	1:B:6:ASP:C	1:B:7:ARG:N	1:B:7:ARG:CA	1:B:7:ARG:C	1	1.31	1.31
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	8	0.75	1.31
(1,283)	1:B:70:ALA:C	1:B:71:ARG:N	1:B:71:ARG:CA	1:B:71:ARG:C	2	0.73	1.25
(1,293)	1:B:75:THR:C	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	5	0.64	1.18
(1,331)	1:B:97:ALA:C	1:B:98:ASP:N	1:B:98:ASP:CA	1:B:98:ASP:C	2	0.93	1.15
(1,223)	1:B:37:GLY:C	1:B:38:GLU:N	1:B:38:GLU:CA	1:B:38:GLU:C	5	0.79	1.11
(1,125)	1:A:75:THR:C	1:A:76:ARG:N	1:A:76:ARG:CA	1:A:76:ARG:C	2	0.56	0.77
(1,123)	1:A:74:GLY:C	1:A:75:THR:N	1:A:75:THR:CA	1:A:75:THR:C	1	0.75	0.75
(1,297)	1:B:77:GLN:C	1:B:78:TYR:N	1:B:78:TYR:CA	1:B:78:TYR:C	1	0.71	0.71
(1,119)	1:A:72:ARG:C	1:A:73:GLU:N	1:A:73:GLU:CA	1:A:73:GLU:C	1	0.58	0.58
(1,299)	1:B:78:TYR:C	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	3	0.39	0.5
(1,287)	1:B:72:ARG:C	1:B:73:GLU:N	1:B:73:GLU:CA	1:B:73:GLU:C	1	0.47	0.47
(1,285)	1:B:71:ARG:C	1:B:72:ARG:N	1:B:72:ARG:CA	1:B:72:ARG:C	3	0.29	0.47
(1,35)	1:A:26:ARG:C	1:A:27:ARG:N	1:A:27:ARG:CA	1:A:27:ARG:C	1	0.42	0.42
(1,221)	1:B:35:ALA:C	1:B:36:GLN:N	1:B:36:GLN:CA	1:B:36:GLN:C	1	0.41	0.41
(1,129)	1:A:77:GLN:C	1:A:78:TYR:N	1:A:78:TYR:CA	1:A:78:TYR:C	1	0.28	0.28
(1,115)	1:A:70:ALA:C	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	2	0.2	0.24
(1,291)	1:B:74:GLY:C	1:B:75:THR:N	1:B:75:THR:CA	1:B:75:THR:C	2	0.23	0.24

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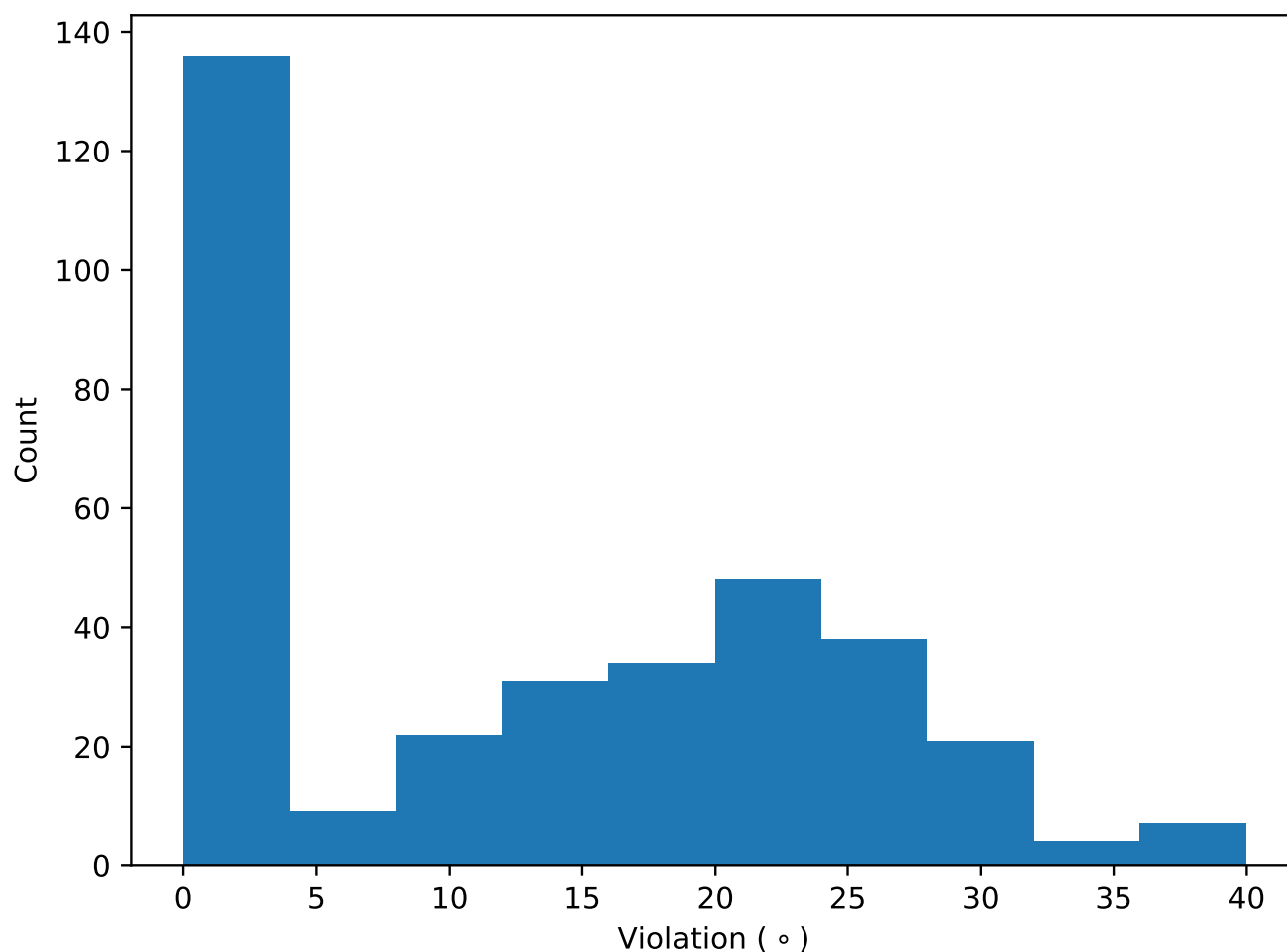
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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models	Mean ( ° )	Max ( ° )
(1,117)	1:A:71:ARG:C	1:A:72:ARG:N	1:A:72:ARG:CA	1:A:72:ARG:C	1	0.07	0.07
(1,75)	1:A:47:ALA:C	1:A:48:THR:N	1:A:48:THR:CA	1:A:48:THR:C	1	0.06	0.06

## 9.8 All violated dihedral angle restraints

### 9.8.1 Histogram : Distribution of violations

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



### 9.8.2 Table: All violated dihedral angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation ( ° )
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	14	39.96
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	12	38.81
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	1	37.8
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	11	37.74

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation ( ° )
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	8	37.57
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	4	36.89
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	6	36.22
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	17	35.48
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	16	34.79
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	5	32.67
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	9	32.31
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	13	30.17
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	6	29.8
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	18	29.69
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	10	29.69
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	19	29.54
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	10	29.39
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	6	29.34
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	2	29.26
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	9	29.18
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	20	29.18
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	1	28.94
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	8	28.87
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	4	28.83
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	1	28.56
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	20	28.48
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	14	28.48
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	2	28.44
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	3	28.38
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	17	28.25
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	4	28.04
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	19	28.01
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	12	27.69
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	20	27.58
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	10	27.57
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	4	27.55
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	17	27.46
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	1	27.46
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	5	27.41
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	3	27.33
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	12	27.33
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	13	27.27
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	5	27.1
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	8	27.05
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	13	27.05
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	9	26.8
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	15	26.41
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	3	26.36
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	7	26.32
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	18	26.26
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	11	26.26
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	16	26.15
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	8	25.88
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	20	25.74
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	13	25.47

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation ( ° )
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	19	25.13
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	15	25.09
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	17	25.01
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	7	24.99
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	16	24.89
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	18	24.88
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	10	24.86
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	19	24.82
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	20	24.5
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	14	24.38
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	7	24.24
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	1	24.22
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	9	24.05
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	10	24.03
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	2	24.03
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	2	23.92
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	3	23.85
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	13	23.82
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	13	23.76
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	3	23.74
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	2	23.73
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	18	23.72
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	18	23.45
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	11	23.43
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	20	23.43
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	12	23.35
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	16	23.15
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	7	23.07
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	11	23.07
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	13	23.02
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	10	23.01
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	6	22.78
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	3	22.77
(1,294)	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	1:B:77:GLN:N	2	22.75
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	15	22.58
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	9	22.41
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	8	22.32
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	7	22.3
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	17	22.14
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	17	21.98
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	15	21.97
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	20	21.88
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	14	21.87
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	13	21.82
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	14	21.58
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	6	21.49
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	13	21.46
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	13	21.44
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	7	21.34
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	4	20.95
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	1	20.9

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation ( ° )
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	5	20.75
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	4	20.69
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	6	20.63
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	4	20.6
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	11	20.49
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	15	20.4
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	9	20.27
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	19	20.25
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	10	20.04
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	11	20.01
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	19	20.0
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	17	20.0
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	6	19.72
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	8	19.7
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	5	19.63
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	9	19.53
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	11	19.39
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	18	19.34
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	10	19.3
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	5	19.26
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	19	19.25
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	2	19.1
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	3	19.01
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	5	18.53
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	6	18.45
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	8	18.44
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	5	18.35
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	19	18.21
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	15	18.2
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	15	18.14
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	1	18.02
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	14	18.01
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	19	17.83
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	12	17.76
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	18	17.45
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	12	17.38
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	16	17.33
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	12	17.27
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	19	17.13
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	4	17.02
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	11	16.94
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	17	16.92
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	16	16.83
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	18	16.35
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	15	16.34
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	12	16.33
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	3	15.54
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	14	15.49
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	9	15.44
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	3	15.28
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	4	15.23

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation ( ° )
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	10	15.15
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	11	15.14
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	1	15.11
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	16	14.99
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	1	14.78
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	20	14.64
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	10	14.56
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	20	14.55
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	2	14.49
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	3	14.48
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	20	14.46
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	8	14.41
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	14	14.22
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	2	14.12
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	7	13.56
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	2	13.39
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	18	13.36
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	9	13.31
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	12	13.22
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	4	13.17
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	15	13.13
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	11	12.72
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	15	12.71
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	12	12.69
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	20	12.58
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	8	12.39
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	16	11.87
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	5	11.85
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	16	11.85
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	1	11.82
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	9	11.79
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	8	11.69
(1,226)	1:B:39:ARG:N	1:B:39:ARG:CA	1:B:39:ARG:C	1:B:40:ALA:N	17	11.24
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	2	10.95
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	12	10.03
(1,110)	1:A:68:VAL:N	1:A:68:VAL:CA	1:A:68:VAL:C	1:A:69:GLU:N	14	9.85
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	7	9.55
(1,132)	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1:A:80:ARG:N	6	9.35
(1,250)	1:B:51:ASN:N	1:B:51:ASN:CA	1:B:51:ASN:C	1:B:52:LEU:N	3	9.31
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	5	9.07
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	15	8.89
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	14	8.86
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	16	8.85
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	9	8.52
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	7	8.4
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	7	8.27
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	18	8.17
(1,82)	1:A:51:ASN:N	1:A:51:ASN:CA	1:A:51:ASN:C	1:A:52:LEU:N	1	8.09
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	8	7.7
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	4	7.68
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	17	7.61

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation ( ° )
(1,278)	1:B:68:VAL:N	1:B:68:VAL:CA	1:B:68:VAL:C	1:B:69:GLU:N	14	7.5
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	19	5.76
(1,58)	1:A:39:ARG:N	1:A:39:ARG:CA	1:A:39:ARG:C	1:A:40:ALA:N	5	5.76
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	17	5.58
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	6	5.46
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	16	5.13
(1,300)	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	1:B:80:ARG:N	13	3.82
(1,272)	1:B:62:LEU:N	1:B:62:LEU:CA	1:B:62:LEU:C	1:B:63:LYS:N	3	3.16
(1,168)	1:A:100:HIS:N	1:A:100:HIS:CA	1:A:100:HIS:C	1:A:101:LEU:N	3	2.88
(1,80)	1:A:50:MET:N	1:A:50:MET:CA	1:A:50:MET:C	1:A:51:ASN:N	10	2.83
(1,248)	1:B:50:MET:N	1:B:50:MET:CA	1:B:50:MET:C	1:B:51:ASN:N	7	2.48
(1,104)	1:A:62:LEU:N	1:A:62:LEU:CA	1:A:62:LEU:C	1:A:63:LYS:N	14	2.15
(1,274)	1:B:63:LYS:N	1:B:63:LYS:CA	1:B:63:LYS:C	1:B:64:SER:N	3	2.11
(1,118)	1:A:72:ARG:N	1:A:72:ARG:CA	1:A:72:ARG:C	1:A:73:GLU:N	13	1.95
(1,116)	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	1:A:72:ARG:N	2	1.82
(1,131)	1:A:78:TYR:C	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	12	1.81
(1,222)	1:B:36:GLN:N	1:B:36:GLN:CA	1:B:36:GLN:C	1:B:37:GLY:N	9	1.75
(1,104)	1:A:62:LEU:N	1:A:62:LEU:CA	1:A:62:LEU:C	1:A:63:LYS:N	15	1.71
(1,204)	1:B:27:ARG:N	1:B:27:ARG:CA	1:B:27:ARG:C	1:B:28:LEU:N	5	1.65
(1,36)	1:A:27:ARG:N	1:A:27:ARG:CA	1:A:27:ARG:C	1:A:28:LEU:N	9	1.63
(1,131)	1:A:78:TYR:C	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	18	1.59
(1,206)	1:B:28:LEU:N	1:B:28:LEU:CA	1:B:28:LEU:C	1:B:29:GLN:N	9	1.54
(1,202)	1:B:26:ARG:N	1:B:26:ARG:CA	1:B:26:ARG:C	1:B:27:ARG:N	17	1.5
(1,168)	1:A:100:HIS:N	1:A:100:HIS:CA	1:A:100:HIS:C	1:A:101:LEU:N	16	1.46
(1,168)	1:A:100:HIS:N	1:A:100:HIS:CA	1:A:100:HIS:C	1:A:101:LEU:N	14	1.43
(1,106)	1:A:63:LYS:N	1:A:63:LYS:CA	1:A:63:LYS:C	1:A:64:SER:N	14	1.42
(1,116)	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	1:A:72:ARG:N	4	1.38
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	16	1.37
(1,106)	1:A:63:LYS:N	1:A:63:LYS:CA	1:A:63:LYS:C	1:A:64:SER:N	15	1.36
(1,166)	1:A:99:GLU:N	1:A:99:GLU:CA	1:A:99:GLU:C	1:A:100:HIS:N	3	1.34
(1,116)	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	1:A:72:ARG:N	10	1.32
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	10	1.31
(1,169)	1:B:6:ASP:C	1:B:7:ARG:N	1:B:7:ARG:CA	1:B:7:ARG:C	1	1.31
(1,284)	1:B:71:ARG:N	1:B:71:ARG:CA	1:B:71:ARG:C	1:B:72:ARG:N	9	1.29
(1,336)	1:B:100:HIS:N	1:B:100:HIS:CA	1:B:100:HIS:C	1:B:101:LEU:N	11	1.25
(1,283)	1:B:70:ALA:C	1:B:71:ARG:N	1:B:71:ARG:CA	1:B:71:ARG:C	17	1.25
(1,200)	1:B:22:LEU:N	1:B:22:LEU:CA	1:B:22:LEU:C	1:B:23:ALA:N	14	1.22
(1,293)	1:B:75:THR:C	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	8	1.18
(1,331)	1:B:97:ALA:C	1:B:98:ASP:N	1:B:98:ASP:CA	1:B:98:ASP:C	18	1.15
(1,34)	1:A:26:ARG:N	1:A:26:ARG:CA	1:A:26:ARG:C	1:A:27:ARG:N	2	1.14
(1,204)	1:B:27:ARG:N	1:B:27:ARG:CA	1:B:27:ARG:C	1:B:28:LEU:N	16	1.13
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	6	1.12
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	5	1.12
(1,200)	1:B:22:LEU:N	1:B:22:LEU:CA	1:B:22:LEU:C	1:B:23:ALA:N	19	1.12
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	18	1.11
(1,223)	1:B:37:GLY:C	1:B:38:GLU:N	1:B:38:GLU:CA	1:B:38:GLU:C	2	1.11
(1,36)	1:A:27:ARG:N	1:A:27:ARG:CA	1:A:27:ARG:C	1:A:28:LEU:N	12	1.09
(1,32)	1:A:22:LEU:N	1:A:22:LEU:CA	1:A:22:LEU:C	1:A:23:ALA:N	4	1.08
(1,32)	1:A:22:LEU:N	1:A:22:LEU:CA	1:A:22:LEU:C	1:A:23:ALA:N	1	1.07
(1,336)	1:B:100:HIS:N	1:B:100:HIS:CA	1:B:100:HIS:C	1:B:101:LEU:N	2	1.05
(1,336)	1:B:100:HIS:N	1:B:100:HIS:CA	1:B:100:HIS:C	1:B:101:LEU:N	5	1.02

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation ( ° )
(1,78)	1:A:49:GLY:N	1:A:49:GLY:CA	1:A:49:GLY:C	1:A:50:MET:N	16	1.01
(1,223)	1:B:37:GLY:C	1:B:38:GLU:N	1:B:38:GLU:CA	1:B:38:GLU:C	20	0.96
(1,296)	1:B:77:GLN:N	1:B:77:GLN:CA	1:B:77:GLN:C	1:B:78:TYR:N	8	0.84
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	2	0.84
(1,131)	1:A:78:TYR:C	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	17	0.84
(1,200)	1:B:22:LEU:N	1:B:22:LEU:CA	1:B:22:LEU:C	1:B:23:ALA:N	10	0.83
(1,223)	1:B:37:GLY:C	1:B:38:GLU:N	1:B:38:GLU:CA	1:B:38:GLU:C	11	0.82
(1,293)	1:B:75:THR:C	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	13	0.81
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	11	0.78
(1,170)	1:B:7:ARG:N	1:B:7:ARG:CA	1:B:7:ARG:C	1:B:8:LYS:N	18	0.77
(1,125)	1:A:75:THR:C	1:A:76:ARG:N	1:A:76:ARG:CA	1:A:76:ARG:C	6	0.77
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	9	0.75
(1,123)	1:A:74:GLY:C	1:A:75:THR:N	1:A:75:THR:CA	1:A:75:THR:C	17	0.75
(1,286)	1:B:72:ARG:N	1:B:72:ARG:CA	1:B:72:ARG:C	1:B:73:GLU:N	10	0.74
(1,331)	1:B:97:ALA:C	1:B:98:ASP:N	1:B:98:ASP:CA	1:B:98:ASP:C	4	0.72
(1,297)	1:B:77:GLN:C	1:B:78:TYR:N	1:B:78:TYR:CA	1:B:78:TYR:C	9	0.71
(1,296)	1:B:77:GLN:N	1:B:77:GLN:CA	1:B:77:GLN:C	1:B:78:TYR:N	11	0.7
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	8	0.68
(1,336)	1:B:100:HIS:N	1:B:100:HIS:CA	1:B:100:HIS:C	1:B:101:LEU:N	14	0.67
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	7	0.66
(1,296)	1:B:77:GLN:N	1:B:77:GLN:CA	1:B:77:GLN:C	1:B:78:TYR:N	3	0.64
(1,223)	1:B:37:GLY:C	1:B:38:GLU:N	1:B:38:GLU:CA	1:B:38:GLU:C	19	0.64
(1,296)	1:B:77:GLN:N	1:B:77:GLN:CA	1:B:77:GLN:C	1:B:78:TYR:N	1	0.63
(1,131)	1:A:78:TYR:C	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	13	0.62
(1,32)	1:A:22:LEU:N	1:A:22:LEU:CA	1:A:22:LEU:C	1:A:23:ALA:N	18	0.61
(1,32)	1:A:22:LEU:N	1:A:22:LEU:CA	1:A:22:LEU:C	1:A:23:ALA:N	19	0.61
(1,32)	1:A:22:LEU:N	1:A:22:LEU:CA	1:A:22:LEU:C	1:A:23:ALA:N	14	0.6
(1,119)	1:A:72:ARG:C	1:A:73:GLU:N	1:A:73:GLU:CA	1:A:73:GLU:C	16	0.58
(1,299)	1:B:78:TYR:C	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	4	0.5
(1,168)	1:A:100:HIS:N	1:A:100:HIS:CA	1:A:100:HIS:C	1:A:101:LEU:N	18	0.49
(1,287)	1:B:72:ARG:C	1:B:73:GLU:N	1:B:73:GLU:CA	1:B:73:GLU:C	11	0.47
(1,285)	1:B:71:ARG:C	1:B:72:ARG:N	1:B:72:ARG:CA	1:B:72:ARG:C	9	0.47
(1,299)	1:B:78:TYR:C	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	11	0.46
(1,293)	1:B:75:THR:C	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	12	0.46
(1,78)	1:A:49:GLY:N	1:A:49:GLY:CA	1:A:49:GLY:C	1:A:50:MET:N	19	0.44
(1,282)	1:B:70:ALA:N	1:B:70:ALA:CA	1:B:70:ALA:C	1:B:71:ARG:N	1	0.44
(1,223)	1:B:37:GLY:C	1:B:38:GLU:N	1:B:38:GLU:CA	1:B:38:GLU:C	8	0.44
(1,164)	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	1:A:99:GLU:N	12	0.44
(1,118)	1:A:72:ARG:N	1:A:72:ARG:CA	1:A:72:ARG:C	1:A:73:GLU:N	3	0.44
(1,35)	1:A:26:ARG:C	1:A:27:ARG:N	1:A:27:ARG:CA	1:A:27:ARG:C	10	0.42
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	3	0.42
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	9	0.42
(1,221)	1:B:35:ALA:C	1:B:36:GLN:N	1:B:36:GLN:CA	1:B:36:GLN:C	6	0.41
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	16	0.4
(1,293)	1:B:75:THR:C	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	2	0.4
(1,131)	1:A:78:TYR:C	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	15	0.4
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	15	0.39
(1,336)	1:B:100:HIS:N	1:B:100:HIS:CA	1:B:100:HIS:C	1:B:101:LEU:N	9	0.37
(1,332)	1:B:98:ASP:N	1:B:98:ASP:CA	1:B:98:ASP:C	1:B:99:GLU:N	4	0.37
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	20	0.37
(1,293)	1:B:75:THR:C	1:B:76:ARG:N	1:B:76:ARG:CA	1:B:76:ARG:C	19	0.36

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model	Violation ( ° )
(1,125)	1:A:75:THR:C	1:A:76:ARG:N	1:A:76:ARG:CA	1:A:76:ARG:C	9	0.36
(1,118)	1:A:72:ARG:N	1:A:72:ARG:CA	1:A:72:ARG:C	1:A:73:GLU:N	7	0.36
(1,118)	1:A:72:ARG:N	1:A:72:ARG:CA	1:A:72:ARG:C	1:A:73:GLU:N	17	0.36
(1,200)	1:B:22:LEU:N	1:B:22:LEU:CA	1:B:22:LEU:C	1:B:23:ALA:N	18	0.33
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	3	0.32
(1,162)	1:A:97:ALA:N	1:A:97:ALA:CA	1:A:97:ALA:C	1:A:98:ASP:N	6	0.32
(1,288)	1:B:73:GLU:N	1:B:73:GLU:CA	1:B:73:GLU:C	1:B:74:GLY:N	3	0.31
(1,116)	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	1:A:72:ARG:N	12	0.29
(1,129)	1:A:77:GLN:C	1:A:78:TYR:N	1:A:78:TYR:CA	1:A:78:TYR:C	18	0.28
(1,36)	1:A:27:ARG:N	1:A:27:ARG:CA	1:A:27:ARG:C	1:A:28:LEU:N	14	0.26
(1,168)	1:A:100:HIS:N	1:A:100:HIS:CA	1:A:100:HIS:C	1:A:101:LEU:N	13	0.26
(1,291)	1:B:74:GLY:C	1:B:75:THR:N	1:B:75:THR:CA	1:B:75:THR:C	14	0.24
(1,115)	1:A:70:ALA:C	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	13	0.24
(1,336)	1:B:100:HIS:N	1:B:100:HIS:CA	1:B:100:HIS:C	1:B:101:LEU:N	12	0.23
(1,291)	1:B:74:GLY:C	1:B:75:THR:N	1:B:75:THR:CA	1:B:75:THR:C	5	0.23
(1,78)	1:A:49:GLY:N	1:A:49:GLY:CA	1:A:49:GLY:C	1:A:50:MET:N	13	0.22
(1,285)	1:B:71:ARG:C	1:B:72:ARG:N	1:B:72:ARG:CA	1:B:72:ARG:C	13	0.21
(1,283)	1:B:70:ALA:C	1:B:71:ARG:N	1:B:71:ARG:CA	1:B:71:ARG:C	12	0.21
(1,114)	1:A:70:ALA:N	1:A:70:ALA:CA	1:A:70:ALA:C	1:A:71:ARG:N	5	0.21
(1,55)	1:A:37:GLY:C	1:A:38:GLU:N	1:A:38:GLU:CA	1:A:38:GLU:C	1	0.2
(1,299)	1:B:78:TYR:C	1:B:79:TYR:N	1:B:79:TYR:CA	1:B:79:TYR:C	18	0.2
(1,285)	1:B:71:ARG:C	1:B:72:ARG:N	1:B:72:ARG:CA	1:B:72:ARG:C	10	0.19
(1,112)	1:A:69:GLU:N	1:A:69:GLU:CA	1:A:69:GLU:C	1:A:70:ALA:N	20	0.19
(1,34)	1:A:26:ARG:N	1:A:26:ARG:CA	1:A:26:ARG:C	1:A:27:ARG:N	6	0.18
(1,334)	1:B:99:GLU:N	1:B:99:GLU:CA	1:B:99:GLU:C	1:B:100:HIS:N	18	0.18
(1,114)	1:A:70:ALA:N	1:A:70:ALA:CA	1:A:70:ALA:C	1:A:71:ARG:N	4	0.17
(1,78)	1:A:49:GLY:N	1:A:49:GLY:CA	1:A:49:GLY:C	1:A:50:MET:N	8	0.16
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	19	0.16
(1,131)	1:A:78:TYR:C	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	1	0.16
(1,115)	1:A:70:ALA:C	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	5	0.16
(1,246)	1:B:49:GLY:N	1:B:49:GLY:CA	1:B:49:GLY:C	1:B:50:MET:N	10	0.11
(1,131)	1:A:78:TYR:C	1:A:79:TYR:N	1:A:79:TYR:CA	1:A:79:TYR:C	5	0.1
(1,36)	1:A:27:ARG:N	1:A:27:ARG:CA	1:A:27:ARG:C	1:A:28:LEU:N	7	0.09
(1,204)	1:B:27:ARG:N	1:B:27:ARG:CA	1:B:27:ARG:C	1:B:28:LEU:N	3	0.09
(1,78)	1:A:49:GLY:N	1:A:49:GLY:CA	1:A:49:GLY:C	1:A:50:MET:N	20	0.08
(1,32)	1:A:22:LEU:N	1:A:22:LEU:CA	1:A:22:LEU:C	1:A:23:ALA:N	11	0.07
(1,117)	1:A:71:ARG:C	1:A:72:ARG:N	1:A:72:ARG:CA	1:A:72:ARG:C	7	0.07
(1,75)	1:A:47:ALA:C	1:A:48:THR:N	1:A:48:THR:CA	1:A:48:THR:C	3	0.06
(1,116)	1:A:71:ARG:N	1:A:71:ARG:CA	1:A:71:ARG:C	1:A:72:ARG:N	5	0.06
(1,78)	1:A:49:GLY:N	1:A:49:GLY:CA	1:A:49:GLY:C	1:A:50:MET:N	12	0.02