



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 06:42 PM UTC

PDB ID : 8K6Z / pdb_00008k6z
BMRB ID : 36585
Title : NMR structure of human leptin
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Deposited on : 2023-07-26

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

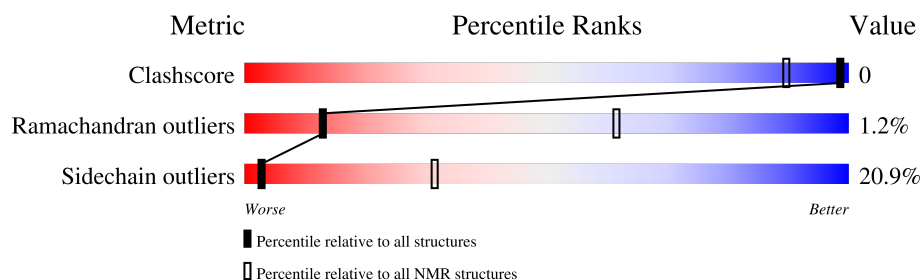
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 88%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	146	 81% 10% 10%

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:2-A:26, A:40-A:146 (132)	0.55	8

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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2276 atoms, of which 1153 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Leptin.

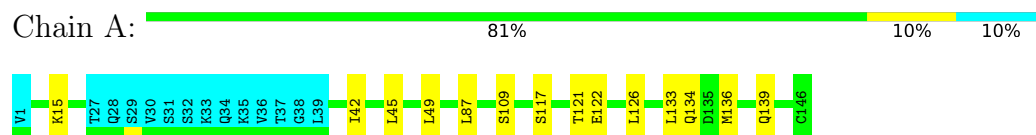
Mol	Chain	Residues	Atoms						Trace
1	A	146	Total	C	H	N	O	S	0
			2276	709	1153	190	219	5	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: Leptin

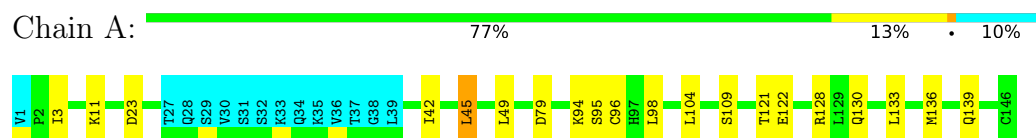


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

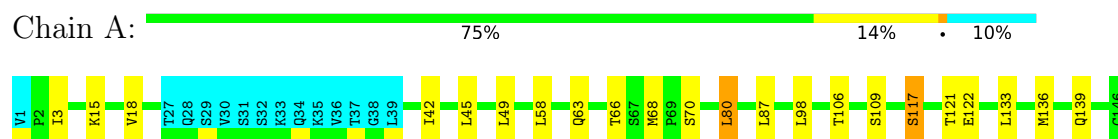
4.2.1 Score per residue for model 1

- Molecule 1: Leptin



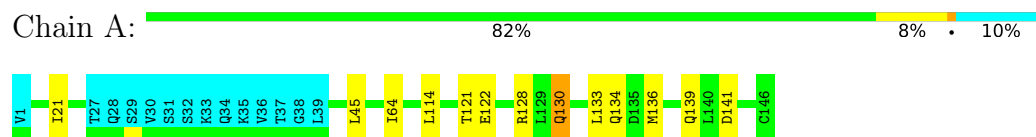
4.2.2 Score per residue for model 2

- Molecule 1: Leptin



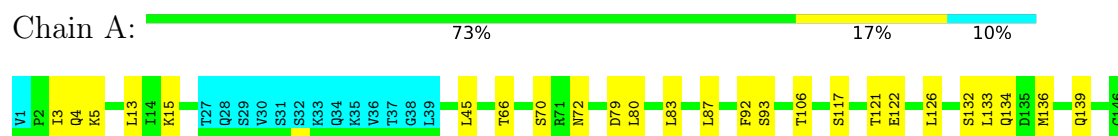
4.2.3 Score per residue for model 3

- Molecule 1: Leptin



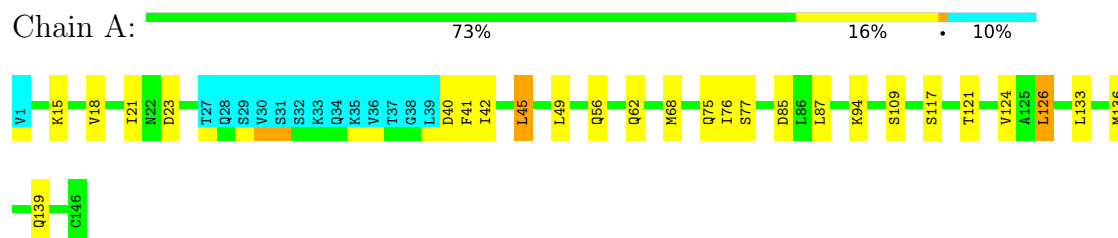
4.2.4 Score per residue for model 4

- Molecule 1: Leptin



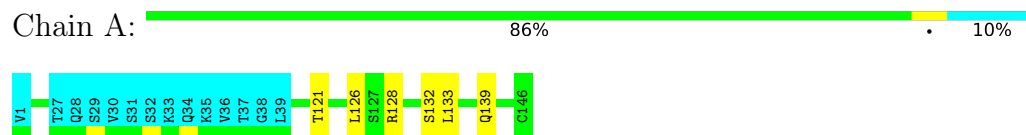
4.2.5 Score per residue for model 5

- Molecule 1: Leptin



4.2.6 Score per residue for model 6

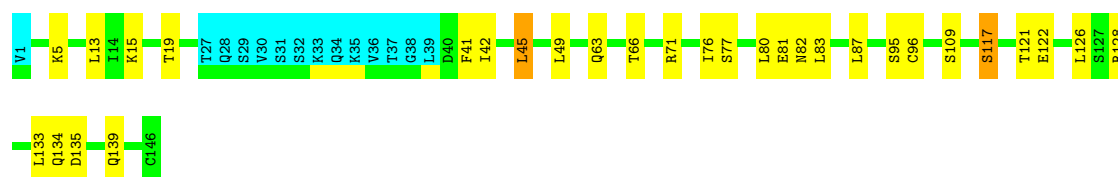
- Molecule 1: Leptin



4.2.7 Score per residue for model 7

- Molecule 1: Leptin

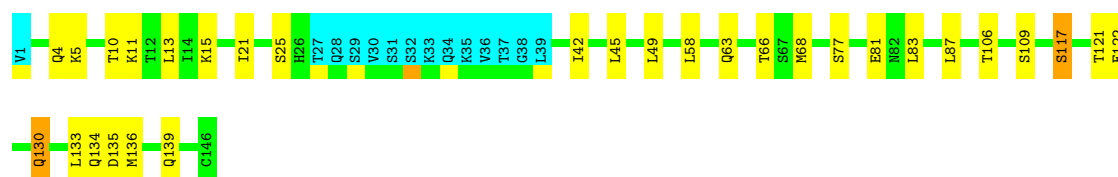




4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Leptin

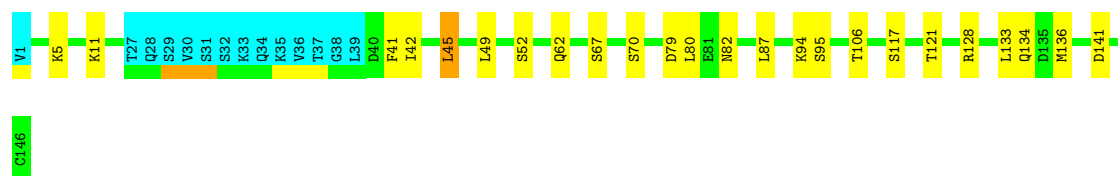
Chain A: 70% 19% 10%



4.2.9 Score per residue for model 9

- Molecule 1: Leptin

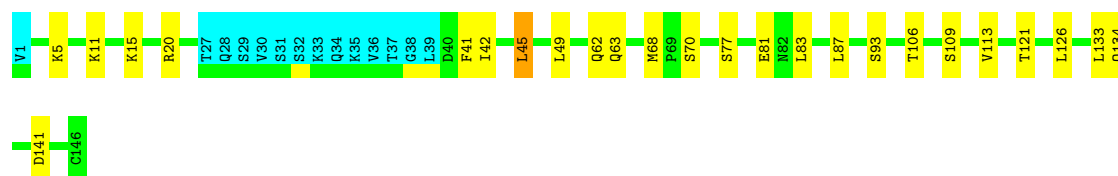
Chain A: 74% 16% 10%



4.2.10 Score per residue for model 10

- Molecule 1: Leptin

Chain A: 73% 16% 10%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry*.

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure calculation	
Amber	refinement	

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1764
Number of shifts mapped to atoms	1747
Number of unparsed shifts	0
Number of shifts with mapping errors	17
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.83±0.03	0±0/1039 (0.0± 0.0%)	1.43±0.04	0±0/1413 (0.0± 0.0%)
All	All	0.83	0/10390 (0.0%)	1.43	2/14130 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	72	ASN	CA-CB-CG	5.14	117.74	112.60	4	1
1	A	79	ASP	CA-CB-CG	5.01	117.61	112.60	1	1

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	1022	1041	1041	0±1
All	All	10220	10410	10410	5

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 0.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:ILE:HG23	1:A:126:LEU:HD22	0.50	1.82	5	1
1:A:21:ILE:HG21	1:A:130:GLN:HB2	0.43	1.91	8	2
1:A:58:LEU:HD22	1:A:80:LEU:HD11	0.43	1.89	2	1
1:A:64:ILE:HD13	1:A:114:LEU:HD12	0.42	1.90	3	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	131/146 (90%)	113±21 (86±16%)	9±2 (7±1%)	2±1 (1±1%)	14	63
All	All	1234/1460 (85%)	1131 (92%)	88 (7%)	15 (1%)	13	61

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	45	LEU	7
1	A	117	SER	4
1	A	130	GLN	2
1	A	40	ASP	1
1	A	124	VAL	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	120/133 (90%)	78±30 (65±25%)	21±7 (17±6%)	4	38
All	All	986/1330 (74%)	780 (79%)	206 (21%)	3	31

All 59 unique residues with a non-rotameric sidechain are listed below. They are sorted by the

frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	121	THR	10
1	A	133	LEU	10
1	A	139	GLN	8
1	A	42	ILE	7
1	A	45	LEU	7
1	A	49	LEU	7
1	A	136	MET	7
1	A	87	LEU	7
1	A	109	SER	6
1	A	122	GLU	6
1	A	15	LYS	6
1	A	134	GLN	6
1	A	128	ARG	5
1	A	106	THR	5
1	A	117	SER	5
1	A	5	LYS	5
1	A	126	LEU	5
1	A	11	LYS	4
1	A	63	GLN	4
1	A	66	THR	4
1	A	68	MET	4
1	A	70	SER	4
1	A	80	LEU	4
1	A	83	LEU	4
1	A	41	PHE	4
1	A	77	SER	4
1	A	3	ILE	3
1	A	94	LYS	3
1	A	95	SER	3
1	A	141	ASP	3
1	A	13	LEU	3
1	A	62	GLN	3
1	A	81	GLU	3
1	A	23	ASP	2
1	A	96	CYS	2
1	A	98	LEU	2
1	A	18	VAL	2
1	A	4	GLN	2
1	A	79	ASP	2
1	A	93	SER	2
1	A	132	SER	2
1	A	76	ILE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	82	ASN	2
1	A	135	ASP	2
1	A	104	LEU	1
1	A	130	GLN	1
1	A	92	PHE	1
1	A	56	GLN	1
1	A	75	GLN	1
1	A	85	ASP	1
1	A	19	THR	1
1	A	71	ARG	1
1	A	10	THR	1
1	A	25	SER	1
1	A	58	LEU	1
1	A	52	SER	1
1	A	67	SER	1
1	A	20	ARG	1
1	A	113	VAL	1

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 oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

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	1764
Number of shifts mapped to atoms	1747
Number of unparsed shifts	0
Number of shifts with mapping errors	17
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. All 17 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	146	GLY	H	8.522	0.02	1
1	A	146	LYS	H	8.229	0.02	1
1	A	146	LYS	HA	4.234	0.02	1
1	A	146	GLY	HA2	3.847	0.02	2
1	A	146	GLY	HA3	4.139	0.02	2
1	A	146	LYS	HB2	1.664	0.02	2
1	A	146	LYS	HD2	1.342	0.02	2
1	A	146	LYS	HE2	2.905	0.02	2
1	A	146	LYS	HG2	1.62	0.02	2
1	A	146	GLY	CA	44.895	0.3	1
1	A	146	LYS	CA	56.168	0.3	1
1	A	146	LYS	CB	33.4	0.3	1
1	A	146	LYS	CD	24.788	0.3	1
1	A	146	LYS	CE	42.276	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	146	LYS	CG	28.764	0.3	1
1	A	146	GLY	N	106.278	0.2	1
1	A	146	LYS	N	120.967	0.2	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	148	-0.58 ± 0.09	Should be checked
$^{13}\text{C}_\beta$	139	0.28 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	142	-0.01 ± 0.19	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 88%, i.e. 1584 atoms were assigned a chemical shift out of a possible 1800. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	523/655 (80%)	265/265 (100%)	132/264 (50%)	126/126 (100%)
Sidechain	987/1055 (94%)	671/694 (97%)	301/331 (91%)	15/30 (50%)
Aromatic	74/90 (82%)	37/46 (80%)	35/38 (92%)	2/6 (33%)
Overall	1584/1800 (88%)	973/1005 (97%)	468/633 (74%)	143/162 (88%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 1746 atoms were assigned a chemical shift out of a possible 1981. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	579/726 (80%)	293/294 (100%)	146/292 (50%)	140/140 (100%)
Sidechain	1093/1165 (94%)	743/766 (97%)	333/365 (91%)	17/34 (50%)
Aromatic	74/90 (82%)	37/46 (80%)	35/38 (92%)	2/6 (33%)
Overall	1746/1981 (88%)	1073/1106 (97%)	514/695 (74%)	159/180 (88%)

7.1.4 Statistically unusual chemical shifts [i](#)

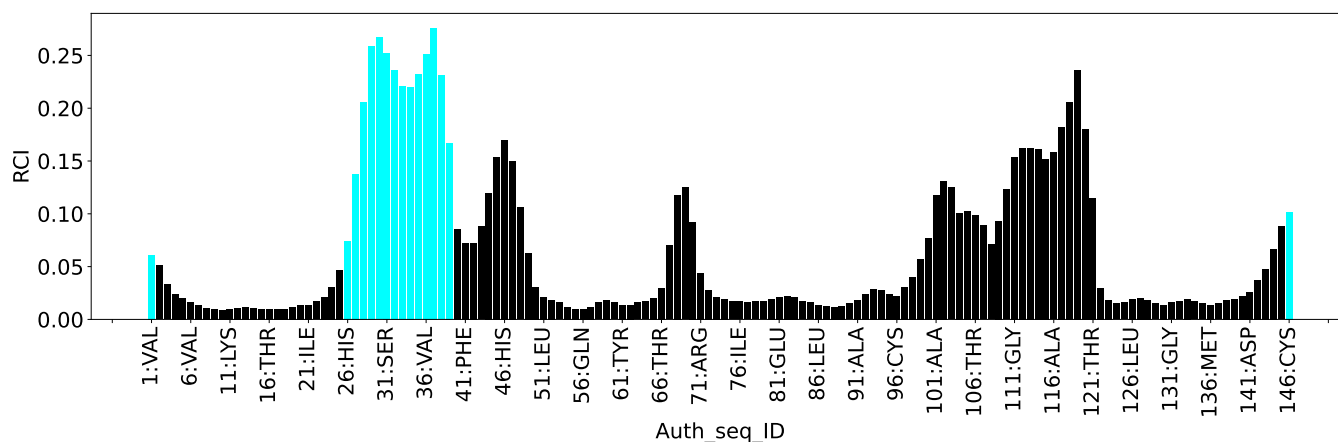
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	78	ASN	CG	2.83	164.52 – 188.90	-71.3

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	7121
Intra-residue ($ i-j =0$)	2978
Sequential ($ i-j =1$)	1508
Medium range ($ i-j >1$ and $ i-j <5$)	1487
Long range ($ i-j \geq 5$)	1147
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	1
Total dihedral-angle restraints	219
Number of unmapped restraints	0
Number of restraints per residue	50.3
Number of long range restraints per residue ¹	7.9

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	42.7	0.2
0.2-0.5 (Medium)	56.3	0.5
>0.5 (Large)	10.3	1.96

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	46.3	9.94
10.0-20.0 (Medium)	4.6	19.92
>20.0 (Large)	0.2	21.74

9 Distance violation analysis ⓘ

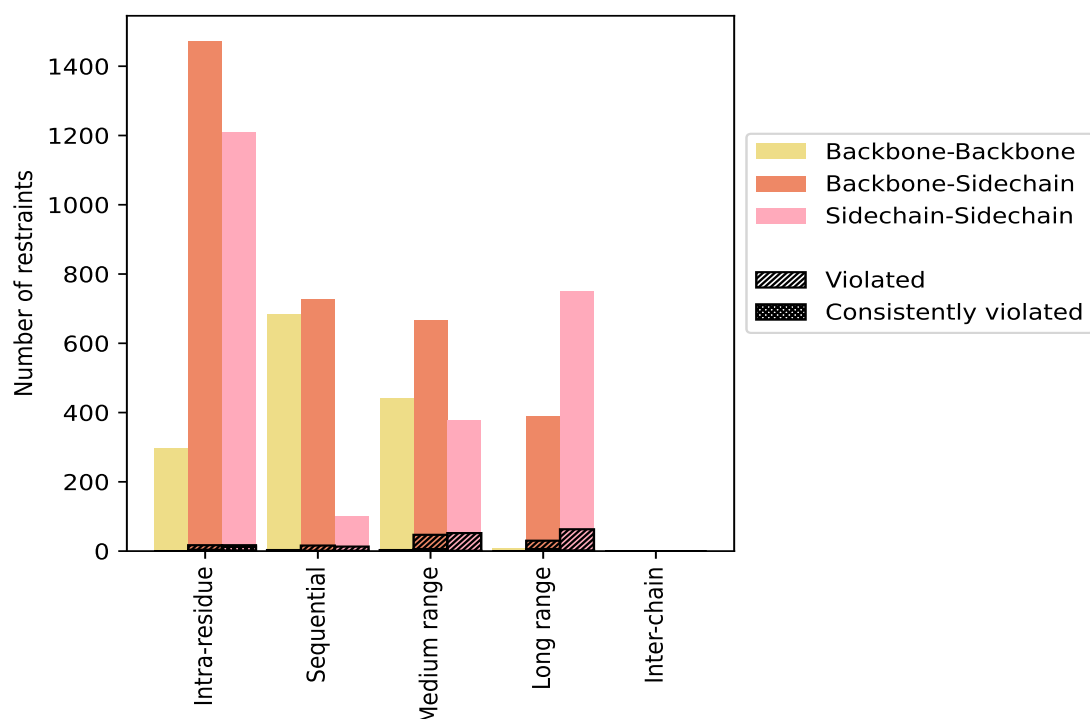
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	2978	41.8	34	1.1	0.5	17	0.6	0.2
Backbone-Backbone	296	4.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1472	20.7	17	1.2	0.2	4	0.3	0.1
Sidechain-Sidechain	1210	17.0	17	1.4	0.2	13	1.1	0.2
Sequential (i-j =1)	1508	21.2	32	2.1	0.4	2	0.1	0.0
Backbone-Backbone	682	9.6	3	0.4	0.0	0	0.0	0.0
Backbone-Sidechain	726	10.2	16	2.2	0.2	1	0.1	0.0
Sidechain-Sidechain	100	1.4	13	13.0	0.2	1	1.0	0.0
Medium range (i-j >1 & i-j <5)	1487	20.9	102	6.9	1.4	7	0.5	0.1
Backbone-Backbone	442	6.2	3	0.7	0.0	0	0.0	0.0
Backbone-Sidechain	667	9.4	47	7.0	0.7	6	0.9	0.1
Sidechain-Sidechain	378	5.3	52	13.8	0.7	1	0.3	0.0
Long range (i-j ≥5)	1147	16.1	93	8.1	1.3	8	0.7	0.1
Backbone-Backbone	8	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	390	5.5	30	7.7	0.4	6	1.5	0.1
Sidechain-Sidechain	749	10.5	63	8.4	0.9	2	0.3	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	1	0.0	0	0.0	0.0	0	0.0	0.0
Total	7121	100.0	261	3.7	3.7	34	0.5	0.5
Backbone-Backbone	1428	20.1	6	0.4	0.1	0	0.0	0.0
Backbone-Sidechain	3255	45.7	110	3.4	1.5	17	0.5	0.2
Sidechain-Sidechain	2438	34.2	145	5.9	2.0	17	0.7	0.2

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

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

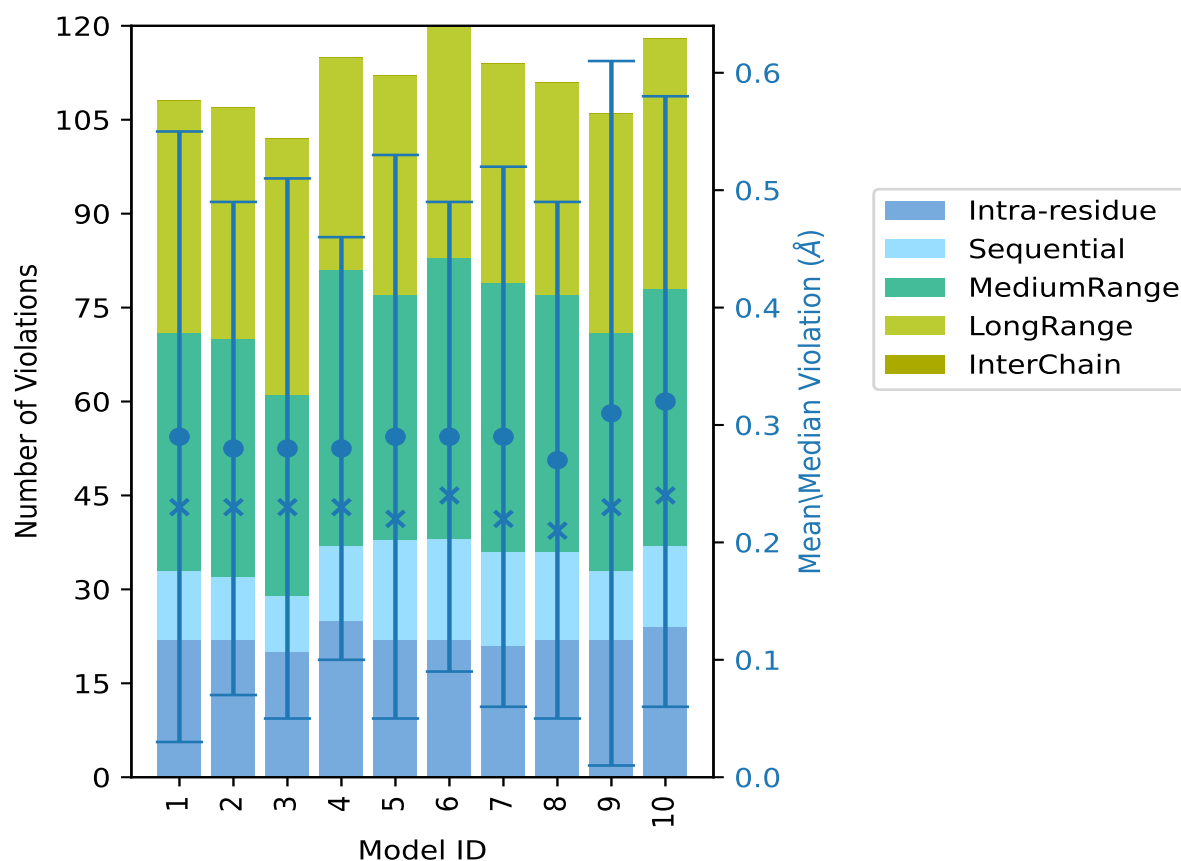
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	22	11	38	37	0	108	0.29	1.96	0.26	0.23
2	22	10	38	37	0	107	0.28	1.51	0.21	0.23
3	20	9	32	41	0	102	0.28	1.49	0.23	0.23
4	25	12	44	34	0	115	0.28	1.58	0.18	0.23
5	22	16	39	35	0	112	0.29	1.59	0.24	0.22
6	22	16	45	37	0	120	0.29	1.45	0.2	0.24
7	21	15	43	35	0	114	0.29	1.55	0.23	0.22
8	22	14	41	34	0	111	0.27	1.44	0.22	0.21
9	22	11	38	35	0	106	0.31	1.69	0.3	0.23
10	24	13	41	40	0	118	0.32	1.56	0.26	0.24

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 6859(IR:2944, SQ:1476, MR:1385, LR:1054, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
3	9	25	31	0	68	1	10.0
6	4	24	13	0	47	2	20.0
3	3	9	13	0	28	3	30.0

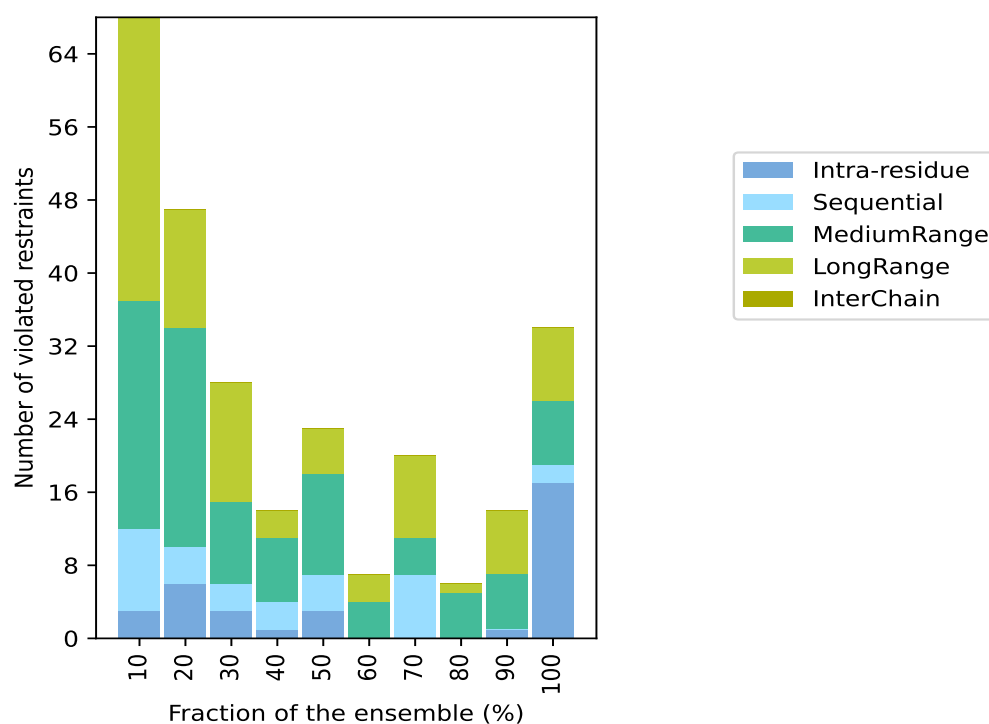
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	3	7	3	0	14	4	40.0
3	4	11	5	0	23	5	50.0
0	0	4	3	0	7	6	60.0
0	7	4	9	0	20	7	70.0
0	0	5	1	0	6	8	80.0
1	0	6	7	0	14	9	90.0
17	2	7	8	0	34	10	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶ Number of models with violations

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

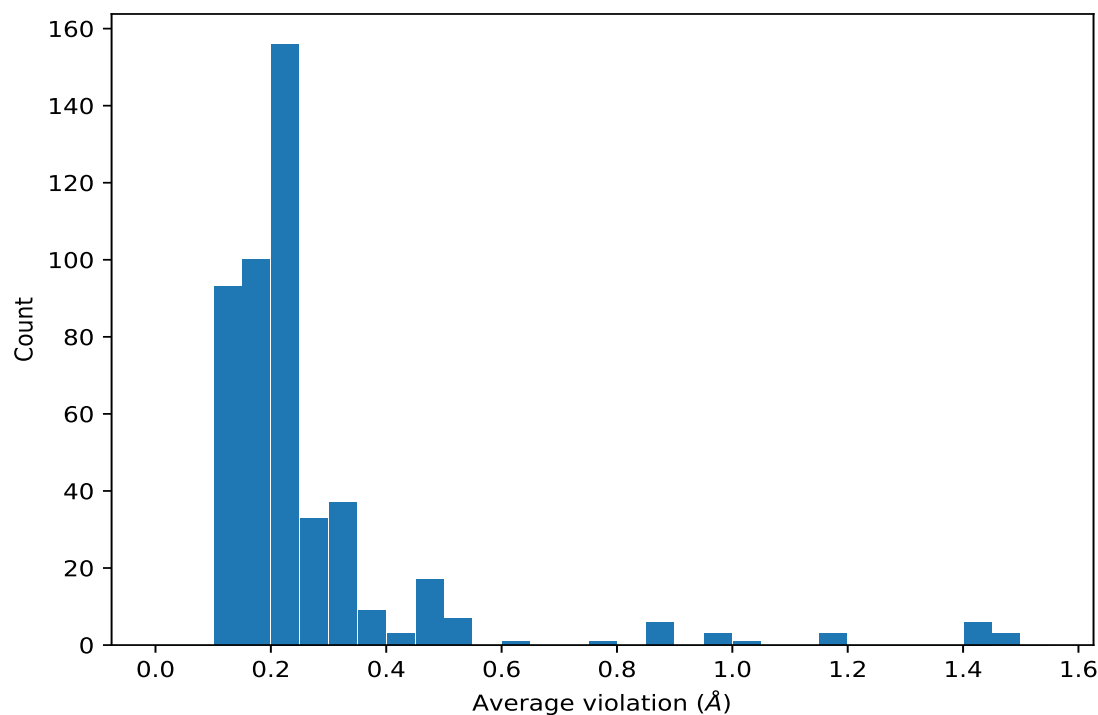


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	10	1.17	0.47	1.12
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	10	1.17	0.47	1.12
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	10	1.17	0.47	1.12
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	10	0.98	0.47	0.86
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	10	0.75	0.16	0.69
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	10	0.63	0.21	0.67
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	10	0.54	0.1	0.54
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	10	0.54	0.1	0.54
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	10	0.54	0.1	0.54
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	10	0.5	0.09	0.5
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	10	0.5	0.09	0.5
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	10	0.5	0.09	0.5
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	10	0.47	0.06	0.45
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	10	0.46	0.13	0.48
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	10	0.45	0.1	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	10	0.45	0.1	0.45
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	10	0.45	0.1	0.45
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	10	0.44	0.06	0.43
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	10	0.37	0.1	0.36
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	10	0.33	0.17	0.28
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	10	0.33	0.05	0.32
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	10	0.32	0.03	0.31
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	10	0.27	0.12	0.26
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	10	0.27	0.06	0.27
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	10	0.25	0.06	0.26
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	10	0.25	0.06	0.26
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	10	0.25	0.06	0.26
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	10	0.25	0.05	0.24
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	10	0.24	0.01	0.24
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	10	0.24	0.01	0.24
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	10	0.24	0.01	0.24
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	10	0.24	0.01	0.24
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	10	0.24	0.01	0.24
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	10	0.24	0.01	0.24
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	10	0.24	0.01	0.24
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	10	0.24	0.01	0.24
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	10	0.24	0.01	0.24
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	10	0.24	0.01	0.24
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	10	0.23	0.0	0.23
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	10	0.23	0.0	0.23
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	10	0.23	0.01	0.23
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	10	0.23	0.01	0.23
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	10	0.23	0.01	0.23
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	10	0.23	0.01	0.23
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	10	0.23	0.01	0.23
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	10	0.23	0.01	0.23
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	10	0.23	0.03	0.23
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	10	0.23	0.0	0.23
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	10	0.23	0.0	0.23
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	10	0.22	0.0	0.22
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	10	0.22	0.0	0.22
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	10	0.21	0.0	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	10	0.21	0.0	0.21
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	10	0.21	0.0	0.21
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	10	0.21	0.0	0.21
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	10	0.2	0.02	0.2
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	10	0.2	0.02	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	10	0.17	0.03	0.16
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	9	0.48	0.13	0.53
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	9	0.48	0.13	0.53
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	9	0.48	0.13	0.53
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	9	0.38	0.08	0.41
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	9	0.38	0.08	0.41
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	9	0.38	0.08	0.41
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	9	0.34	0.1	0.36
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	9	0.34	0.1	0.36
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	9	0.34	0.1	0.36
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	9	0.31	0.06	0.32
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	9	0.31	0.06	0.32
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	9	0.27	0.03	0.27
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	9	0.27	0.03	0.27
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	9	0.27	0.03	0.27
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	9	0.25	0.1	0.22
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	9	0.22	0.07	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	9	0.22	0.07	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	9	0.22	0.07	0.27
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	9	0.2	0.06	0.18
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	9	0.2	0.06	0.18
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	9	0.2	0.06	0.18
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	9	0.2	0.06	0.18
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	9	0.2	0.06	0.18
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	9	0.2	0.06	0.18
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	9	0.2	0.06	0.18
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	9	0.2	0.06	0.18
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	9	0.2	0.06	0.18
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	9	0.2	0.06	0.19
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	9	0.19	0.02	0.19
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	9	0.19	0.02	0.19
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	9	0.19	0.02	0.19
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	9	0.18	0.04	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	9	0.16	0.04	0.17
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	9	0.14	0.02	0.14
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	8	0.3	0.06	0.3
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	8	0.3	0.06	0.3
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	8	0.3	0.06	0.3
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	8	0.27	0.07	0.28
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	8	0.27	0.07	0.28
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	8	0.27	0.07	0.28
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	8	0.22	0.04	0.21
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	8	0.22	0.04	0.21
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	8	0.22	0.04	0.21
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	8	0.21	0.08	0.18
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	8	0.21	0.08	0.18
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	8	0.21	0.08	0.18
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	8	0.2	0.05	0.2
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	8	0.2	0.05	0.2
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	8	0.2	0.05	0.2
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	8	0.2	0.05	0.2
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	8	0.2	0.05	0.2
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	8	0.2	0.05	0.2
(2,1539)	1:67:A:SER:H	1:68:A:MET:HB2	7	0.5	0.12	0.48
(2,1538)	1:68:A:MET:HB3	1:67:A:SER:H	7	0.35	0.1	0.33
(2,1527)	1:68:A:MET:HE1	1:65:A:LEU:H	7	0.33	0.13	0.32
(2,1527)	1:68:A:MET:HE2	1:65:A:LEU:H	7	0.33	0.13	0.32
(2,1527)	1:68:A:MET:HE3	1:65:A:LEU:H	7	0.33	0.13	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1650)	1:73:A:VAL:HB	1:70:A:SER:H	7	0.31	0.04	0.29
(2,1651)	1:70:A:SER:H	1:73:A:VAL:HB	7	0.31	0.04	0.29
(2,224)	1:8:A:ASP:HB2	1:5:A:LYS:HB3	7	0.25	0.08	0.25
(2,1541)	1:68:A:MET:HE1	1:67:A:SER:H	7	0.24	0.05	0.22
(2,1541)	1:68:A:MET:HE2	1:67:A:SER:H	7	0.24	0.05	0.22
(2,1541)	1:68:A:MET:HE3	1:67:A:SER:H	7	0.24	0.05	0.22
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE1	7	0.24	0.05	0.22
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE2	7	0.24	0.05	0.22
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE3	7	0.24	0.05	0.22
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD11	7	0.23	0.09	0.2
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD12	7	0.23	0.09	0.2
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD13	7	0.23	0.09	0.2
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD11	7	0.23	0.09	0.2
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD12	7	0.23	0.09	0.2
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD13	7	0.23	0.09	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD11	7	0.23	0.09	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD12	7	0.23	0.09	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD13	7	0.23	0.09	0.2
(2,2970)	1:130:A:GLN:HE21	1:18:A:VAL:HA	7	0.22	0.07	0.24
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG21	7	0.21	0.07	0.2
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG22	7	0.21	0.07	0.2
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG23	7	0.21	0.07	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG21	7	0.21	0.06	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG22	7	0.21	0.06	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG23	7	0.21	0.06	0.2
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG21	7	0.2	0.11	0.14
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG22	7	0.2	0.11	0.14
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG23	7	0.2	0.11	0.14
(2,2843)	1:46:A:HIS:HE1	1:127:A:SER:HA	7	0.19	0.03	0.2
(2,2295)	1:100:A:TRP:HE3	1:84:A:ARG:HB2	7	0.19	0.04	0.19
(2,2679)	1:121:A:THR:HG21	1:120:A:SER:HA	7	0.18	0.03	0.18
(2,2679)	1:121:A:THR:HG22	1:120:A:SER:HA	7	0.18	0.03	0.18
(2,2679)	1:121:A:THR:HG23	1:120:A:SER:HA	7	0.18	0.03	0.18
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG21	7	0.18	0.02	0.18
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG22	7	0.18	0.02	0.18
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG23	7	0.18	0.02	0.18
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD21	7	0.16	0.03	0.16
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD22	7	0.16	0.03	0.16
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD23	7	0.16	0.03	0.16
(2,2304)	1:100:A:TRP:HZ3	1:84:A:ARG:H	7	0.14	0.01	0.14
(2,2305)	1:84:A:ARG:H	1:100:A:TRP:HZ3	7	0.14	0.01	0.14
(2,3113)	1:134:A:GLN:HE21	1:131:A:GLY:HA2	6	1.03	0.62	1.43

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD11	6	0.35	0.07	0.36
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD12	6	0.35	0.07	0.36
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD13	6	0.35	0.07	0.36
(2,988)	1:45:A:LEU:HD11	1:42:A:ILE:HB	6	0.32	0.09	0.29
(2,988)	1:45:A:LEU:HD12	1:42:A:ILE:HB	6	0.32	0.09	0.29
(2,988)	1:45:A:LEU:HD13	1:42:A:ILE:HB	6	0.32	0.09	0.29
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB1	6	0.19	0.04	0.18
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB2	6	0.19	0.04	0.18
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB3	6	0.19	0.04	0.18
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB1	6	0.19	0.04	0.18
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB2	6	0.19	0.04	0.18
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB3	6	0.19	0.04	0.18
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG21	6	0.18	0.06	0.16
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG22	6	0.18	0.06	0.16
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG23	6	0.18	0.06	0.16
(2,1190)	1:51:A:LEU:HD11	1:54:A:MET:HB2	6	0.18	0.05	0.16
(2,1190)	1:51:A:LEU:HD12	1:54:A:MET:HB2	6	0.18	0.05	0.16
(2,1190)	1:51:A:LEU:HD13	1:54:A:MET:HB2	6	0.18	0.05	0.16
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD21	6	0.16	0.02	0.16
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD22	6	0.16	0.02	0.16
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD23	6	0.16	0.02	0.16
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB1	5	1.48	0.09	1.51
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB2	5	1.48	0.09	1.51
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB3	5	1.48	0.09	1.51
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD21	5	0.88	0.22	0.8
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD22	5	0.88	0.22	0.8
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD23	5	0.88	0.22	0.8
(2,2987)	1:130:A:GLN:HE21	1:21:A:ILE:H	5	0.44	0.18	0.45
(2,100)	1:4:A:GLN:HE21	1:4:A:GLN:HA	5	0.42	0.1	0.43
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG21	5	0.37	0.34	0.19
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG22	5	0.37	0.34	0.19
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG23	5	0.37	0.34	0.19
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD11	5	0.35	0.15	0.39
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD12	5	0.35	0.15	0.39
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD13	5	0.35	0.15	0.39
(2,118)	1:2:A:PRO:HB2	1:5:A:LYS:HG2	5	0.34	0.06	0.34
(2,2056)	1:88:A:HIS:HD2	1:87:A:LEU:HB3	5	0.33	0.04	0.34
(2,324)	1:12:A:THR:H	1:11:A:LYS:HD2	5	0.24	0.16	0.15
(2,1393)	1:63:A:GLN:HE21	1:63:A:GLN:HA	5	0.23	0.03	0.24
(2,813)	1:36:A:VAL:HG11	1:35:A:LYS:HA	5	0.22	0.07	0.2
(2,813)	1:36:A:VAL:HG12	1:35:A:LYS:HA	5	0.22	0.07	0.2
(2,813)	1:36:A:VAL:HG13	1:35:A:LYS:HA	5	0.22	0.07	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2240)	1:97:A:HIS:HE1	1:95:A:SER:H	5	0.22	0.05	0.23
(2,3003)	1:126:A:LEU:HD11	1:130:A:GLN:HA	5	0.21	0.1	0.17
(2,3003)	1:126:A:LEU:HD12	1:130:A:GLN:HA	5	0.21	0.1	0.17
(2,3003)	1:126:A:LEU:HD13	1:130:A:GLN:HA	5	0.21	0.1	0.17
(2,2296)	1:100:A:TRP:HE3	1:84:A:ARG:HD3	5	0.19	0.05	0.18
(2,3009)	1:130:A:GLN:HG3	1:127:A:SER:HA	5	0.19	0.06	0.19
(2,1515)	1:68:A:MET:HE1	1:64:A:ILE:HA	5	0.19	0.05	0.17
(2,1515)	1:68:A:MET:HE2	1:64:A:ILE:HA	5	0.19	0.05	0.17
(2,1515)	1:68:A:MET:HE3	1:64:A:ILE:HA	5	0.19	0.05	0.17
(2,729)	1:29:A:SER:H	1:27:A:THR:HB	5	0.18	0.09	0.16
(2,2131)	1:91:A:ALA:HA	1:3:A:ILE:HG13	5	0.17	0.06	0.14
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG21	5	0.15	0.03	0.15
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG22	5	0.15	0.03	0.15
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG23	5	0.15	0.03	0.15
(2,3490)	1:143:A:SER:H	1:141:A:ASP:HA	5	0.15	0.05	0.15
(2,2767)	1:124:A:VAL:HB	1:121:A:THR:HA	5	0.15	0.04	0.15
(2,1566)	1:68:A:MET:HE1	1:69:A:PRO:HD2	5	0.14	0.05	0.12
(2,1566)	1:68:A:MET:HE2	1:69:A:PRO:HD2	5	0.14	0.05	0.12
(2,1566)	1:68:A:MET:HE3	1:69:A:PRO:HD2	5	0.14	0.05	0.12
(2,2203)	1:94:A:LYS:HB2	1:94:A:LYS:HD2	5	0.12	0.01	0.12
(2,886)	1:41:A:PHE:HD1	1:40:A:ASP:HB3	4	0.32	0.12	0.34
(2,886)	1:41:A:PHE:HD2	1:40:A:ASP:HB3	4	0.32	0.12	0.34
(2,391)	1:12:A:THR:HG21	1:15:A:LYS:HB2	4	0.29	0.05	0.31
(2,391)	1:12:A:THR:HG22	1:15:A:LYS:HB2	4	0.29	0.05	0.31
(2,391)	1:12:A:THR:HG23	1:15:A:LYS:HB2	4	0.29	0.05	0.31
(2,2948)	1:129:A:LEU:H	1:128:A:ARG:HD2	4	0.22	0.09	0.22
(2,1163)	1:53:A:LYS:HD2	1:53:A:LYS:HB2	4	0.22	0.05	0.2
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG21	4	0.22	0.05	0.2
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG22	4	0.22	0.05	0.2
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG23	4	0.22	0.05	0.2
(2,779)	1:34:A:GLN:HG2	1:31:A:SER:HB2	4	0.19	0.1	0.15
(2,2515)	1:111:A:GLY:H	1:110:A:LEU:HG	4	0.19	0.05	0.17
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD11	4	0.17	0.04	0.18
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD12	4	0.17	0.04	0.18
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD13	4	0.17	0.04	0.18
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG11	4	0.16	0.06	0.14
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG12	4	0.16	0.06	0.14
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG13	4	0.16	0.06	0.14
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD11	4	0.16	0.05	0.15
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD12	4	0.16	0.05	0.15
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD13	4	0.16	0.05	0.15
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD11	4	0.15	0.04	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD12	4	0.15	0.04	0.15
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD13	4	0.15	0.04	0.15
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD11	4	0.15	0.04	0.15
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD12	4	0.15	0.04	0.15
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD13	4	0.15	0.04	0.15
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD11	4	0.15	0.04	0.15
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD12	4	0.15	0.04	0.15
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD13	4	0.15	0.04	0.15
(2,3108)	1:134:A:GLN:HG2	1:18:A:VAL:HA	4	0.15	0.03	0.15
(2,3087)	1:130:A:GLN:HA	1:133:A:LEU:HG	4	0.15	0.03	0.14
(2,3088)	1:133:A:LEU:HG	1:130:A:GLN:HA	4	0.15	0.03	0.14
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD11	3	0.48	0.27	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD12	3	0.48	0.27	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD13	3	0.48	0.27	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD21	3	0.48	0.27	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD22	3	0.48	0.27	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD23	3	0.48	0.27	0.55
(2,937)	1:41:A:PHE:HZ	1:43:A:PRO:HA	3	0.36	0.1	0.32
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG11	3	0.34	0.01	0.35
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG12	3	0.34	0.01	0.35
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG13	3	0.34	0.01	0.35
(2,1733)	1:75:A:GLN:HE21	1:75:A:GLN:HA	3	0.34	0.15	0.42
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD21	3	0.32	0.02	0.33
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD22	3	0.32	0.02	0.33
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD23	3	0.32	0.02	0.33
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD21	3	0.32	0.02	0.33
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD22	3	0.32	0.02	0.33
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD23	3	0.32	0.02	0.33
(2,2992)	1:21:A:ILE:HD11	1:130:A:GLN:HG2	3	0.26	0.04	0.24
(2,2992)	1:21:A:ILE:HD12	1:130:A:GLN:HG2	3	0.26	0.04	0.24
(2,2992)	1:21:A:ILE:HD13	1:130:A:GLN:HG2	3	0.26	0.04	0.24
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD21	3	0.23	0.03	0.24
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD22	3	0.23	0.03	0.24
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD23	3	0.23	0.03	0.24
(2,2109)	1:90:A:LEU:HD21	1:7:A:GLN:HB2	3	0.23	0.03	0.24
(2,2109)	1:90:A:LEU:HD22	1:7:A:GLN:HB2	3	0.23	0.03	0.24
(2,2109)	1:90:A:LEU:HD23	1:7:A:GLN:HB2	3	0.23	0.03	0.24
(2,3190)	1:136:A:MET:HB3	1:133:A:LEU:HA	3	0.23	0.03	0.22
(2,2911)	1:128:A:ARG:HG2	1:128:A:ARG:HD2	3	0.21	0.01	0.21
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD11	3	0.21	0.07	0.26
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD12	3	0.21	0.07	0.26
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD13	3	0.21	0.07	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD11	3	0.21	0.07	0.26
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD12	3	0.21	0.07	0.26
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD13	3	0.21	0.07	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD11	3	0.21	0.07	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD12	3	0.21	0.07	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD13	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB1	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB2	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB3	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB1	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB2	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB3	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB1	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB2	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB3	3	0.21	0.07	0.26
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD11	3	0.2	0.05	0.17
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD12	3	0.2	0.05	0.17
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD13	3	0.2	0.05	0.17
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD21	3	0.2	0.04	0.17
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD22	3	0.2	0.04	0.17
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD23	3	0.2	0.04	0.17
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG21	3	0.2	0.09	0.14
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG22	3	0.2	0.09	0.14
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG23	3	0.2	0.09	0.14
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG21	3	0.2	0.09	0.14
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG22	3	0.2	0.09	0.14
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG23	3	0.2	0.09	0.14
(2,704)	1:27:A:THR:HG21	1:28:A:GLN:HA	3	0.2	0.03	0.19
(2,704)	1:27:A:THR:HG22	1:28:A:GLN:HA	3	0.2	0.03	0.19
(2,704)	1:27:A:THR:HG23	1:28:A:GLN:HA	3	0.2	0.03	0.19
(2,1537)	1:68:A:MET:HB3	1:67:A:SER:HB2	3	0.19	0.05	0.17
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD11	3	0.17	0.05	0.18
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD12	3	0.17	0.05	0.18
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD13	3	0.17	0.05	0.18
(2,3163)	1:49:A:LEU:HD11	1:136:A:MET:HB2	3	0.17	0.05	0.18
(2,3163)	1:49:A:LEU:HD12	1:136:A:MET:HB2	3	0.17	0.05	0.18
(2,3163)	1:49:A:LEU:HD13	1:136:A:MET:HB2	3	0.17	0.05	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB1	3	0.17	0.02	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB2	3	0.17	0.02	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB3	3	0.17	0.02	0.18
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB1	3	0.17	0.02	0.18
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB2	3	0.17	0.02	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB3	3	0.17	0.02	0.18
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB1	3	0.17	0.02	0.18
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB2	3	0.17	0.02	0.18
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB3	3	0.17	0.02	0.18
(2,2798)	1:119:A:TYR:HE1	1:125:A:ALA:H	3	0.17	0.05	0.14
(2,2798)	1:119:A:TYR:HE2	1:125:A:ALA:H	3	0.17	0.05	0.14
(2,2903)	1:128:A:ARG:HE	1:128:A:ARG:HA	3	0.16	0.02	0.15
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD11	3	0.15	0.03	0.13
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD12	3	0.15	0.03	0.13
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD13	3	0.15	0.03	0.13
(2,3450)	1:142:A:LEU:HD11	1:138:A:TRP:HZ2	3	0.15	0.03	0.13
(2,3450)	1:142:A:LEU:HD12	1:138:A:TRP:HZ2	3	0.15	0.03	0.13
(2,3450)	1:142:A:LEU:HD13	1:138:A:TRP:HZ2	3	0.15	0.03	0.13
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD11	3	0.14	0.0	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD12	3	0.14	0.0	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD13	3	0.14	0.0	0.14
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG21	3	0.13	0.01	0.13
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG22	3	0.13	0.01	0.13
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG23	3	0.13	0.01	0.13
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG21	3	0.13	0.01	0.13
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG22	3	0.13	0.01	0.13
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG23	3	0.13	0.01	0.13
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG21	3	0.13	0.01	0.13
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG22	3	0.13	0.01	0.13
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG23	3	0.13	0.01	0.13
(2,426)	1:16:A:THR:H	1:15:A:LYS:HD2	3	0.12	0.01	0.11
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD21	3	0.12	0.02	0.12
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD22	3	0.12	0.02	0.12
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD23	3	0.12	0.02	0.12
(2,3461)	1:142:A:LEU:HD11	1:139:A:GLN:HE21	2	1.45	0.11	1.45
(2,3461)	1:142:A:LEU:HD12	1:139:A:GLN:HE21	2	1.45	0.11	1.45
(2,3461)	1:142:A:LEU:HD13	1:139:A:GLN:HE21	2	1.45	0.11	1.45
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD11	2	1.45	0.11	1.45
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD12	2	1.45	0.11	1.45
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD13	2	1.45	0.11	1.45
(2,3347)	1:135:A:ASP:HB2	1:139:A:GLN:HE21	2	0.96	0.56	0.96
(2,3348)	1:139:A:GLN:HE21	1:135:A:ASP:HB2	2	0.96	0.56	0.96
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD11	2	0.86	0.07	0.86
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD12	2	0.86	0.07	0.86
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD13	2	0.86	0.07	0.86
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG21	2	0.47	0.28	0.47
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG22	2	0.47	0.28	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG23	2	0.47	0.28	0.47
(2,325)	1:12:A:THR:H	1:11:A:LYS:HE2	2	0.36	0.11	0.36
(2,2414)	1:105:A:GLU:H	1:56:A:GLN:HE22	2	0.26	0.11	0.26
(2,2415)	1:56:A:GLN:HE22	1:105:A:GLU:H	2	0.26	0.11	0.26
(2,2765)	1:120:A:SER:H	1:124:A:VAL:HB	2	0.26	0.06	0.26
(2,203)	1:7:A:GLN:HE21	1:7:A:GLN:HA	2	0.26	0.08	0.26
(2,1143)	1:49:A:LEU:HD21	1:53:A:LYS:HE2	2	0.25	0.01	0.25
(2,1143)	1:49:A:LEU:HD22	1:53:A:LYS:HE2	2	0.25	0.01	0.25
(2,1143)	1:49:A:LEU:HD23	1:53:A:LYS:HE2	2	0.25	0.01	0.25
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD21	2	0.25	0.01	0.25
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD22	2	0.25	0.01	0.25
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD23	2	0.25	0.01	0.25
(2,755)	1:30:A:VAL:HB	1:32:A:SER:HB2	2	0.24	0.1	0.24
(2,3173)	1:136:A:MET:HE1	1:57:A:THR:HA	2	0.24	0.05	0.24
(2,3173)	1:136:A:MET:HE2	1:57:A:THR:HA	2	0.24	0.05	0.24
(2,3173)	1:136:A:MET:HE3	1:57:A:THR:HA	2	0.24	0.05	0.24
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG21	2	0.22	0.06	0.22
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG22	2	0.22	0.06	0.22
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG23	2	0.22	0.06	0.22
(2,141)	1:5:A:LYS:H	1:5:A:LYS:HE2	2	0.22	0.08	0.22
(2,3058)	1:132:A:SER:H	1:130:A:GLN:HG3	2	0.21	0.05	0.21
(2,989)	1:45:A:LEU:H	1:42:A:ILE:HB	2	0.2	0.0	0.2
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD21	2	0.2	0.02	0.2
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD22	2	0.2	0.02	0.2
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD23	2	0.2	0.02	0.2
(2,1656)	1:73:A:VAL:H	1:71:A:ARG:HB2	2	0.19	0.05	0.19
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD21	2	0.18	0.04	0.18
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD22	2	0.18	0.04	0.18
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD23	2	0.18	0.04	0.18
(2,730)	1:29:A:SER:H	1:27:A:THR:HG21	2	0.18	0.02	0.18
(2,730)	1:29:A:SER:H	1:27:A:THR:HG22	2	0.18	0.02	0.18
(2,730)	1:29:A:SER:H	1:27:A:THR:HG23	2	0.18	0.02	0.18
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG21	2	0.18	0.02	0.18
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG22	2	0.18	0.02	0.18
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG23	2	0.18	0.02	0.18
(2,1175)	1:53:A:LYS:H	1:53:A:LYS:HE2	2	0.18	0.0	0.18
(2,3234)	1:137:A:LEU:HD21	1:11:A:LYS:HE2	2	0.17	0.05	0.17
(2,3234)	1:137:A:LEU:HD22	1:11:A:LYS:HE2	2	0.17	0.05	0.17
(2,3234)	1:137:A:LEU:HD23	1:11:A:LYS:HE2	2	0.17	0.05	0.17
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD21	2	0.17	0.05	0.17
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD22	2	0.17	0.05	0.17
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD23	2	0.17	0.05	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2616)	1:117:A:SER:HB2	1:117:A:SER:HA	2	0.16	0.02	0.16
(2,1567)	1:68:A:MET:HG2	1:69:A:PRO:HD2	2	0.16	0.01	0.16
(2,2696)	1:68:A:MET:HE1	1:122:A:GLU:HG2	2	0.16	0.04	0.16
(2,2696)	1:68:A:MET:HE2	1:122:A:GLU:HG2	2	0.16	0.04	0.16
(2,2696)	1:68:A:MET:HE3	1:122:A:GLU:HG2	2	0.16	0.04	0.16
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE1	2	0.16	0.04	0.16
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE2	2	0.16	0.04	0.16
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE3	2	0.16	0.04	0.16
(2,589)	1:24:A:ILE:HD11	1:21:A:ILE:HA	2	0.16	0.02	0.16
(2,589)	1:24:A:ILE:HD12	1:21:A:ILE:HA	2	0.16	0.02	0.16
(2,589)	1:24:A:ILE:HD13	1:21:A:ILE:HA	2	0.16	0.02	0.16
(2,2693)	1:68:A:MET:HE1	1:122:A:GLU:HB3	2	0.16	0.05	0.16
(2,2693)	1:68:A:MET:HE2	1:122:A:GLU:HB3	2	0.16	0.05	0.16
(2,2693)	1:68:A:MET:HE3	1:122:A:GLU:HB3	2	0.16	0.05	0.16
(2,293)	1:11:A:LYS:HE2	1:11:A:LYS:HA	2	0.15	0.01	0.15
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD21	2	0.15	0.01	0.15
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD22	2	0.15	0.01	0.15
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD23	2	0.15	0.01	0.15
(2,1030)	1:46:A:HIS:HD2	1:47:A:PRO:HD3	2	0.15	0.04	0.15
(2,832)	1:37:A:THR:H	1:35:A:LYS:HD2	2	0.15	0.04	0.15
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG21	2	0.14	0.04	0.14
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG22	2	0.14	0.04	0.14
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG23	2	0.14	0.04	0.14
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG21	2	0.14	0.04	0.14
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG22	2	0.14	0.04	0.14
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG23	2	0.14	0.04	0.14
(2,2817)	1:76:A:ILE:HD11	1:126:A:LEU:HA	2	0.14	0.01	0.14
(2,2817)	1:76:A:ILE:HD12	1:126:A:LEU:HA	2	0.14	0.01	0.14
(2,2817)	1:76:A:ILE:HD13	1:126:A:LEU:HA	2	0.14	0.01	0.14
(2,3122)	1:134:A:GLN:HE21	1:134:A:GLN:HA	2	0.14	0.01	0.14
(2,655)	1:26:A:HIS:HD2	1:23:A:ASP:HA	2	0.13	0.02	0.13
(2,1014)	1:46:A:HIS:HD2	1:45:A:LEU:HB2	2	0.12	0.02	0.12
(2,1011)	1:46:A:HIS:HD2	1:42:A:ILE:HG13	2	0.12	0.02	0.12
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD21	2	0.12	0.02	0.12
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD22	2	0.12	0.02	0.12
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD23	2	0.12	0.02	0.12
(2,2395)	1:104:A:LEU:HD21	1:63:A:GLN:HE21	2	0.12	0.0	0.12
(2,2395)	1:104:A:LEU:HD22	1:63:A:GLN:HE21	2	0.12	0.0	0.12
(2,2395)	1:104:A:LEU:HD23	1:63:A:GLN:HE21	2	0.12	0.0	0.12
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD21	2	0.12	0.0	0.12
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD22	2	0.12	0.0	0.12
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD23	2	0.12	0.0	0.12

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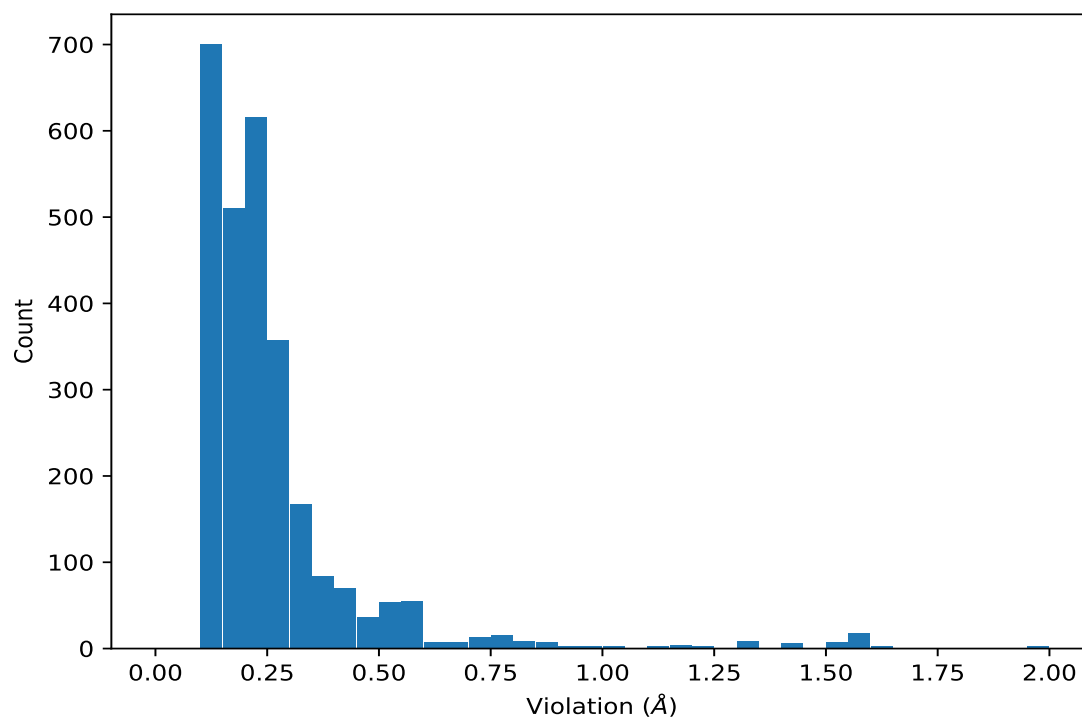
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2626)	1:119:A:TYR:HE1	1:38:A:GLY:HA2	2	0.12	0.0	0.12
(2,2626)	1:119:A:TYR:HE2	1:38:A:GLY:HA2	2	0.12	0.0	0.12

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

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



9.5.2 Table : All distance violations [i](#)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	1	1.96
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	1	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	1	1.96
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	9	1.69
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	9	1.63
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	9	1.63
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	9	1.63
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	5	1.59
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	5	1.59
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	5	1.59
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB1	4	1.58
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB2	4	1.58
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB3	4	1.58
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD11	10	1.56
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD12	10	1.56
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD13	10	1.56
(2,3461)	1:142:A:LEU:HD11	1:139:A:GLN:HE21	10	1.56
(2,3461)	1:142:A:LEU:HD12	1:139:A:GLN:HE21	10	1.56
(2,3461)	1:142:A:LEU:HD13	1:139:A:GLN:HE21	10	1.56
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	10	1.56
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	10	1.56
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	10	1.56
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB1	7	1.55
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB2	7	1.55
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB3	7	1.55
(2,3348)	1:139:A:GLN:HE21	1:135:A:ASP:HB2	9	1.52
(2,3347)	1:135:A:ASP:HB2	1:139:A:GLN:HE21	9	1.52
(2,3113)	1:134:A:GLN:HE21	1:131:A:GLY:HA2	5	1.51
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB1	2	1.51
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB2	2	1.51
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB3	2	1.51
(2,3113)	1:134:A:GLN:HE21	1:131:A:GLY:HA2	1	1.5
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	3	1.49
(2,3113)	1:134:A:GLN:HE21	1:131:A:GLY:HA2	6	1.45
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	8	1.44
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB1	8	1.42
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB2	8	1.42
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB3	8	1.42
(2,3113)	1:134:A:GLN:HE21	1:131:A:GLY:HA2	2	1.41
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	1	1.4
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD11	7	1.34
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD12	7	1.34
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD13	7	1.34
(2,3461)	1:142:A:LEU:HD11	1:139:A:GLN:HE21	7	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3461)	1:142:A:LEU:HD12	1:139:A:GLN:HE21	7	1.34
(2,3461)	1:142:A:LEU:HD13	1:139:A:GLN:HE21	7	1.34
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB1	6	1.33
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB2	6	1.33
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB3	6	1.33
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	3	1.24
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	3	1.24
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	3	1.24
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD21	3	1.18
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD22	3	1.18
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD23	3	1.18
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	5	1.16
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD21	5	1.1
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD22	5	1.1
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD23	5	1.1
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	10	1.06
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG21	9	1.04
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG22	9	1.04
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG23	9	1.04
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	8	0.99
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	8	0.99
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	8	0.99
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD11	3	0.94
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD12	3	0.94
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD13	3	0.94
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	8	0.88
(2,3337)	1:139:A:GLN:HE21	1:48:A:ILE:HD11	7	0.87
(2,3337)	1:139:A:GLN:HE21	1:48:A:ILE:HD12	7	0.87
(2,3337)	1:139:A:GLN:HE21	1:48:A:ILE:HD13	7	0.87
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	7	0.87
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	10	0.87
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	6	0.87
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	2	0.85
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	4	0.82
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	4	0.82
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	4	0.82
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	3	0.81
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	4	0.81
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD21	10	0.8
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD22	10	0.8
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD23	10	0.8
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD11	10	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD12	10	0.79
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD13	10	0.79
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD11	10	0.77
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD12	10	0.77
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD13	10	0.77
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD21	10	0.77
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD22	10	0.77
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD23	10	0.77
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	6	0.75
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	6	0.75
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	6	0.75
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	8	0.75
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG21	1	0.75
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG22	1	0.75
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG23	1	0.75
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	2	0.74
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	2	0.74
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	2	0.74
(2,3389)	1:140:A:LEU:HD21	1:11:A:LYS:HE2	9	0.73
(2,3389)	1:140:A:LEU:HD22	1:11:A:LYS:HE2	9	0.73
(2,3389)	1:140:A:LEU:HD23	1:11:A:LYS:HE2	9	0.73
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	9	0.72
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD21	1	0.71
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD22	1	0.71
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD23	1	0.71
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	8	0.71
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	8	0.71
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	8	0.71
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	4	0.7
(2,1539)	1:67:A:SER:H	1:68:A:MET:HB2	6	0.69
(2,2987)	1:130:A:GLN:HE21	1:21:A:ILE:H	2	0.68
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	3	0.68
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	10	0.65
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	10	0.65
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	10	0.65
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	4	0.65
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	1	0.64
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	7	0.64
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	4	0.62
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	5	0.62
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	5	0.62
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	5	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	8	0.62
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	9	0.61
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD11	6	0.6
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD12	6	0.6
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD13	6	0.6
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	7	0.6
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	7	0.6
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	7	0.6
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD21	9	0.6
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD22	9	0.6
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD23	9	0.6
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	2	0.6
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	2	0.6
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	2	0.6
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	10	0.6
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	2	0.59
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	8	0.59
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	8	0.59
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	8	0.59
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	5	0.59
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	5	0.58
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	3	0.57
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	3	0.57
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	3	0.57
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	9	0.57
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	9	0.57
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	9	0.57
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	6	0.57
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	6	0.57
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	6	0.57
(2,1539)	1:67:A:SER:H	1:68:A:MET:HB2	10	0.57
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	1	0.57
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	3	0.56
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	3	0.56
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	3	0.56
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	8	0.56
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	8	0.56
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	8	0.56
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	6	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD11	3	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD12	3	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD13	3	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD21	3	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD22	3	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD23	3	0.55
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	10	0.55
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	10	0.55
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	10	0.55
(2,1539)	1:67:A:SER:H	1:68:A:MET:HB2	5	0.55
(2,324)	1:12:A:THR:H	1:11:A:LYS:HD2	10	0.55
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	2	0.55
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	2	0.55
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	2	0.55
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	9	0.55
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	9	0.55
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	9	0.55
(2,100)	1:4:A:GLN:HE21	1:4:A:GLN:HA	7	0.55
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	5	0.54
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	4	0.54
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	4	0.54
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	4	0.54
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	7	0.54
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	7	0.54
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	7	0.54
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	9	0.53
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	9	0.53
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	9	0.53
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	3	0.53
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	3	0.53
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	3	0.53
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	5	0.53
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	6	0.53
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	1	0.52
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	1	0.52
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	1	0.52
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	4	0.52
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	6	0.52
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	6	0.52
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	6	0.52
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	2	0.51
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	2	0.51
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	2	0.51
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	4	0.51
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	4	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	4	0.51
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	9	0.51
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	9	0.51
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	9	0.51
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	10	0.51
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	2	0.51
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	5	0.51
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	5	0.51
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	5	0.51
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	8	0.5
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	8	0.5
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	8	0.5
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	2	0.5
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	2	0.5
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	2	0.5
(2,1527)	1:68:A:MET:HE1	1:65:A:LEU:H	2	0.5
(2,1527)	1:68:A:MET:HE2	1:65:A:LEU:H	2	0.5
(2,1527)	1:68:A:MET:HE3	1:65:A:LEU:H	2	0.5
(2,1527)	1:68:A:MET:HE1	1:65:A:LEU:H	6	0.5
(2,1527)	1:68:A:MET:HE2	1:65:A:LEU:H	6	0.5
(2,1527)	1:68:A:MET:HE3	1:65:A:LEU:H	6	0.5
(2,988)	1:45:A:LEU:HD11	1:42:A:ILE:HB	10	0.5
(2,988)	1:45:A:LEU:HD12	1:42:A:ILE:HB	10	0.5
(2,988)	1:45:A:LEU:HD13	1:42:A:ILE:HB	10	0.5
(2,937)	1:41:A:PHE:HZ	1:43:A:PRO:HA	3	0.5
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	4	0.5
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	2	0.5
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	10	0.49
(2,2987)	1:130:A:GLN:HE21	1:21:A:ILE:H	7	0.49
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	5	0.49
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	5	0.49
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	5	0.49
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	1	0.48
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	1	0.48
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	1	0.48
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	1	0.48
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	4	0.48
(2,1733)	1:75:A:GLN:HE21	1:75:A:GLN:HA	6	0.48
(2,1539)	1:67:A:SER:H	1:68:A:MET:HB2	4	0.48
(2,1539)	1:67:A:SER:H	1:68:A:MET:HB2	7	0.48
(2,1538)	1:68:A:MET:HB3	1:67:A:SER:H	1	0.48
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	7	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	7	0.47
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	7	0.47
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	10	0.47
(2,325)	1:12:A:THR:H	1:11:A:LYS:HE2	9	0.47
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	4	0.46
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD11	4	0.46
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD12	4	0.46
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD13	4	0.46
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	6	0.46
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	6	0.46
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	6	0.46
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	7	0.46
(2,1538)	1:68:A:MET:HB3	1:67:A:SER:H	9	0.46
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	4	0.46
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	7	0.46
(2,2987)	1:130:A:GLN:HE21	1:21:A:ILE:H	5	0.45
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	4	0.45
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	4	0.45
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	4	0.45
(2,886)	1:41:A:PHE:HD1	1:40:A:ASP:HB3	7	0.45
(2,886)	1:41:A:PHE:HD2	1:40:A:ASP:HB3	7	0.45
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	8	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	6	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	6	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	6	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	9	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	9	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	9	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	10	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	10	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	10	0.44
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	4	0.44
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	4	0.44
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	4	0.44
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	5	0.44
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	5	0.44
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	5	0.44
(2,1539)	1:67:A:SER:H	1:68:A:MET:HB2	8	0.44
(2,118)	1:2:A:PRO:HB2	1:5:A:LYS:HG2	6	0.44
(2,100)	1:4:A:GLN:HE21	1:4:A:GLN:HA	6	0.44
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	5	0.43
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	7	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	9	0.43
(2,2987)	1:130:A:GLN:HE21	1:21:A:ILE:H	6	0.43
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG21	6	0.43
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG22	6	0.43
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG23	6	0.43
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	7	0.43
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD11	10	0.43
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD12	10	0.43
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD13	10	0.43
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD11	10	0.43
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD12	10	0.43
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD13	10	0.43
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD11	10	0.43
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD12	10	0.43
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD13	10	0.43
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	7	0.43
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	8	0.43
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	9	0.43
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	6	0.43
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	7	0.43
(2,100)	1:4:A:GLN:HE21	1:4:A:GLN:HA	10	0.43
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	1	0.42
(2,1733)	1:75:A:GLN:HE21	1:75:A:GLN:HA	1	0.42
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	6	0.42
(2,100)	1:4:A:GLN:HE21	1:4:A:GLN:HA	9	0.42
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD11	7	0.41
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD12	7	0.41
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD13	7	0.41
(2,3003)	1:126:A:LEU:HD11	1:130:A:GLN:HA	1	0.41
(2,3003)	1:126:A:LEU:HD12	1:130:A:GLN:HA	1	0.41
(2,3003)	1:126:A:LEU:HD13	1:130:A:GLN:HA	1	0.41
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	5	0.41
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	5	0.41
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	5	0.41
(2,1538)	1:68:A:MET:HB3	1:67:A:SER:H	3	0.41
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	1	0.41
(2,886)	1:41:A:PHE:HD1	1:40:A:ASP:HB3	10	0.41
(2,886)	1:41:A:PHE:HD2	1:40:A:ASP:HB3	10	0.41
(2,3348)	1:139:A:GLN:HE21	1:135:A:ASP:HB2	5	0.4
(2,3347)	1:135:A:ASP:HB2	1:139:A:GLN:HE21	5	0.4
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	5	0.4
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	10	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	1	0.4
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	1	0.4
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	1	0.4
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	10	0.4
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	10	0.4
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	10	0.4
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	9	0.4
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	3	0.39
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	2	0.39
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	6	0.39
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD11	1	0.39
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD12	1	0.39
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD13	1	0.39
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD11	8	0.39
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD12	8	0.39
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD13	8	0.39
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	1	0.39
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	2	0.39
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	2	0.39
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	2	0.39
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	9	0.39
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	10	0.39
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	10	0.39
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	10	0.39
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	7	0.38
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	7	0.38
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	7	0.38
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	2	0.38
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	2	0.38
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	4	0.38
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	4	0.38
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	4	0.38
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	1	0.38
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	3	0.38
(2,2056)	1:88:A:HIS:HD2	1:87:A:LEU:HB3	3	0.38
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	2	0.38
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	4	0.37
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	4	0.37
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	4	0.37
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	5	0.37
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	5	0.37
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2415)	1:56:A:GLN:HE22	1:105:A:GLU:H	6	0.37
(2,2414)	1:105:A:GLU:H	1:56:A:GLN:HE22	6	0.37
(2,1651)	1:70:A:SER:H	1:73:A:VAL:HB	1	0.37
(2,1650)	1:73:A:VAL:HB	1:70:A:SER:H	1	0.37
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	9	0.37
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	9	0.37
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	9	0.37
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	3	0.37
(2,224)	1:8:A:ASP:HB2	1:5:A:LYS:HB3	3	0.37
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	6	0.36
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD11	8	0.36
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD12	8	0.36
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD13	8	0.36
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD11	9	0.36
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD12	9	0.36
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD13	9	0.36
(2,2927)	1:129:A:LEU:HD11	1:61:A:TYR:HE1	3	0.36
(2,2927)	1:129:A:LEU:HD11	1:61:A:TYR:HE2	3	0.36
(2,2927)	1:129:A:LEU:HD12	1:61:A:TYR:HE1	3	0.36
(2,2927)	1:129:A:LEU:HD12	1:61:A:TYR:HE2	3	0.36
(2,2927)	1:129:A:LEU:HD13	1:61:A:TYR:HE1	3	0.36
(2,2927)	1:129:A:LEU:HD13	1:61:A:TYR:HE2	3	0.36
(2,2926)	1:61:A:TYR:HE1	1:129:A:LEU:HD11	3	0.36
(2,2926)	1:61:A:TYR:HE1	1:129:A:LEU:HD12	3	0.36
(2,2926)	1:61:A:TYR:HE1	1:129:A:LEU:HD13	3	0.36
(2,2926)	1:61:A:TYR:HE2	1:129:A:LEU:HD11	3	0.36
(2,2926)	1:61:A:TYR:HE2	1:129:A:LEU:HD12	3	0.36
(2,2926)	1:61:A:TYR:HE2	1:129:A:LEU:HD13	3	0.36
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	6	0.36
(2,2664)	1:68:A:MET:HE1	1:120:A:SER:HB2	3	0.36
(2,2664)	1:68:A:MET:HE2	1:120:A:SER:HB2	3	0.36
(2,2664)	1:68:A:MET:HE3	1:120:A:SER:HB2	3	0.36
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	7	0.36
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	7	0.36
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	5	0.36
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	5	0.36
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	5	0.36
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	7	0.36
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	7	0.36
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	7	0.36
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	3	0.36
(2,1527)	1:68:A:MET:HE1	1:65:A:LEU:H	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1527)	1:68:A:MET:HE2	1:65:A:LEU:H	7	0.36
(2,1527)	1:68:A:MET:HE3	1:65:A:LEU:H	7	0.36
(2,779)	1:34:A:GLN:HG2	1:31:A:SER:HB2	5	0.36
(2,729)	1:29:A:SER:H	1:27:A:THR:HB	9	0.36
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	7	0.36
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	7	0.36
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	7	0.36
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	2	0.35
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	4	0.35
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	6	0.35
(2,2056)	1:88:A:HIS:HD2	1:87:A:LEU:HB3	6	0.35
(2,1651)	1:70:A:SER:H	1:73:A:VAL:HB	10	0.35
(2,1650)	1:73:A:VAL:HB	1:70:A:SER:H	10	0.35
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	2	0.35
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	2	0.35
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	2	0.35
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	6	0.35
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	6	0.35
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	6	0.35
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD21	6	0.35
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD22	6	0.35
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD23	6	0.35
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD21	6	0.35
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD22	6	0.35
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD23	6	0.35
(2,755)	1:30:A:VAL:HB	1:32:A:SER:HB2	6	0.35
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	1	0.35
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	1	0.35
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	1	0.35
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	4	0.35
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	4	0.35
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	4	0.35
(2,118)	1:2:A:PRO:HB2	1:5:A:LYS:HG2	4	0.35
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG11	4	0.35
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG12	4	0.35
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG13	4	0.35
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG11	6	0.35
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG12	6	0.35
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG13	6	0.35
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG21	10	0.34
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG22	10	0.34
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG23	10	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	10	0.34
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	10	0.34
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	10	0.34
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	8	0.34
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	8	0.34
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	8	0.34
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	2	0.34
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	9	0.34
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	9	0.34
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	8	0.34
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	8	0.34
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	8	0.34
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	6	0.34
(2,2527)	1:41:A:PHE:HE2	1:113:A:VAL:HG21	5	0.34
(2,2527)	1:41:A:PHE:HE2	1:113:A:VAL:HG22	5	0.34
(2,2527)	1:41:A:PHE:HE2	1:113:A:VAL:HG23	5	0.34
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	5	0.34
(2,2056)	1:88:A:HIS:HD2	1:87:A:LEU:HB3	5	0.34
(2,988)	1:45:A:LEU:HD11	1:42:A:ILE:HB	7	0.34
(2,988)	1:45:A:LEU:HD12	1:42:A:ILE:HB	7	0.34
(2,988)	1:45:A:LEU:HD13	1:42:A:ILE:HB	7	0.34
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG21	2	0.34
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG22	2	0.34
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG23	2	0.34
(2,203)	1:7:A:GLN:HE21	1:7:A:GLN:HA	9	0.34
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	6	0.34
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	6	0.34
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	6	0.34
(2,118)	1:2:A:PRO:HB2	1:5:A:LYS:HG2	9	0.34
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	9	0.33
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	5	0.33
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	5	0.33
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	5	0.33
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	5	0.33
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	5	0.33
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	5	0.33
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	5	0.33
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	5	0.33
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	5	0.33
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	5	0.33
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	5	0.33
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	5	0.33
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	5	0.33
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	5	0.33
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	5	0.33
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	5	0.33
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	5	0.33
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	2	0.33
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	2	0.33
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	2	0.33
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	10	0.33
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	10	0.33
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	10	0.33
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	7	0.33
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	7	0.33
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	7	0.33
(2,2056)	1:88:A:HIS:HD2	1:87:A:LEU:HB3	4	0.33
(2,1651)	1:70:A:SER:H	1:73:A:VAL:HB	6	0.33
(2,1650)	1:73:A:VAL:HB	1:70:A:SER:H	6	0.33
(2,1538)	1:68:A:MET:HB3	1:67:A:SER:H	10	0.33
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD21	8	0.33
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD22	8	0.33
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD23	8	0.33
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD21	8	0.33
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD22	8	0.33
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD23	8	0.33
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG21	6	0.33
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG22	6	0.33
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG23	6	0.33
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG11	7	0.33
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG12	7	0.33
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG13	7	0.33
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	1	0.32
(2,2992)	1:21:A:ILE:HD11	1:130:A:GLN:HG2	1	0.32
(2,2992)	1:21:A:ILE:HD12	1:130:A:GLN:HG2	1	0.32
(2,2992)	1:21:A:ILE:HD13	1:130:A:GLN:HG2	1	0.32
(2,2948)	1:129:A:LEU:H	1:128:A:ARG:HD2	5	0.32
(2,2765)	1:120:A:SER:H	1:124:A:VAL:HB	10	0.32
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	8	0.32
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	8	0.32
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG21	10	0.32
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG22	10	0.32
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG23	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG21	10	0.32
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG22	10	0.32
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG23	10	0.32
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	8	0.32
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	1	0.32
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	8	0.32
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	7	0.32
(2,1527)	1:68:A:MET:HE1	1:65:A:LEU:H	4	0.32
(2,1527)	1:68:A:MET:HE2	1:65:A:LEU:H	4	0.32
(2,1527)	1:68:A:MET:HE3	1:65:A:LEU:H	4	0.32
(2,937)	1:41:A:PHE:HZ	1:43:A:PRO:HA	1	0.32
(2,813)	1:36:A:VAL:HG11	1:35:A:LYS:HA	5	0.32
(2,813)	1:36:A:VAL:HG12	1:35:A:LYS:HA	5	0.32
(2,813)	1:36:A:VAL:HG13	1:35:A:LYS:HA	5	0.32
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	4	0.32
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	4	0.32
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	4	0.32
(2,391)	1:12:A:THR:HG21	1:15:A:LYS:HB2	2	0.32
(2,391)	1:12:A:THR:HG22	1:15:A:LYS:HB2	2	0.32
(2,391)	1:12:A:THR:HG23	1:15:A:LYS:HB2	2	0.32
(2,391)	1:12:A:THR:HG21	1:15:A:LYS:HB2	7	0.32
(2,391)	1:12:A:THR:HG22	1:15:A:LYS:HB2	7	0.32
(2,391)	1:12:A:THR:HG23	1:15:A:LYS:HB2	7	0.32
(2,224)	1:8:A:ASP:HB2	1:5:A:LYS:HB3	8	0.32
(2,118)	1:2:A:PRO:HB2	1:5:A:LYS:HG2	7	0.32
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	10	0.31
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	10	0.31
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	10	0.31
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	3	0.31
(2,2705)	1:122:A:GLU:HB3	1:121:A:THR:HB	1	0.31
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	6	0.31
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	6	0.31
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	3	0.31
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	1	0.31
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	8	0.31
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	10	0.31
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE1	10	0.31
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE2	10	0.31
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE3	10	0.31
(2,1541)	1:68:A:MET:HE1	1:67:A:SER:H	10	0.31
(2,1541)	1:68:A:MET:HE2	1:67:A:SER:H	10	0.31
(2,1541)	1:68:A:MET:HE3	1:67:A:SER:H	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1527)	1:68:A:MET:HE1	1:65:A:LEU:H	8	0.31
(2,1527)	1:68:A:MET:HE2	1:65:A:LEU:H	8	0.31
(2,1527)	1:68:A:MET:HE3	1:65:A:LEU:H	8	0.31
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	1	0.31
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	1	0.31
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	1	0.31
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	3	0.31
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	5	0.3
(2,2970)	1:130:A:GLN:HE21	1:18:A:VAL:HA	2	0.3
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG21	9	0.3
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG22	9	0.3
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG23	9	0.3
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	4	0.3
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	8	0.3
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	10	0.3
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	10	0.3
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	10	0.3
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	10	0.3
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	10	0.3
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	10	0.3
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	10	0.3
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	10	0.3
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	10	0.3
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	10	0.3
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	10	0.3
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	10	0.3
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	10	0.3
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	10	0.3
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	10	0.3
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	10	0.3
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	10	0.3
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	10	0.3
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	4	0.3
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	4	0.3
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	10	0.3
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	4	0.3
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	1	0.3
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	5	0.3
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	10	0.3
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	5	0.3
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	9	0.3
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	3	0.3
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	3	0.3
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	1	0.3
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	1	0.3
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	1	0.3
(2,1538)	1:68:A:MET:HB3	1:67:A:SER:H	2	0.3
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	7	0.3
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	7	0.3
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	7	0.3
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	8	0.3
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	8	0.3
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	8	0.3
(2,1163)	1:53:A:LYS:HD2	1:53:A:LYS:HB2	2	0.3
(2,988)	1:45:A:LEU:HD11	1:42:A:ILE:HB	3	0.3
(2,988)	1:45:A:LEU:HD12	1:42:A:ILE:HB	3	0.3
(2,988)	1:45:A:LEU:HD13	1:42:A:ILE:HB	3	0.3
(2,833)	1:36:A:VAL:HA	1:37:A:THR:HB	9	0.3
(2,391)	1:12:A:THR:HG21	1:15:A:LYS:HB2	4	0.3
(2,391)	1:12:A:THR:HG22	1:15:A:LYS:HB2	4	0.3
(2,391)	1:12:A:THR:HG23	1:15:A:LYS:HB2	4	0.3
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	6	0.3
(2,141)	1:5:A:LYS:H	1:5:A:LYS:HE2	10	0.3
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	6	0.29
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	6	0.29
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	6	0.29
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	9	0.29
(2,2948)	1:129:A:LEU:H	1:128:A:ARG:HD2	10	0.29
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	4	0.29
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	4	0.29
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	4	0.29
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG21	5	0.29
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG22	5	0.29
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG23	5	0.29
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	7	0.29
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	7	0.29
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	7	0.29
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	2	0.29
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	4	0.29
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	4	0.29
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	4	0.29
(2,2107)	1:90:A:LEU:HD21	1:7:A:GLN:HB3	9	0.29
(2,2107)	1:90:A:LEU:HD22	1:7:A:GLN:HB3	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2107)	1:90:A:LEU:HD23	1:7:A:GLN:HB3	9	0.29
(2,2106)	1:7:A:GLN:HB3	1:90:A:LEU:HD21	9	0.29
(2,2106)	1:7:A:GLN:HB3	1:90:A:LEU:HD22	9	0.29
(2,2106)	1:7:A:GLN:HB3	1:90:A:LEU:HD23	9	0.29
(2,1651)	1:70:A:SER:H	1:73:A:VAL:HB	7	0.29
(2,1650)	1:73:A:VAL:HB	1:70:A:SER:H	7	0.29
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE1	6	0.29
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE2	6	0.29
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE3	6	0.29
(2,1541)	1:68:A:MET:HE1	1:67:A:SER:H	6	0.29
(2,1541)	1:68:A:MET:HE2	1:67:A:SER:H	6	0.29
(2,1541)	1:68:A:MET:HE3	1:67:A:SER:H	6	0.29
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG21	5	0.29
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG22	5	0.29
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG23	5	0.29
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD21	2	0.29
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD22	2	0.29
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD23	2	0.29
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD21	2	0.29
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD22	2	0.29
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD23	2	0.29
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG21	4	0.29
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG22	4	0.29
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG23	4	0.29
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	2	0.28
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	2	0.28
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	2	0.28
(2,3190)	1:136:A:MET:HB3	1:133:A:LEU:HA	3	0.28
(2,3173)	1:136:A:MET:HE1	1:57:A:THR:HA	10	0.28
(2,3173)	1:136:A:MET:HE2	1:57:A:THR:HA	10	0.28
(2,3173)	1:136:A:MET:HE3	1:57:A:THR:HA	10	0.28
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD11	2	0.28
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD12	2	0.28
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD13	2	0.28
(2,2970)	1:130:A:GLN:HE21	1:18:A:VAL:HA	5	0.28
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	1	0.28
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	1	0.28
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	1	0.28
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	3	0.28
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	3	0.28
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	3	0.28
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	8	0.28
(2,1651)	1:70:A:SER:H	1:73:A:VAL:HB	4	0.28
(2,1651)	1:70:A:SER:H	1:73:A:VAL:HB	5	0.28
(2,1651)	1:70:A:SER:H	1:73:A:VAL:HB	8	0.28
(2,1650)	1:73:A:VAL:HB	1:70:A:SER:H	4	0.28
(2,1650)	1:73:A:VAL:HB	1:70:A:SER:H	5	0.28
(2,1650)	1:73:A:VAL:HB	1:70:A:SER:H	8	0.28
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE1	5	0.28
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE2	5	0.28
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE3	5	0.28
(2,1541)	1:68:A:MET:HE1	1:67:A:SER:H	5	0.28
(2,1541)	1:68:A:MET:HE2	1:67:A:SER:H	5	0.28
(2,1541)	1:68:A:MET:HE3	1:67:A:SER:H	5	0.28
(2,1538)	1:68:A:MET:HB3	1:67:A:SER:H	5	0.28
(2,1515)	1:68:A:MET:HE1	1:64:A:ILE:HA	6	0.28
(2,1515)	1:68:A:MET:HE2	1:64:A:ILE:HA	6	0.28
(2,1515)	1:68:A:MET:HE3	1:64:A:ILE:HA	6	0.28
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	1	0.28
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	7	0.28
(2,988)	1:45:A:LEU:HD11	1:42:A:ILE:HB	4	0.28
(2,988)	1:45:A:LEU:HD12	1:42:A:ILE:HB	4	0.28
(2,988)	1:45:A:LEU:HD13	1:42:A:ILE:HB	4	0.28
(2,813)	1:36:A:VAL:HG11	1:35:A:LYS:HA	9	0.28
(2,813)	1:36:A:VAL:HG12	1:35:A:LYS:HA	9	0.28
(2,813)	1:36:A:VAL:HG13	1:35:A:LYS:HA	9	0.28
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG21	10	0.28
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG22	10	0.28
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG23	10	0.28
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	8	0.27
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	8	0.27
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	8	0.27
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	7	0.27
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	10	0.27
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD11	7	0.27
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD12	7	0.27
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD13	7	0.27
(2,2970)	1:130:A:GLN:HE21	1:18:A:VAL:HA	7	0.27
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	8	0.27
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	8	0.27
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	8	0.27
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG11	10	0.27
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG12	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG13	10	0.27
(2,2515)	1:111:A:GLY:H	1:110:A:LEU:HG	6	0.27
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	6	0.27
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	6	0.27
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	6	0.27
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	6	0.27
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	9	0.27
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	2	0.27
(2,2296)	1:100:A:TRP:HE3	1:84:A:ARG:HD3	4	0.27
(2,2260)	1:98:A:LEU:HD11	1:55:A:ASP:HB2	4	0.27
(2,2260)	1:98:A:LEU:HD12	1:55:A:ASP:HB2	4	0.27
(2,2260)	1:98:A:LEU:HD13	1:55:A:ASP:HB2	4	0.27
(2,2240)	1:97:A:HIS:HE1	1:95:A:SER:H	9	0.27
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	2	0.27
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	2	0.27
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	2	0.27
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	5	0.27
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	5	0.27
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	5	0.27
(2,2131)	1:91:A:ALA:HA	1:3:A:ILE:HG13	10	0.27
(2,2109)	1:90:A:LEU:HD21	1:7:A:GLN:HB2	3	0.27
(2,2109)	1:90:A:LEU:HD22	1:7:A:GLN:HB2	3	0.27
(2,2109)	1:90:A:LEU:HD23	1:7:A:GLN:HB2	3	0.27
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD21	3	0.27
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD22	3	0.27
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD23	3	0.27
(2,988)	1:45:A:LEU:HD11	1:42:A:ILE:HB	1	0.27
(2,988)	1:45:A:LEU:HD12	1:42:A:ILE:HB	1	0.27
(2,988)	1:45:A:LEU:HD13	1:42:A:ILE:HB	1	0.27
(2,811)	1:35:A:LYS:H	1:35:A:LYS:HE2	8	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	2	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	2	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	2	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	5	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	5	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	5	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	6	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	6	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	6	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	7	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	7	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,224)	1:8:A:ASP:HB2	1:5:A:LYS:HB3	9	0.27
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	3	0.26
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	3	0.26
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	3	0.26
(2,3058)	1:132:A:SER:H	1:130:A:GLN:HG3	7	0.26
(2,3009)	1:130:A:GLN:HG3	1:127:A:SER:HA	3	0.26
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	2	0.26
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	3	0.26
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	3	0.26
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	2	0.26
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	2	0.26
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	2	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB1	1	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB2	1	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB3	1	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB1	1	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB2	1	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB3	1	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB1	1	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB2	1	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB3	1	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB1	10	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB2	10	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB3	10	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB1	10	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB2	10	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB3	10	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB1	10	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB2	10	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB3	10	0.26
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD11	1	0.26
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD12	1	0.26
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD13	1	0.26
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD11	1	0.26
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD12	1	0.26
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD13	1	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD11	1	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD12	1	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD13	1	0.26
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD11	10	0.26
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD12	10	0.26
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD13	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD11	10	0.26
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD12	10	0.26
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD13	10	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD11	10	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD12	10	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD13	10	0.26
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	3	0.26
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	3	0.26
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	3	0.26
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	3	0.26
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	3	0.26
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	3	0.26
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD11	5	0.26
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD12	5	0.26
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD13	5	0.26
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD11	5	0.26
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD12	5	0.26
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD13	5	0.26
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD11	5	0.26
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD12	5	0.26
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD13	5	0.26
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD11	6	0.26
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD12	6	0.26
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD13	6	0.26
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD11	6	0.26
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD12	6	0.26
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD13	6	0.26
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD11	6	0.26
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD12	6	0.26
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD13	6	0.26
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD21	1	0.26
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD22	1	0.26
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD23	1	0.26
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	5	0.26
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	5	0.26
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	5	0.26
(2,2240)	1:97:A:HIS:HE1	1:95:A:SER:H	3	0.26
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	6	0.26
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	6	0.26
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	6	0.26
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	8	0.26
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	8	0.26
(2,2056)	1:88:A:HIS:HD2	1:87:A:LEU:HB3	8	0.26
(2,1539)	1:67:A:SER:H	1:68:A:MET:HB2	2	0.26
(2,1537)	1:68:A:MET:HB3	1:67:A:SER:HB2	1	0.26
(2,1393)	1:63:A:GLN:HE21	1:63:A:GLN:HA	2	0.26
(2,1393)	1:63:A:GLN:HE21	1:63:A:GLN:HA	7	0.26
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	4	0.26
(2,1190)	1:51:A:LEU:HD11	1:54:A:MET:HB2	7	0.26
(2,1190)	1:51:A:LEU:HD12	1:54:A:MET:HB2	7	0.26
(2,1190)	1:51:A:LEU:HD13	1:54:A:MET:HB2	7	0.26
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD21	4	0.26
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD22	4	0.26
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD23	4	0.26
(2,1143)	1:49:A:LEU:HD21	1:53:A:LYS:HE2	4	0.26
(2,1143)	1:49:A:LEU:HD22	1:53:A:LYS:HE2	4	0.26
(2,1143)	1:49:A:LEU:HD23	1:53:A:LYS:HE2	4	0.26
(2,937)	1:41:A:PHE:HZ	1:43:A:PRO:HA	4	0.26
(2,886)	1:41:A:PHE:HD1	1:40:A:ASP:HB3	3	0.26
(2,886)	1:41:A:PHE:HD2	1:40:A:ASP:HB3	3	0.26
(2,776)	1:28:A:GLN:HG2	1:34:A:GLN:HB2	9	0.26
(2,3009)	1:130:A:GLN:HG3	1:127:A:SER:HA	1	0.25
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	6	0.25
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	6	0.25
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	6	0.25
(2,2843)	1:46:A:HIS:HE1	1:127:A:SER:HA	1	0.25
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	7	0.25
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB1	9	0.25
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB2	9	0.25
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB3	9	0.25
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB1	9	0.25
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB2	9	0.25
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB3	9	0.25
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	4	0.25
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	4	0.25
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	4	0.25
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	2	0.25
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	3	0.25
(2,2295)	1:100:A:TRP:HE3	1:84:A:ARG:HB2	8	0.25
(2,1350)	1:59:A:ALA:HB1	1:62:A:GLN:HB3	6	0.25
(2,1350)	1:59:A:ALA:HB2	1:62:A:GLN:HB3	6	0.25
(2,1350)	1:59:A:ALA:HB3	1:62:A:GLN:HB3	6	0.25
(2,700)	1:28:A:GLN:HG2	1:25:A:SER:HB2	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,325)	1:12:A:THR:H	1:11:A:LYS:HE2	10	0.25
(2,224)	1:8:A:ASP:HB2	1:5:A:LYS:HB3	2	0.25
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	2	0.25
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	4	0.25
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	9	0.25
(2,118)	1:2:A:PRO:HB2	1:5:A:LYS:HG2	10	0.25
(2,100)	1:4:A:GLN:HE21	1:4:A:GLN:HA	4	0.25
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	2	0.25
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	2	0.25
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	10	0.25
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	10	0.25
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	2	0.25
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	2	0.25
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	9	0.25
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	9	0.25
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	2	0.25
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	2	0.25
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	9	0.25
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	9	0.25
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	8	0.25
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	8	0.25
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	10	0.25
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	10	0.25
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	5	0.25
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	5	0.25
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	6	0.25
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	6	0.25
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	1	0.25
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	1	0.25
(2,3490)	1:143:A:SER:H	1:141:A:ASP:HA	9	0.24
(2,3161)	1:49:A:LEU:HD11	1:136:A:MET:HB3	10	0.24
(2,3161)	1:49:A:LEU:HD12	1:136:A:MET:HB3	10	0.24
(2,3161)	1:49:A:LEU:HD13	1:136:A:MET:HB3	10	0.24
(2,3160)	1:136:A:MET:HB3	1:49:A:LEU:HD11	10	0.24
(2,3160)	1:136:A:MET:HB3	1:49:A:LEU:HD12	10	0.24
(2,3160)	1:136:A:MET:HB3	1:49:A:LEU:HD13	10	0.24
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD11	6	0.24
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD12	6	0.24
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD13	6	0.24
(2,2992)	1:21:A:ILE:HD11	1:130:A:GLN:HG2	4	0.24
(2,2992)	1:21:A:ILE:HD12	1:130:A:GLN:HG2	4	0.24
(2,2992)	1:21:A:ILE:HD13	1:130:A:GLN:HG2	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2970)	1:130:A:GLN:HE21	1:18:A:VAL:HA	4	0.24
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	2	0.24
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	2	0.24
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	2	0.24
(2,2798)	1:119:A:TYR:HE1	1:125:A:ALA:H	10	0.24
(2,2798)	1:119:A:TYR:HE2	1:125:A:ALA:H	10	0.24
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	1	0.24
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	1	0.24
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	1	0.24
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	10	0.24
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	10	0.24
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	10	0.24
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	1	0.24
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	1	0.24
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	1	0.24
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	10	0.24
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	10	0.24
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	10	0.24
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	6	0.24
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	8	0.24
(2,2295)	1:100:A:TRP:HE3	1:84:A:ARG:HB2	6	0.24
(2,2109)	1:90:A:LEU:HD21	1:7:A:GLN:HB2	4	0.24
(2,2109)	1:90:A:LEU:HD22	1:7:A:GLN:HB2	4	0.24
(2,2109)	1:90:A:LEU:HD23	1:7:A:GLN:HB2	4	0.24
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD21	4	0.24
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD22	4	0.24
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD23	4	0.24
(2,1791)	1:77:A:SER:H	1:75:A:GLN:HB2	6	0.24
(2,1656)	1:73:A:VAL:H	1:71:A:ARG:HB2	4	0.24
(2,1500)	1:67:A:SER:H	1:63:A:GLN:HA	2	0.24
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	4	0.24
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	4	0.24
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	4	0.24
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG21	1	0.24
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG22	1	0.24
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG23	1	0.24
(2,1393)	1:63:A:GLN:HE21	1:63:A:GLN:HA	6	0.24
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD21	1	0.24
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD22	1	0.24
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD23	1	0.24
(2,1143)	1:49:A:LEU:HD21	1:53:A:LYS:HE2	1	0.24
(2,1143)	1:49:A:LEU:HD22	1:53:A:LYS:HE2	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1143)	1:49:A:LEU:HD23	1:53:A:LYS:HE2	1	0.24
(2,704)	1:27:A:THR:HG21	1:28:A:GLN:HA	3	0.24
(2,704)	1:27:A:THR:HG22	1:28:A:GLN:HA	3	0.24
(2,704)	1:27:A:THR:HG23	1:28:A:GLN:HA	3	0.24
(2,586)	1:24:A:ILE:H	1:20:A:ARG:HA	3	0.24
(2,224)	1:8:A:ASP:HB2	1:5:A:LYS:HB3	5	0.24
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	4	0.24
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	4	0.24
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	7	0.24
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	7	0.24
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	3	0.24
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	3	0.24
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	4	0.24
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	4	0.24
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	6	0.24
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	6	0.24
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	7	0.24
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	7	0.24
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	8	0.24
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	8	0.24
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	10	0.24
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	10	0.24
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	2	0.24
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	2	0.24
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	4	0.24
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	4	0.24
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	9	0.24
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	9	0.24
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	10	0.24
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	10	0.24
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	1	0.24
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	1	0.24
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	6	0.24
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	6	0.24
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	8	0.24
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	8	0.24
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	10	0.24
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	10	0.24
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	1	0.24
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	1	0.24
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	2	0.24
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	4	0.24
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	4	0.24
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	6	0.24
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	6	0.24
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	9	0.24
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	9	0.24
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	10	0.24
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	10	0.24
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	2	0.24
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	2	0.24
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	4	0.24
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	4	0.24
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	5	0.24
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	5	0.24
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	6	0.24
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	6	0.24
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	7	0.24
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	7	0.24
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	8	0.24
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	8	0.24
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	3	0.24
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	3	0.24
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	5	0.24
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	5	0.24
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	6	0.24
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	6	0.24
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	8	0.24
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	8	0.24
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	2	0.24
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	2	0.24
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	3	0.24
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	3	0.24
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	7	0.24
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	7	0.24
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	8	0.24
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	8	0.24
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	9	0.24
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	9	0.24
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	5	0.24
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	5	0.24
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	6	0.24
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	1	0.23
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	1	0.23
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	1	0.23
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG21	2	0.23
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG22	2	0.23
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG23	2	0.23
(2,3188)	1:136:A:MET:HE1	1:132:A:SER:HB2	6	0.23
(2,3188)	1:136:A:MET:HE2	1:132:A:SER:HB2	6	0.23
(2,3188)	1:136:A:MET:HE3	1:132:A:SER:HB2	6	0.23
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	3	0.23
(2,2911)	1:128:A:ARG:HG2	1:128:A:ARG:HD2	4	0.23
(2,2679)	1:121:A:THR:HG21	1:120:A:SER:HA	9	0.23
(2,2679)	1:121:A:THR:HG22	1:120:A:SER:HA	9	0.23
(2,2679)	1:121:A:THR:HG23	1:120:A:SER:HA	9	0.23
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	10	0.23
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	10	0.23
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	10	0.23
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	9	0.23
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	9	0.23
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	9	0.23
(2,2455)	1:108:A:ASP:HB3	1:107:A:LEU:HB2	8	0.23
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	7	0.23
(2,2240)	1:97:A:HIS:HE1	1:95:A:SER:H	2	0.23
(2,2240)	1:97:A:HIS:HE1	1:95:A:SER:H	8	0.23
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	1	0.23
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	1	0.23
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	1	0.23
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	9	0.23
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	9	0.23
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	9	0.23
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD11	9	0.23
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD12	9	0.23
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD13	9	0.23
(2,1566)	1:68:A:MET:HE1	1:69:A:PRO:HD2	6	0.23
(2,1566)	1:68:A:MET:HE2	1:69:A:PRO:HD2	6	0.23
(2,1566)	1:68:A:MET:HE3	1:69:A:PRO:HD2	6	0.23
(2,1190)	1:51:A:LEU:HD11	1:54:A:MET:HB2	9	0.23
(2,1190)	1:51:A:LEU:HD12	1:54:A:MET:HB2	9	0.23
(2,1190)	1:51:A:LEU:HD13	1:54:A:MET:HB2	9	0.23
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	1	0.23
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	4	0.23
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG21	4	0.23
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG22	4	0.23
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG23	4	0.23
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	3	0.23
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	8	0.23
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	10	0.23
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	1	0.23
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	1	0.23
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	2	0.23
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	2	0.23
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	3	0.23
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	3	0.23
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	3	0.23
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	3	0.23
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	5	0.23
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	5	0.23
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	8	0.23
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	8	0.23
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	9	0.23
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	9	0.23
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	1	0.23
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	1	0.23
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	5	0.23
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	5	0.23
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	1	0.23
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	1	0.23
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	3	0.23
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	3	0.23
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	6	0.23
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	6	0.23
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	7	0.23
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	7	0.23
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	8	0.23
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	8	0.23
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	3	0.23
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	3	0.23
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	4	0.23
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	4	0.23
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	5	0.23
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	5	0.23
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	7	0.23
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	3	0.23
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	3	0.23
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	5	0.23
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	5	0.23
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	7	0.23
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	7	0.23
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	1	0.23
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	1	0.23
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	3	0.23
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	3	0.23
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	9	0.23
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	9	0.23
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	2	0.23
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	2	0.23
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	4	0.23
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	4	0.23
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	7	0.23
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	7	0.23
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	8	0.23
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	8	0.23
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	9	0.23
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	9	0.23
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	10	0.23
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	10	0.23
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	1	0.23
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	1	0.23
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	2	0.23
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	2	0.23
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	4	0.23
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	4	0.23
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	7	0.23
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	7	0.23
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	9	0.23
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	9	0.23
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	10	0.23
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	10	0.23
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	1	0.23
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	1	0.23
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	4	0.23
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	4	0.23
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	10	0.23
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	2	0.23
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	2	0.23
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	3	0.23
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	3	0.23
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	4	0.23
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	4	0.23
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	8	0.23
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	8	0.23
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	9	0.23
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	9	0.23
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	10	0.23
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	10	0.23
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD21	6	0.22
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD22	6	0.22
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD23	6	0.22
(2,3234)	1:137:A:LEU:HD21	1:11:A:LYS:HE2	6	0.22
(2,3234)	1:137:A:LEU:HD22	1:11:A:LYS:HE2	6	0.22
(2,3234)	1:137:A:LEU:HD23	1:11:A:LYS:HE2	6	0.22
(2,3190)	1:136:A:MET:HB3	1:133:A:LEU:HA	4	0.22
(2,3172)	1:54:A:MET:HE1	1:136:A:MET:HG2	7	0.22
(2,3172)	1:54:A:MET:HE2	1:136:A:MET:HG2	7	0.22
(2,3172)	1:54:A:MET:HE3	1:136:A:MET:HG2	7	0.22
(2,3163)	1:49:A:LEU:HD11	1:136:A:MET:HB2	7	0.22
(2,3163)	1:49:A:LEU:HD12	1:136:A:MET:HB2	7	0.22
(2,3163)	1:49:A:LEU:HD13	1:136:A:MET:HB2	7	0.22
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD11	7	0.22
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD12	7	0.22
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD13	7	0.22
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	4	0.22
(2,2992)	1:21:A:ILE:HD11	1:130:A:GLN:HG2	7	0.22
(2,2992)	1:21:A:ILE:HD12	1:130:A:GLN:HG2	7	0.22
(2,2992)	1:21:A:ILE:HD13	1:130:A:GLN:HG2	7	0.22
(2,2843)	1:46:A:HIS:HE1	1:127:A:SER:HA	8	0.22
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG21	2	0.22
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG22	2	0.22
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG23	2	0.22
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD11	9	0.22
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD12	9	0.22
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD13	9	0.22
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD11	9	0.22
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD12	9	0.22
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD13	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD11	9	0.22
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD12	9	0.22
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD13	9	0.22
(2,2695)	1:122:A:GLU:HG3	1:68:A:MET:HE1	2	0.22
(2,2695)	1:122:A:GLU:HG3	1:68:A:MET:HE2	2	0.22
(2,2695)	1:122:A:GLU:HG3	1:68:A:MET:HE3	2	0.22
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB1	1	0.22
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB2	1	0.22
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB3	1	0.22
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB1	1	0.22
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB2	1	0.22
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB3	1	0.22
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	7	0.22
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	7	0.22
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	7	0.22
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	2	0.22
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	1	0.22
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	5	0.22
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	9	0.22
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	10	0.22
(2,2296)	1:100:A:TRP:HE3	1:84:A:ARG:HD3	1	0.22
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	6	0.22
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD11	5	0.22
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD12	5	0.22
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD13	5	0.22
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE1	4	0.22
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE2	4	0.22
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE3	4	0.22
(2,1541)	1:68:A:MET:HE1	1:67:A:SER:H	4	0.22
(2,1541)	1:68:A:MET:HE2	1:67:A:SER:H	4	0.22
(2,1541)	1:68:A:MET:HE3	1:67:A:SER:H	4	0.22
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	3	0.22
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	3	0.22
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	9	0.22
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	9	0.22
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	3	0.22
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD21	4	0.22
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD22	4	0.22
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD23	4	0.22
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	4	0.22
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	4	0.22
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	5	0.22
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	6	0.22
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	6	0.22
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	7	0.22
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	7	0.22
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	8	0.22
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	8	0.22
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	9	0.22
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	9	0.22
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	10	0.22
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	10	0.22
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	1	0.22
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	1	0.22
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	6	0.22
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	6	0.22
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	5	0.22
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	5	0.22
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	1	0.22
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	1	0.22
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	3	0.22
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	3	0.22
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	5	0.22
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	5	0.22
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	6	0.22
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	6	0.22
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	7	0.22
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	7	0.22
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG21	5	0.21
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG22	5	0.21
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG23	5	0.21
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	2	0.21
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	2	0.21
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	2	0.21
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	5	0.21
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	5	0.21
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	5	0.21
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG21	1	0.21
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG22	1	0.21
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG23	1	0.21
(2,3113)	1:134:A:GLN:HE21	1:131:A:GLY:HA2	8	0.21
(2,2911)	1:128:A:ARG:HG2	1:128:A:ARG:HD2	2	0.21
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD11	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD12	9	0.21
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD13	9	0.21
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	7	0.21
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	7	0.21
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	7	0.21
(2,2843)	1:46:A:HIS:HE1	1:127:A:SER:HA	2	0.21
(2,2693)	1:68:A:MET:HE1	1:122:A:GLU:HB3	1	0.21
(2,2693)	1:68:A:MET:HE2	1:122:A:GLU:HB3	1	0.21
(2,2693)	1:68:A:MET:HE3	1:122:A:GLU:HB3	1	0.21
(2,2679)	1:121:A:THR:HG21	1:120:A:SER:HA	6	0.21
(2,2679)	1:121:A:THR:HG22	1:120:A:SER:HA	6	0.21
(2,2679)	1:121:A:THR:HG23	1:120:A:SER:HA	6	0.21
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	8	0.21
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	8	0.21
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	8	0.21
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	8	0.21
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	8	0.21
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	8	0.21
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	10	0.21
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	1	0.21
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD21	7	0.21
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD22	7	0.21
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD23	7	0.21
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG21	4	0.21
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG22	4	0.21
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG23	4	0.21
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE1	7	0.21
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE2	7	0.21
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE3	7	0.21
(2,1541)	1:68:A:MET:HE1	1:67:A:SER:H	7	0.21
(2,1541)	1:68:A:MET:HE2	1:67:A:SER:H	7	0.21
(2,1541)	1:68:A:MET:HE3	1:67:A:SER:H	7	0.21
(2,1393)	1:63:A:GLN:HE21	1:63:A:GLN:HA	4	0.21
(2,1163)	1:53:A:LYS:HD2	1:53:A:LYS:HB2	7	0.21
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	1	0.21
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	1	0.21
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	7	0.21
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	7	0.21
(2,774)	1:33:A:LYS:H	1:33:A:LYS:HE2	6	0.21
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	10	0.21
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	10	0.21
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,391)	1:12:A:THR:HG21	1:15:A:LYS:HB2	8	0.21
(2,391)	1:12:A:THR:HG22	1:15:A:LYS:HB2	8	0.21
(2,391)	1:12:A:THR:HG23	1:15:A:LYS:HB2	8	0.21
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	1	0.21
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	7	0.21
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	1	0.21
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	1	0.21
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	2	0.21
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	2	0.21
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	3	0.21
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	3	0.21
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	6	0.21
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	6	0.21
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	7	0.21
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	7	0.21
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	9	0.21
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	9	0.21
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	10	0.21
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	10	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	1	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	1	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	2	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	2	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	3	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	3	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	4	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	4	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	5	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	5	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	6	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	6	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	7	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	7	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	8	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	8	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	9	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	9	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	10	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	10	0.21
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG21	4	0.2
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG22	4	0.2
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG23	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	4	0.2
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	4	0.2
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	4	0.2
(2,3364)	1:139:A:GLN:HE21	1:139:A:GLN:HA	10	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG21	6	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG22	6	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG23	6	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG21	9	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG22	9	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG23	9	0.2
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	1	0.2
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	1	0.2
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	1	0.2
(2,3190)	1:136:A:MET:HB3	1:133:A:LEU:HA	10	0.2
(2,3183)	1:136:A:MET:HE1	1:83:A:LEU:HD21	10	0.2
(2,3183)	1:136:A:MET:HE1	1:83:A:LEU:HD22	10	0.2
(2,3183)	1:136:A:MET:HE1	1:83:A:LEU:HD23	10	0.2
(2,3183)	1:136:A:MET:HE2	1:83:A:LEU:HD21	10	0.2
(2,3183)	1:136:A:MET:HE2	1:83:A:LEU:HD22	10	0.2
(2,3183)	1:136:A:MET:HE2	1:83:A:LEU:HD23	10	0.2
(2,3183)	1:136:A:MET:HE3	1:83:A:LEU:HD21	10	0.2
(2,3183)	1:136:A:MET:HE3	1:83:A:LEU:HD22	10	0.2
(2,3183)	1:136:A:MET:HE3	1:83:A:LEU:HD23	10	0.2
(2,3088)	1:133:A:LEU:HG	1:130:A:GLN:HA	5	0.2
(2,3087)	1:130:A:GLN:HA	1:133:A:LEU:HG	5	0.2
(2,2911)	1:128:A:ARG:HG2	1:128:A:ARG:HD2	5	0.2
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	9	0.2
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	9	0.2
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	9	0.2
(2,2843)	1:46:A:HIS:HE1	1:127:A:SER:HA	4	0.2
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	3	0.2
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	3	0.2
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	3	0.2
(2,2767)	1:124:A:VAL:HB	1:121:A:THR:HA	7	0.2
(2,2765)	1:120:A:SER:H	1:124:A:VAL:HB	3	0.2
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	2	0.2
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	2	0.2
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	2	0.2
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	2	0.2
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	2	0.2
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	2	0.2
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	2	0.2
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	2	0.2
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	8	0.2
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	8	0.2
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	8	0.2
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	8	0.2
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	8	0.2
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	8	0.2
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	8	0.2
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	8	0.2
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	8	0.2
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	2	0.2
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	2	0.2
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	2	0.2
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	2	0.2
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	2	0.2
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	2	0.2
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	2	0.2
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	2	0.2
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	2	0.2
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	8	0.2
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	8	0.2
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	8	0.2
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	8	0.2
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	8	0.2
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	8	0.2
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	8	0.2
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	8	0.2
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	8	0.2
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE1	10	0.2
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE2	10	0.2
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE3	10	0.2
(2,2696)	1:68:A:MET:HE1	1:122:A:GLU:HG2	10	0.2
(2,2696)	1:68:A:MET:HE2	1:122:A:GLU:HG2	10	0.2
(2,2696)	1:68:A:MET:HE3	1:122:A:GLU:HG2	10	0.2
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	7	0.2
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	7	0.2
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	7	0.2
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	1	0.2
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD11	2	0.2
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD12	2	0.2
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD13	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD11	2	0.2
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD12	2	0.2
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD13	2	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD11	2	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD12	2	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD13	2	0.2
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD11	8	0.2
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD12	8	0.2
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD13	8	0.2
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD11	8	0.2
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD12	8	0.2
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD13	8	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD11	8	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD12	8	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD13	8	0.2
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	9	0.2
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	9	0.2
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	9	0.2
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	4	0.2
(2,2288)	1:98:A:LEU:HD11	1:99:A:PRO:HG2	8	0.2
(2,2288)	1:98:A:LEU:HD12	1:99:A:PRO:HG2	8	0.2
(2,2288)	1:98:A:LEU:HD13	1:99:A:PRO:HG2	8	0.2
(2,2095)	1:6:A:VAL:H	1:90:A:LEU:HD11	5	0.2
(2,2095)	1:6:A:VAL:H	1:90:A:LEU:HD12	5	0.2
(2,2095)	1:6:A:VAL:H	1:90:A:LEU:HD13	5	0.2
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD11	3	0.2
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD12	3	0.2
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD13	3	0.2
(2,1723)	1:71:A:ARG:HD2	1:75:A:GLN:HG2	6	0.2
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	2	0.2
(2,989)	1:45:A:LEU:H	1:42:A:ILE:HB	6	0.2
(2,989)	1:45:A:LEU:H	1:42:A:ILE:HB	8	0.2
(2,988)	1:45:A:LEU:HD11	1:42:A:ILE:HB	9	0.2
(2,988)	1:45:A:LEU:HD12	1:42:A:ILE:HB	9	0.2
(2,988)	1:45:A:LEU:HD13	1:42:A:ILE:HB	9	0.2
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	6	0.2
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	6	0.2
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	10	0.2
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	10	0.2
(2,813)	1:36:A:VAL:HG11	1:35:A:LYS:HA	1	0.2
(2,813)	1:36:A:VAL:HG12	1:35:A:LYS:HA	1	0.2
(2,813)	1:36:A:VAL:HG13	1:35:A:LYS:HA	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,813)	1:36:A:VAL:HG11	1:35:A:LYS:HA	6	0.2
(2,813)	1:36:A:VAL:HG12	1:35:A:LYS:HA	6	0.2
(2,813)	1:36:A:VAL:HG13	1:35:A:LYS:HA	6	0.2
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	10	0.2
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG21	7	0.2
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG22	7	0.2
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG23	7	0.2
(2,324)	1:12:A:THR:H	1:11:A:LYS:HD2	9	0.2
(2,224)	1:8:A:ASP:HB2	1:5:A:LYS:HB3	1	0.2
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	4	0.2
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	4	0.2
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	5	0.2
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	5	0.2
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	8	0.2
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	8	0.2
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG21	1	0.19
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG22	1	0.19
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG23	1	0.19
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	6	0.19
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	6	0.19
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	6	0.19
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD21	8	0.19
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD22	8	0.19
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD23	8	0.19
(2,3450)	1:142:A:LEU:HD11	1:138:A:TRP:HZ2	10	0.19
(2,3450)	1:142:A:LEU:HD12	1:138:A:TRP:HZ2	10	0.19
(2,3450)	1:142:A:LEU:HD13	1:138:A:TRP:HZ2	10	0.19
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD11	10	0.19
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD12	10	0.19
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD13	10	0.19
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD21	1	0.19
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD22	1	0.19
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD23	1	0.19
(2,3173)	1:136:A:MET:HE1	1:57:A:THR:HA	8	0.19
(2,3173)	1:136:A:MET:HE2	1:57:A:THR:HA	8	0.19
(2,3173)	1:136:A:MET:HE3	1:57:A:THR:HA	8	0.19
(2,3009)	1:130:A:GLN:HG3	1:127:A:SER:HA	2	0.19
(2,2903)	1:128:A:ARG:HE	1:128:A:ARG:HA	4	0.19
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG21	5	0.19
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG22	5	0.19
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG23	5	0.19
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG21	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG22	8	0.19
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG23	8	0.19
(2,2679)	1:121:A:THR:HG21	1:120:A:SER:HA	7	0.19
(2,2679)	1:121:A:THR:HG22	1:120:A:SER:HA	7	0.19
(2,2679)	1:121:A:THR:HG23	1:120:A:SER:HA	7	0.19
(2,2648)	1:119:A:TYR:H	1:117:A:SER:HB2	6	0.19
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	2	0.19
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	2	0.19
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	2	0.19
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	7	0.19
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	7	0.19
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	7	0.19
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	2	0.19
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	2	0.19
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	2	0.19
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	7	0.19
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	7	0.19
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	7	0.19
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	2	0.19
(2,2515)	1:111:A:GLY:H	1:110:A:LEU:HG	7	0.19
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	2	0.19
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	2	0.19
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	2	0.19
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	7	0.19
(2,2295)	1:100:A:TRP:HE3	1:84:A:ARG:HB2	5	0.19
(2,2295)	1:100:A:TRP:HE3	1:84:A:ARG:HB2	7	0.19
(2,2131)	1:91:A:ALA:HA	1:3:A:ILE:HG13	4	0.19
(2,2109)	1:90:A:LEU:HD21	1:7:A:GLN:HB2	1	0.19
(2,2109)	1:90:A:LEU:HD22	1:7:A:GLN:HB2	1	0.19
(2,2109)	1:90:A:LEU:HD23	1:7:A:GLN:HB2	1	0.19
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD21	1	0.19
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD22	1	0.19
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD23	1	0.19
(2,1527)	1:68:A:MET:HE1	1:65:A:LEU:H	10	0.19
(2,1527)	1:68:A:MET:HE2	1:65:A:LEU:H	10	0.19
(2,1527)	1:68:A:MET:HE3	1:65:A:LEU:H	10	0.19
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	3	0.19
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	10	0.19
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG21	1	0.19
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG22	1	0.19
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG23	1	0.19
(2,1030)	1:46:A:HIS:HD2	1:47:A:PRO:HD3	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	4	0.19
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	4	0.19
(2,832)	1:37:A:THR:H	1:35:A:LYS:HD2	5	0.19
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG21	10	0.19
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG22	10	0.19
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG23	10	0.19
(2,815)	1:36:A:VAL:H	1:35:A:LYS:HA	9	0.19
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG21	4	0.19
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG22	4	0.19
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG23	4	0.19
(2,730)	1:29:A:SER:H	1:27:A:THR:HG21	5	0.19
(2,730)	1:29:A:SER:H	1:27:A:THR:HG22	5	0.19
(2,730)	1:29:A:SER:H	1:27:A:THR:HG23	5	0.19
(2,704)	1:27:A:THR:HG21	1:28:A:GLN:HA	6	0.19
(2,704)	1:27:A:THR:HG22	1:28:A:GLN:HA	6	0.19
(2,704)	1:27:A:THR:HG23	1:28:A:GLN:HA	6	0.19
(2,697)	1:28:A:GLN:HB2	1:25:A:SER:HB3	7	0.19
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	6	0.19
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG21	8	0.18
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG22	8	0.18
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG23	8	0.18
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	3	0.18
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	3	0.18
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	3	0.18
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	7	0.18
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	7	0.18
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	7	0.18
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	10	0.18
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	10	0.18
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	10	0.18
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD21	4	0.18
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD22	4	0.18
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD23	4	0.18
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD21	5	0.18
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD22	5	0.18
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD23	5	0.18
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD21	6	0.18
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD22	6	0.18
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD23	6	0.18
(2,3163)	1:49:A:LEU:HD11	1:136:A:MET:HB2	9	0.18
(2,3163)	1:49:A:LEU:HD12	1:136:A:MET:HB2	9	0.18
(2,3163)	1:49:A:LEU:HD13	1:136:A:MET:HB2	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD11	9	0.18
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD12	9	0.18
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD13	9	0.18
(2,3108)	1:134:A:GLN:HG2	1:18:A:VAL:HA	8	0.18
(2,3003)	1:126:A:LEU:HD11	1:130:A:GLN:HA	3	0.18
(2,3003)	1:126:A:LEU:HD12	1:130:A:GLN:HA	3	0.18
(2,3003)	1:126:A:LEU:HD13	1:130:A:GLN:HA	3	0.18
(2,2970)	1:130:A:GLN:HE21	1:18:A:VAL:HA	3	0.18
(2,2843)	1:46:A:HIS:HE1	1:127:A:SER:HA	7	0.18
(2,2767)	1:124:A:VAL:HB	1:121:A:THR:HA	4	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	3	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	3	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	3	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	3	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	3	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	3	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	3	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	3	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	3	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	4	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	4	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	4	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	4	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	4	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	4	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	4	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	4	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	4	0.18
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	3	0.18
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	3	0.18
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	3	0.18
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	3	0.18
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	3	0.18
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	3	0.18
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	3	0.18
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	3	0.18
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	3	0.18
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	4	0.18
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	4	0.18
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	4	0.18
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	4	0.18
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	4	0.18
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	4	0.18
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	4	0.18
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	4	0.18
(2,2679)	1:121:A:THR:HG21	1:120:A:SER:HA	1	0.18
(2,2679)	1:121:A:THR:HG22	1:120:A:SER:HA	1	0.18
(2,2679)	1:121:A:THR:HG23	1:120:A:SER:HA	1	0.18
(2,2679)	1:121:A:THR:HG21	1:120:A:SER:HA	8	0.18
(2,2679)	1:121:A:THR:HG22	1:120:A:SER:HA	8	0.18
(2,2679)	1:121:A:THR:HG23	1:120:A:SER:HA	8	0.18
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB1	3	0.18
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB2	3	0.18
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB3	3	0.18
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB1	3	0.18
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB2	3	0.18
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB3	3	0.18
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	1	0.18
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	1	0.18
(2,2616)	1:117:A:SER:HB2	1:117:A:SER:HA	4	0.18
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	6	0.18
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	1	0.18
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	1	0.18
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	1	0.18
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	10	0.18
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	10	0.18
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	10	0.18
(2,2398)	1:63:A:GLN:HE22	1:104:A:LEU:HD21	3	0.18
(2,2398)	1:63:A:GLN:HE22	1:104:A:LEU:HD22	3	0.18
(2,2398)	1:63:A:GLN:HE22	1:104:A:LEU:HD23	3	0.18
(2,2397)	1:104:A:LEU:HD21	1:63:A:GLN:HE22	3	0.18
(2,2397)	1:104:A:LEU:HD22	1:63:A:GLN:HE22	3	0.18
(2,2397)	1:104:A:LEU:HD23	1:63:A:GLN:HE22	3	0.18
(2,2296)	1:100:A:TRP:HE3	1:84:A:ARG:HD3	6	0.18
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	7	0.18
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	10	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB1	2	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB2	2	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB3	2	0.18
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB1	2	0.18
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB2	2	0.18
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB3	2	0.18
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB1	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB2	2	0.18
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB3	2	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB1	4	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB2	4	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB3	4	0.18
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB1	4	0.18
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB2	4	0.18
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB3	4	0.18
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB1	4	0.18
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB2	4	0.18
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB3	4	0.18
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD21	9	0.18
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD22	9	0.18
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD23	9	0.18
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE1	8	0.18
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE2	8	0.18
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE3	8	0.18
(2,1541)	1:68:A:MET:HE1	1:67:A:SER:H	8	0.18
(2,1541)	1:68:A:MET:HE2	1:67:A:SER:H	8	0.18
(2,1541)	1:68:A:MET:HE3	1:67:A:SER:H	8	0.18
(2,1515)	1:68:A:MET:HE1	1:64:A:ILE:HA	2	0.18
(2,1515)	1:68:A:MET:HE2	1:64:A:ILE:HA	2	0.18
(2,1515)	1:68:A:MET:HE3	1:64:A:ILE:HA	2	0.18
(2,1393)	1:63:A:GLN:HE21	1:63:A:GLN:HA	8	0.18
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	9	0.18
(2,1190)	1:51:A:LEU:HD11	1:54:A:MET:HB2	2	0.18
(2,1190)	1:51:A:LEU:HD12	1:54:A:MET:HB2	2	0.18
(2,1190)	1:51:A:LEU:HD13	1:54:A:MET:HB2	2	0.18
(2,1175)	1:53:A:LYS:H	1:53:A:LYS:HE2	2	0.18
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	5	0.18
(2,1163)	1:53:A:LYS:HD2	1:53:A:LYS:HB2	1	0.18
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	2	0.18
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	2	0.18
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	8	0.18
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	8	0.18
(2,882)	1:41:A:PHE:HD1	1:39:A:LEU:HD11	7	0.18
(2,882)	1:41:A:PHE:HD1	1:39:A:LEU:HD12	7	0.18
(2,882)	1:41:A:PHE:HD1	1:39:A:LEU:HD13	7	0.18
(2,882)	1:41:A:PHE:HD2	1:39:A:LEU:HD11	7	0.18
(2,882)	1:41:A:PHE:HD2	1:39:A:LEU:HD12	7	0.18
(2,882)	1:41:A:PHE:HD2	1:39:A:LEU:HD13	7	0.18
(2,779)	1:34:A:GLN:HG2	1:31:A:SER:HB2	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	9	0.18
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	5	0.18
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG21	6	0.17
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG22	6	0.17
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG23	6	0.17
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD21	2	0.17
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD22	2	0.17
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD23	2	0.17
(2,3003)	1:126:A:LEU:HD11	1:130:A:GLN:HA	2	0.17
(2,3003)	1:126:A:LEU:HD12	1:130:A:GLN:HA	2	0.17
(2,3003)	1:126:A:LEU:HD13	1:130:A:GLN:HA	2	0.17
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD11	4	0.17
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD12	4	0.17
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD13	4	0.17
(2,2975)	1:130:A:GLN:H	1:18:A:VAL:HG21	9	0.17
(2,2975)	1:130:A:GLN:H	1:18:A:VAL:HG22	9	0.17
(2,2975)	1:130:A:GLN:H	1:18:A:VAL:HG23	9	0.17
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD11	3	0.17
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD12	3	0.17
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD13	3	0.17
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB1	7	0.17
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB2	7	0.17
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB3	7	0.17
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB1	7	0.17
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB2	7	0.17
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB3	7	0.17
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD21	10	0.17
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD22	10	0.17
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD23	10	0.17
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	9	0.17
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	10	0.17
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	3	0.17
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD11	10	0.17
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD12	10	0.17
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD13	10	0.17
(2,1567)	1:68:A:MET:HG2	1:69:A:PRO:HD2	4	0.17
(2,1537)	1:68:A:MET:HB3	1:67:A:SER:HB2	3	0.17
(2,1515)	1:68:A:MET:HE1	1:64:A:ILE:HA	4	0.17
(2,1515)	1:68:A:MET:HE2	1:64:A:ILE:HA	4	0.17
(2,1515)	1:68:A:MET:HE3	1:64:A:ILE:HA	4	0.17
(2,1515)	1:68:A:MET:HE1	1:64:A:ILE:HA	7	0.17
(2,1515)	1:68:A:MET:HE2	1:64:A:ILE:HA	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1515)	1:68:A:MET:HE3	1:64:A:ILE:HA	7	0.17
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	5	0.17
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	5	0.17
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	5	0.17
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG21	2	0.17
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG22	2	0.17
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG23	2	0.17
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG21	2	0.17
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG22	2	0.17
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG23	2	0.17
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG21	3	0.17
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG22	3	0.17
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG23	3	0.17
(2,1269)	1:55:A:ASP:H	1:58:A:LEU:HG	10	0.17
(2,1175)	1:53:A:LYS:H	1:53:A:LYS:HE2	5	0.17
(2,1163)	1:53:A:LYS:HD2	1:53:A:LYS:HB2	4	0.17
(2,1092)	1:48:A:ILE:HG21	1:50:A:THR:HG21	10	0.17
(2,1092)	1:48:A:ILE:HG21	1:50:A:THR:HG22	10	0.17
(2,1092)	1:48:A:ILE:HG21	1:50:A:THR:HG23	10	0.17
(2,1092)	1:48:A:ILE:HG22	1:50:A:THR:HG21	10	0.17
(2,1092)	1:48:A:ILE:HG22	1:50:A:THR:HG22	10	0.17
(2,1092)	1:48:A:ILE:HG22	1:50:A:THR:HG23	10	0.17
(2,1092)	1:48:A:ILE:HG23	1:50:A:THR:HG21	10	0.17
(2,1092)	1:48:A:ILE:HG23	1:50:A:THR:HG22	10	0.17
(2,1092)	1:48:A:ILE:HG23	1:50:A:THR:HG23	10	0.17
(2,1091)	1:50:A:THR:HG21	1:48:A:ILE:HG21	10	0.17
(2,1091)	1:50:A:THR:HG21	1:48:A:ILE:HG22	10	0.17
(2,1091)	1:50:A:THR:HG21	1:48:A:ILE:HG23	10	0.17
(2,1091)	1:50:A:THR:HG22	1:48:A:ILE:HG21	10	0.17
(2,1091)	1:50:A:THR:HG22	1:48:A:ILE:HG22	10	0.17
(2,1091)	1:50:A:THR:HG22	1:48:A:ILE:HG23	10	0.17
(2,1091)	1:50:A:THR:HG23	1:48:A:ILE:HG21	10	0.17
(2,1091)	1:50:A:THR:HG23	1:48:A:ILE:HG22	10	0.17
(2,1091)	1:50:A:THR:HG23	1:48:A:ILE:HG23	10	0.17
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	5	0.17
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	5	0.17
(2,837)	1:37:A:THR:H	1:36:A:VAL:H	7	0.17
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG21	5	0.17
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG22	5	0.17
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG23	5	0.17
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	4	0.17
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG21	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG22	1	0.17
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG23	1	0.17
(2,589)	1:24:A:ILE:HD11	1:21:A:ILE:HA	1	0.17
(2,589)	1:24:A:ILE:HD12	1:21:A:ILE:HA	1	0.17
(2,589)	1:24:A:ILE:HD13	1:21:A:ILE:HA	1	0.17
(2,203)	1:7:A:GLN:HE21	1:7:A:GLN:HA	4	0.17
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	3	0.17
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	3	0.17
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	3	0.17
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	3	0.17
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	3	0.17
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	3	0.17
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	3	0.17
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	3	0.17
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	3	0.17
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	3	0.17
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	3	0.17
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	3	0.17
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	3	0.17
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	3	0.17
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	3	0.17
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	3	0.17
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	3	0.17
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	3	0.17
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG21	2	0.16
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG22	2	0.16
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG23	2	0.16
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD21	5	0.16
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD22	5	0.16
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD23	5	0.16
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD21	6	0.16
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD22	6	0.16
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD23	6	0.16
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD21	9	0.16
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD22	9	0.16
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD23	9	0.16
(2,3108)	1:134:A:GLN:HG2	1:18:A:VAL:HA	7	0.16
(2,3058)	1:132:A:SER:H	1:130:A:GLN:HG3	8	0.16
(2,3057)	1:132:A:SER:H	1:130:A:GLN:HB2	7	0.16
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD11	2	0.16
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD12	2	0.16
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD13	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2948)	1:129:A:LEU:H	1:128:A:ARG:HD2	2	0.16
(2,2882)	1:128:A:ARG:HE	1:124:A:VAL:HG21	4	0.16
(2,2882)	1:128:A:ARG:HE	1:124:A:VAL:HG22	4	0.16
(2,2882)	1:128:A:ARG:HE	1:124:A:VAL:HG23	4	0.16
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	6	0.16
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	6	0.16
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	6	0.16
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	6	0.16
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	6	0.16
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	6	0.16
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	6	0.16
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	6	0.16
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	6	0.16
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	9	0.16
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	9	0.16
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	9	0.16
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	9	0.16
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	9	0.16
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	9	0.16
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	9	0.16
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	9	0.16
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	9	0.16
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	6	0.16
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	6	0.16
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	6	0.16
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	6	0.16
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	6	0.16
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	6	0.16
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	6	0.16
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	6	0.16
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	6	0.16
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	9	0.16
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	9	0.16
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	9	0.16
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	9	0.16
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	9	0.16
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	9	0.16
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	9	0.16
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	9	0.16
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	9	0.16
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD11	5	0.16
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD12	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD13	5	0.16
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD11	5	0.16
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD12	5	0.16
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD13	5	0.16
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD11	5	0.16
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD12	5	0.16
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD13	5	0.16
(2,2679)	1:121:A:THR:HG21	1:120:A:SER:HA	4	0.16
(2,2679)	1:121:A:THR:HG22	1:120:A:SER:HA	4	0.16
(2,2679)	1:121:A:THR:HG23	1:120:A:SER:HA	4	0.16
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB1	10	0.16
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB2	10	0.16
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB3	10	0.16
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB1	10	0.16
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB2	10	0.16
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB3	10	0.16
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	4	0.16
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	4	0.16
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	4	0.16
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	6	0.16
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	6	0.16
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	6	0.16
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD11	4	0.16
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD12	4	0.16
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD13	4	0.16
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD11	4	0.16
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD12	4	0.16
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD13	4	0.16
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD11	4	0.16
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD12	4	0.16
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD13	4	0.16
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD21	6	0.16
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD22	6	0.16
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD23	6	0.16
(2,2413)	1:56:A:GLN:HE21	1:105:A:GLU:H	5	0.16
(2,2296)	1:100:A:TRP:HE3	1:84:A:ARG:HD3	3	0.16
(2,2295)	1:100:A:TRP:HE3	1:84:A:ARG:HB2	10	0.16
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	4	0.16
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	8	0.16
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE1	1	0.16
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE2	1	0.16
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE3	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1541)	1:68:A:MET:HE1	1:67:A:SER:H	1	0.16
(2,1541)	1:68:A:MET:HE2	1:67:A:SER:H	1	0.16
(2,1541)	1:68:A:MET:HE3	1:67:A:SER:H	1	0.16
(2,1538)	1:68:A:MET:HB3	1:67:A:SER:H	8	0.16
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG21	10	0.16
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG22	10	0.16
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG23	10	0.16
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	8	0.16
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG21	2	0.16
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG22	2	0.16
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG23	2	0.16
(2,886)	1:41:A:PHE:HD1	1:40:A:ASP:HB3	4	0.16
(2,886)	1:41:A:PHE:HD2	1:40:A:ASP:HB3	4	0.16
(2,730)	1:29:A:SER:H	1:27:A:THR:HG21	6	0.16
(2,730)	1:29:A:SER:H	1:27:A:THR:HG22	6	0.16
(2,730)	1:29:A:SER:H	1:27:A:THR:HG23	6	0.16
(2,729)	1:29:A:SER:H	1:27:A:THR:HB	5	0.16
(2,729)	1:29:A:SER:H	1:27:A:THR:HB	6	0.16
(2,704)	1:27:A:THR:HG21	1:28:A:GLN:HA	7	0.16
(2,704)	1:27:A:THR:HG22	1:28:A:GLN:HA	7	0.16
(2,704)	1:27:A:THR:HG23	1:28:A:GLN:HA	7	0.16
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	9	0.16
(2,293)	1:11:A:LYS:HE2	1:11:A:LYS:HA	10	0.16
(2,272)	1:11:A:LYS:HD2	1:8:A:ASP:HA	10	0.16
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG21	8	0.16
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG22	8	0.16
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG23	8	0.16
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	5	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	2	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	2	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	2	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	2	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	2	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	2	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	2	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	2	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	2	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	2	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	2	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	2	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	2	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	2	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	2	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	2	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	2	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	5	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	5	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	5	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	5	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	5	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	5	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	5	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	5	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	5	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	5	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	5	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	5	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	5	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	5	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	5	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	5	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	5	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	5	0.16
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG21	10	0.15
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG22	10	0.15
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG23	10	0.15
(2,3490)	1:143:A:SER:H	1:141:A:ASP:HA	1	0.15
(2,3490)	1:143:A:SER:H	1:141:A:ASP:HA	8	0.15
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	8	0.15
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	8	0.15
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	8	0.15
(2,3009)	1:130:A:GLN:HG3	1:127:A:SER:HA	8	0.15
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	8	0.15
(2,2903)	1:128:A:ARG:HE	1:128:A:ARG:HA	5	0.15
(2,2843)	1:46:A:HIS:HE1	1:127:A:SER:HA	3	0.15
(2,2843)	1:46:A:HIS:HE1	1:127:A:SER:HA	6	0.15
(2,2767)	1:124:A:VAL:HB	1:121:A:THR:HA	6	0.15
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG11	3	0.15
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG12	3	0.15
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG13	3	0.15
(2,2730)	1:28:A:GLN:HB2	1:123:A:VAL:HG21	8	0.15
(2,2730)	1:28:A:GLN:HB2	1:123:A:VAL:HG22	8	0.15
(2,2730)	1:28:A:GLN:HB2	1:123:A:VAL:HG23	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2616)	1:117:A:SER:HB2	1:117:A:SER:HA	8	0.15
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	4	0.15
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	4	0.15
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	4	0.15
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	4	0.15
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	4	0.15
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	4	0.15
(2,2515)	1:111:A:GLY:H	1:110:A:LEU:HG	2	0.15
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	3	0.15
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	3	0.15
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	3	0.15
(2,2415)	1:56:A:GLN:HE22	1:105:A:GLU:H	7	0.15
(2,2414)	1:105:A:GLU:H	1:56:A:GLN:HE22	7	0.15
(2,2305)	1:84:A:ARG:H	1:100:A:TRP:HZ3	2	0.15
(2,2305)	1:84:A:ARG:H	1:100:A:TRP:HZ3	8	0.15
(2,2304)	1:100:A:TRP:HZ3	1:84:A:ARG:H	2	0.15
(2,2304)	1:100:A:TRP:HZ3	1:84:A:ARG:H	8	0.15
(2,2295)	1:100:A:TRP:HE3	1:84:A:ARG:HB2	2	0.15
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	5	0.15
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD11	6	0.15
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD12	6	0.15
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD13	6	0.15
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG21	2	0.15
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG22	2	0.15
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG23	2	0.15
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG21	3	0.15
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG22	3	0.15
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG23	3	0.15
(2,1567)	1:68:A:MET:HG2	1:69:A:PRO:HD2	7	0.15
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	5	0.15
(2,1014)	1:46:A:HIS:HD2	1:45:A:LEU:HB2	6	0.15
(2,655)	1:26:A:HIS:HD2	1:23:A:ASP:HA	10	0.15
(2,324)	1:12:A:THR:H	1:11:A:LYS:HD2	5	0.15
(2,324)	1:12:A:THR:H	1:11:A:LYS:HD2	7	0.15
(2,3549)	1:146:A:CYS:H	1:50:A:THR:HG21	7	0.14
(2,3549)	1:146:A:CYS:H	1:50:A:THR:HG22	7	0.14
(2,3549)	1:146:A:CYS:H	1:50:A:THR:HG23	7	0.14
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD21	8	0.14
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD22	8	0.14
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD23	8	0.14
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG21	3	0.14
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG22	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG23	3	0.14
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG21	8	0.14
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG22	8	0.14
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG23	8	0.14
(2,3256)	1:15:A:LYS:HE2	1:137:A:LEU:HD21	8	0.14
(2,3256)	1:15:A:LYS:HE2	1:137:A:LEU:HD22	8	0.14
(2,3256)	1:15:A:LYS:HE2	1:137:A:LEU:HD23	8	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD21	2	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD22	2	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD23	2	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD21	3	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD22	3	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD23	3	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD21	4	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD22	4	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD23	4	0.14
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD21	4	0.14
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD22	4	0.14
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD23	4	0.14
(2,3122)	1:134:A:GLN:HE21	1:134:A:GLN:HA	3	0.14
(2,3108)	1:134:A:GLN:HG2	1:18:A:VAL:HA	4	0.14
(2,3088)	1:133:A:LEU:HG	1:130:A:GLN:HA	7	0.14
(2,3087)	1:130:A:GLN:HA	1:133:A:LEU:HG	7	0.14
(2,3003)	1:126:A:LEU:HD11	1:130:A:GLN:HA	5	0.14
(2,3003)	1:126:A:LEU:HD12	1:130:A:GLN:HA	5	0.14
(2,3003)	1:126:A:LEU:HD13	1:130:A:GLN:HA	5	0.14
(2,3003)	1:126:A:LEU:HD11	1:130:A:GLN:HA	8	0.14
(2,3003)	1:126:A:LEU:HD12	1:130:A:GLN:HA	8	0.14
(2,3003)	1:126:A:LEU:HD13	1:130:A:GLN:HA	8	0.14
(2,2903)	1:128:A:ARG:HE	1:128:A:ARG:HA	2	0.14
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG21	2	0.14
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG22	2	0.14
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG23	2	0.14
(2,2817)	1:76:A:ILE:HD11	1:126:A:LEU:HA	2	0.14
(2,2817)	1:76:A:ILE:HD12	1:126:A:LEU:HA	2	0.14
(2,2817)	1:76:A:ILE:HD13	1:126:A:LEU:HA	2	0.14
(2,2798)	1:119:A:TYR:HE1	1:125:A:ALA:H	8	0.14
(2,2798)	1:119:A:TYR:HE2	1:125:A:ALA:H	8	0.14
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG21	6	0.14
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG22	6	0.14
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG23	6	0.14
(2,2679)	1:121:A:THR:HG21	1:120:A:SER:HA	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2679)	1:121:A:THR:HG22	1:120:A:SER:HA	5	0.14
(2,2679)	1:121:A:THR:HG23	1:120:A:SER:HA	5	0.14
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	5	0.14
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	5	0.14
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	5	0.14
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG21	5	0.14
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG22	5	0.14
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG23	5	0.14
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG21	5	0.14
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG22	5	0.14
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG23	5	0.14
(2,2515)	1:111:A:GLY:H	1:110:A:LEU:HG	8	0.14
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	3	0.14
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	6	0.14
(2,2305)	1:84:A:ARG:H	1:100:A:TRP:HZ3	5	0.14
(2,2305)	1:84:A:ARG:H	1:100:A:TRP:HZ3	7	0.14
(2,2304)	1:100:A:TRP:HZ3	1:84:A:ARG:H	5	0.14
(2,2304)	1:100:A:TRP:HZ3	1:84:A:ARG:H	7	0.14
(2,2203)	1:94:A:LYS:HB2	1:94:A:LYS:HD2	8	0.14
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB1	10	0.14
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB2	10	0.14
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB3	10	0.14
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB1	10	0.14
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB2	10	0.14
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB3	10	0.14
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB1	10	0.14
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB2	10	0.14
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB3	10	0.14
(2,2131)	1:91:A:ALA:HA	1:3:A:ILE:HG13	1	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD11	3	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD12	3	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD13	3	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD11	9	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD12	9	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD13	9	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD11	10	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD12	10	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD13	10	0.14
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG21	6	0.14
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG22	6	0.14
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG23	6	0.14
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG21	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG22	6	0.14
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG23	6	0.14
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG21	6	0.14
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG22	6	0.14
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG23	6	0.14
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG21	5	0.14
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG22	5	0.14
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG23	5	0.14
(2,1656)	1:73:A:VAL:H	1:71:A:ARG:HB2	7	0.14
(2,1566)	1:68:A:MET:HE1	1:69:A:PRO:HD2	7	0.14
(2,1566)	1:68:A:MET:HE2	1:69:A:PRO:HD2	7	0.14
(2,1566)	1:68:A:MET:HE3	1:69:A:PRO:HD2	7	0.14
(2,1190)	1:51:A:LEU:HD11	1:54:A:MET:HB2	8	0.14
(2,1190)	1:51:A:LEU:HD12	1:54:A:MET:HB2	8	0.14
(2,1190)	1:51:A:LEU:HD13	1:54:A:MET:HB2	8	0.14
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	6	0.14
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	9	0.14
(2,755)	1:30:A:VAL:HB	1:32:A:SER:HB2	5	0.14
(2,589)	1:24:A:ILE:HD11	1:21:A:ILE:HA	4	0.14
(2,589)	1:24:A:ILE:HD12	1:21:A:ILE:HA	4	0.14
(2,589)	1:24:A:ILE:HD13	1:21:A:ILE:HA	4	0.14
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	9	0.14
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	9	0.14
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	9	0.14
(2,426)	1:16:A:THR:H	1:15:A:LYS:HD2	6	0.14
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD21	8	0.14
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD22	8	0.14
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD23	8	0.14
(2,324)	1:12:A:THR:H	1:11:A:LYS:HD2	6	0.14
(2,293)	1:11:A:LYS:HE2	1:11:A:LYS:HA	9	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	4	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	4	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	4	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	4	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	4	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	4	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	4	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	4	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	4	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	4	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	4	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	4	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	4	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	4	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	4	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	4	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	4	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	8	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	8	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	8	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	8	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	8	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	8	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	8	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	8	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	8	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	8	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	8	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	8	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	8	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	8	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	8	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	8	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	8	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	8	0.14
(2,3450)	1:142:A:LEU:HD11	1:138:A:TRP:HZ2	5	0.13
(2,3450)	1:142:A:LEU:HD12	1:138:A:TRP:HZ2	5	0.13
(2,3450)	1:142:A:LEU:HD13	1:138:A:TRP:HZ2	5	0.13
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD11	5	0.13
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD12	5	0.13
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD13	5	0.13
(2,3122)	1:134:A:GLN:HE21	1:134:A:GLN:HA	10	0.13
(2,3088)	1:133:A:LEU:HG	1:130:A:GLN:HA	9	0.13
(2,3087)	1:130:A:GLN:HA	1:133:A:LEU:HG	9	0.13
(2,2987)	1:130:A:GLN:HE21	1:21:A:ILE:H	4	0.13
(2,2970)	1:130:A:GLN:HE21	1:18:A:VAL:HA	1	0.13
(2,2970)	1:130:A:GLN:HE21	1:18:A:VAL:HA	6	0.13
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	5	0.13
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	5	0.13
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	5	0.13
(2,2817)	1:76:A:ILE:HD11	1:126:A:LEU:HA	5	0.13
(2,2817)	1:76:A:ILE:HD12	1:126:A:LEU:HA	5	0.13
(2,2817)	1:76:A:ILE:HD13	1:126:A:LEU:HA	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2767)	1:124:A:VAL:HB	1:121:A:THR:HA	9	0.13
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG21	1	0.13
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG22	1	0.13
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG23	1	0.13
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	1	0.13
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	1	0.13
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	1	0.13
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	1	0.13
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	1	0.13
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	1	0.13
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	1	0.13
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	1	0.13
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	1	0.13
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	1	0.13
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	1	0.13
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	1	0.13
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	1	0.13
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	1	0.13
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	1	0.13
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	1	0.13
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	1	0.13
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	1	0.13
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD11	2	0.13
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD12	2	0.13
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD13	2	0.13
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD11	2	0.13
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD12	2	0.13
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD13	2	0.13
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD11	2	0.13
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD12	2	0.13
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD13	2	0.13
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG11	4	0.13
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG12	4	0.13
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG13	4	0.13
(2,2724)	1:26:A:HIS:HD2	1:123:A:VAL:HG21	1	0.13
(2,2724)	1:26:A:HIS:HD2	1:123:A:VAL:HG22	1	0.13
(2,2724)	1:26:A:HIS:HD2	1:123:A:VAL:HG23	1	0.13
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB1	5	0.13
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB2	5	0.13
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB3	5	0.13
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB1	5	0.13
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB2	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB3	5	0.13
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	8	0.13
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	8	0.13
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	8	0.13
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	6	0.13
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	6	0.13
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	6	0.13
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	5	0.13
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD11	3	0.13
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD12	3	0.13
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD13	3	0.13
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD11	3	0.13
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD12	3	0.13
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD13	3	0.13
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD11	3	0.13
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD12	3	0.13
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD13	3	0.13
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG21	1	0.13
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG22	1	0.13
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG23	1	0.13
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG21	1	0.13
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG22	1	0.13
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG23	1	0.13
(2,2305)	1:84:A:ARG:H	1:100:A:TRP:HZ3	3	0.13
(2,2305)	1:84:A:ARG:H	1:100:A:TRP:HZ3	9	0.13
(2,2304)	1:100:A:TRP:HZ3	1:84:A:ARG:H	3	0.13
(2,2304)	1:100:A:TRP:HZ3	1:84:A:ARG:H	9	0.13
(2,2296)	1:100:A:TRP:HE3	1:84:A:ARG:HD3	7	0.13
(2,2240)	1:97:A:HIS:HE1	1:95:A:SER:H	7	0.13
(2,2203)	1:94:A:LYS:HB2	1:94:A:LYS:HD2	1	0.13
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	9	0.13
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG21	2	0.13
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG22	2	0.13
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG23	2	0.13
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG21	2	0.13
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG22	2	0.13
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG23	2	0.13
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG21	2	0.13
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG22	2	0.13
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG23	2	0.13
(2,1733)	1:75:A:GLN:HE21	1:75:A:GLN:HA	5	0.13
(2,1537)	1:68:A:MET:HB3	1:67:A:SER:HB2	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1527)	1:68:A:MET:HE1	1:65:A:LEU:H	5	0.13
(2,1527)	1:68:A:MET:HE2	1:65:A:LEU:H	5	0.13
(2,1527)	1:68:A:MET:HE3	1:65:A:LEU:H	5	0.13
(2,1517)	1:64:A:ILE:HD11	1:68:A:MET:HE1	6	0.13
(2,1517)	1:64:A:ILE:HD11	1:68:A:MET:HE2	6	0.13
(2,1517)	1:64:A:ILE:HD11	1:68:A:MET:HE3	6	0.13
(2,1517)	1:64:A:ILE:HD12	1:68:A:MET:HE1	6	0.13
(2,1517)	1:64:A:ILE:HD12	1:68:A:MET:HE2	6	0.13
(2,1517)	1:64:A:ILE:HD12	1:68:A:MET:HE3	6	0.13
(2,1517)	1:64:A:ILE:HD13	1:68:A:MET:HE1	6	0.13
(2,1517)	1:64:A:ILE:HD13	1:68:A:MET:HE2	6	0.13
(2,1517)	1:64:A:ILE:HD13	1:68:A:MET:HE3	6	0.13
(2,1516)	1:68:A:MET:HE1	1:64:A:ILE:HD11	6	0.13
(2,1516)	1:68:A:MET:HE1	1:64:A:ILE:HD12	6	0.13
(2,1516)	1:68:A:MET:HE1	1:64:A:ILE:HD13	6	0.13
(2,1516)	1:68:A:MET:HE2	1:64:A:ILE:HD11	6	0.13
(2,1516)	1:68:A:MET:HE2	1:64:A:ILE:HD12	6	0.13
(2,1516)	1:68:A:MET:HE2	1:64:A:ILE:HD13	6	0.13
(2,1516)	1:68:A:MET:HE3	1:64:A:ILE:HD11	6	0.13
(2,1516)	1:68:A:MET:HE3	1:64:A:ILE:HD12	6	0.13
(2,1516)	1:68:A:MET:HE3	1:64:A:ILE:HD13	6	0.13
(2,1515)	1:68:A:MET:HE1	1:64:A:ILE:HA	8	0.13
(2,1515)	1:68:A:MET:HE2	1:64:A:ILE:HA	8	0.13
(2,1515)	1:68:A:MET:HE3	1:64:A:ILE:HA	8	0.13
(2,1402)	1:64:A:ILE:HD11	1:60:A:VAL:HG11	5	0.13
(2,1402)	1:64:A:ILE:HD11	1:60:A:VAL:HG12	5	0.13
(2,1402)	1:64:A:ILE:HD11	1:60:A:VAL:HG13	5	0.13
(2,1402)	1:64:A:ILE:HD12	1:60:A:VAL:HG11	5	0.13
(2,1402)	1:64:A:ILE:HD12	1:60:A:VAL:HG12	5	0.13
(2,1402)	1:64:A:ILE:HD12	1:60:A:VAL:HG13	5	0.13
(2,1402)	1:64:A:ILE:HD13	1:60:A:VAL:HG11	5	0.13
(2,1402)	1:64:A:ILE:HD13	1:60:A:VAL:HG12	5	0.13
(2,1402)	1:64:A:ILE:HD13	1:60:A:VAL:HG13	5	0.13
(2,1332)	1:61:A:TYR:HE1	1:58:A:LEU:HD21	3	0.13
(2,1332)	1:61:A:TYR:HE1	1:58:A:LEU:HD22	3	0.13
(2,1332)	1:61:A:TYR:HE1	1:58:A:LEU:HD23	3	0.13
(2,1332)	1:61:A:TYR:HE2	1:58:A:LEU:HD21	3	0.13
(2,1332)	1:61:A:TYR:HE2	1:58:A:LEU:HD22	3	0.13
(2,1332)	1:61:A:TYR:HE2	1:58:A:LEU:HD23	3	0.13
(2,1257)	1:56:A:GLN:H	1:57:A:THR:HB	10	0.13
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD21	7	0.13
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD22	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD23	7	0.13
(2,1011)	1:46:A:HIS:HD2	1:42:A:ILE:HG13	2	0.13
(2,814)	1:36:A:VAL:HG21	1:35:A:LYS:HD2	2	0.13
(2,814)	1:36:A:VAL:HG22	1:35:A:LYS:HD2	2	0.13
(2,814)	1:36:A:VAL:HG23	1:35:A:LYS:HD2	2	0.13
(2,729)	1:29:A:SER:H	1:27:A:THR:HB	10	0.13
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	1	0.13
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG21	9	0.13
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG22	9	0.13
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG23	9	0.13
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	8	0.13
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	8	0.13
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	8	0.13
(2,141)	1:5:A:LYS:H	1:5:A:LYS:HE2	1	0.13
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	9	0.13
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	9	0.13
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	9	0.13
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	9	0.13
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	9	0.13
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	9	0.13
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	9	0.13
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	9	0.13
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	9	0.13
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	9	0.13
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	9	0.13
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	9	0.13
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	9	0.13
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	9	0.13
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	9	0.13
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	9	0.13
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	9	0.13
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	9	0.13
(2,3490)	1:143:A:SER:H	1:141:A:ASP:HA	4	0.12
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD21	1	0.12
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD22	1	0.12
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD23	1	0.12
(2,3450)	1:142:A:LEU:HD11	1:138:A:TRP:HZ2	1	0.12
(2,3450)	1:142:A:LEU:HD12	1:138:A:TRP:HZ2	1	0.12
(2,3450)	1:142:A:LEU:HD13	1:138:A:TRP:HZ2	1	0.12
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD11	1	0.12
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD12	1	0.12
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD13	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD21	2	0.12
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD22	2	0.12
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD23	2	0.12
(2,3234)	1:137:A:LEU:HD21	1:11:A:LYS:HE2	2	0.12
(2,3234)	1:137:A:LEU:HD22	1:11:A:LYS:HE2	2	0.12
(2,3234)	1:137:A:LEU:HD23	1:11:A:LYS:HE2	2	0.12
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD21	2	0.12
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD22	2	0.12
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD23	2	0.12
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	9	0.12
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	9	0.12
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	9	0.12
(2,3113)	1:134:A:GLN:HE21	1:131:A:GLY:HA2	7	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG21	1	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG22	1	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG23	1	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG21	4	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG22	4	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG23	4	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG21	7	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG22	7	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG23	7	0.12
(2,2798)	1:119:A:TYR:HE1	1:125:A:ALA:H	2	0.12
(2,2798)	1:119:A:TYR:HE2	1:125:A:ALA:H	2	0.12
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE1	9	0.12
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE2	9	0.12
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE3	9	0.12
(2,2696)	1:68:A:MET:HE1	1:122:A:GLU:HG2	9	0.12
(2,2696)	1:68:A:MET:HE2	1:122:A:GLU:HG2	9	0.12
(2,2696)	1:68:A:MET:HE3	1:122:A:GLU:HG2	9	0.12
(2,2626)	1:119:A:TYR:HE1	1:38:A:GLY:HA2	6	0.12
(2,2626)	1:119:A:TYR:HE2	1:38:A:GLY:HA2	6	0.12
(2,2452)	1:108:A:ASP:H	1:106:A:THR:HB	8	0.12
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD21	3	0.12
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD22	3	0.12
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD23	3	0.12
(2,2395)	1:104:A:LEU:HD21	1:63:A:GLN:HE21	3	0.12
(2,2395)	1:104:A:LEU:HD22	1:63:A:GLN:HE21	3	0.12
(2,2395)	1:104:A:LEU:HD23	1:63:A:GLN:HE21	3	0.12
(2,2295)	1:100:A:TRP:HE3	1:84:A:ARG:HB2	3	0.12
(2,2203)	1:94:A:LYS:HB2	1:94:A:LYS:HD2	3	0.12
(2,2203)	1:94:A:LYS:HB2	1:94:A:LYS:HD2	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	2	0.12
(2,2131)	1:91:A:ALA:HA	1:3:A:ILE:HG13	6	0.12
(2,1916)	1:83:A:LEU:HB3	1:80:A:LEU:HD21	10	0.12
(2,1916)	1:83:A:LEU:HB3	1:80:A:LEU:HD22	10	0.12
(2,1916)	1:83:A:LEU:HB3	1:80:A:LEU:HD23	10	0.12
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD11	6	0.12
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD12	6	0.12
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD13	6	0.12
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG21	8	0.12
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG22	8	0.12
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG23	8	0.12
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG21	8	0.12
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG22	8	0.12
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG23	8	0.12
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG21	8	0.12
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG22	8	0.12
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG23	8	0.12
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG21	7	0.12
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG22	7	0.12
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG23	7	0.12
(2,1566)	1:68:A:MET:HE1	1:69:A:PRO:HD2	4	0.12
(2,1566)	1:68:A:MET:HE2	1:69:A:PRO:HD2	4	0.12
(2,1566)	1:68:A:MET:HE3	1:69:A:PRO:HD2	4	0.12
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	8	0.12
(2,1190)	1:51:A:LEU:HD11	1:54:A:MET:HB2	1	0.12
(2,1190)	1:51:A:LEU:HD12	1:54:A:MET:HB2	1	0.12
(2,1190)	1:51:A:LEU:HD13	1:54:A:MET:HB2	1	0.12
(2,1190)	1:51:A:LEU:HD11	1:54:A:MET:HB2	3	0.12
(2,1190)	1:51:A:LEU:HD12	1:54:A:MET:HB2	3	0.12
(2,1190)	1:51:A:LEU:HD13	1:54:A:MET:HB2	3	0.12
(2,884)	1:41:A:PHE:H	1:39:A:LEU:HB2	3	0.12
(2,813)	1:36:A:VAL:HG11	1:35:A:LYS:HA	7	0.12
(2,813)	1:36:A:VAL:HG12	1:35:A:LYS:HA	7	0.12
(2,813)	1:36:A:VAL:HG13	1:35:A:LYS:HA	7	0.12
(2,779)	1:34:A:GLN:HG2	1:31:A:SER:HB2	6	0.12
(2,761)	1:32:A:SER:H	1:33:A:LYS:H	6	0.12
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	8	0.12
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG21	5	0.12
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG22	5	0.12
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG23	5	0.12
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	1	0.12
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	1	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	1	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	1	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	1	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	1	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	1	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	1	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	1	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	1	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	1	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	1	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	1	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	1	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	1	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	1	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	1	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	1	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	1	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	1	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	7	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	7	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	7	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	7	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	7	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	7	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	7	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	7	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	7	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	7	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	7	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	7	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	7	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	7	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	7	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	7	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	7	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	7	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	10	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	10	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	10	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	10	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	10	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	10	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	10	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	10	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	10	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	10	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	10	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	10	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	10	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	10	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	10	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	10	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	10	0.12
(2,3490)	1:143:A:SER:H	1:141:A:ASP:HA	5	0.11
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD21	3	0.11
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD22	3	0.11
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD23	3	0.11
(2,3454)	1:138:A:TRP:HE1	1:142:A:LEU:HD21	9	0.11
(2,3454)	1:138:A:TRP:HE1	1:142:A:LEU:HD22	9	0.11
(2,3454)	1:138:A:TRP:HE1	1:142:A:LEU:HD23	9	0.11
(2,3167)	1:136:A:MET:HB2	1:54:A:MET:HE1	9	0.11
(2,3167)	1:136:A:MET:HB2	1:54:A:MET:HE2	9	0.11
(2,3167)	1:136:A:MET:HB2	1:54:A:MET:HE3	9	0.11
(2,3163)	1:49:A:LEU:HD11	1:136:A:MET:HB2	8	0.11
(2,3163)	1:49:A:LEU:HD12	1:136:A:MET:HB2	8	0.11
(2,3163)	1:49:A:LEU:HD13	1:136:A:MET:HB2	8	0.11
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD11	8	0.11
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD12	8	0.11
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD13	8	0.11
(2,3108)	1:134:A:GLN:HG2	1:18:A:VAL:HA	3	0.11
(2,3088)	1:133:A:LEU:HG	1:130:A:GLN:HA	2	0.11
(2,3087)	1:130:A:GLN:HA	1:133:A:LEU:HG	2	0.11
(2,3009)	1:130:A:GLN:HG3	1:127:A:SER:HA	7	0.11
(2,2948)	1:129:A:LEU:H	1:128:A:ARG:HD2	8	0.11
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG21	10	0.11
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG22	10	0.11
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG23	10	0.11
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG11	7	0.11
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG12	7	0.11
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG13	7	0.11
(2,2704)	1:122:A:GLU:H	1:73:A:VAL:HG11	9	0.11
(2,2704)	1:122:A:GLU:H	1:73:A:VAL:HG12	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2704)	1:122:A:GLU:H	1:73:A:VAL:HG13	9	0.11
(2,2626)	1:119:A:TYR:HE1	1:38:A:GLY:HA2	5	0.11
(2,2626)	1:119:A:TYR:HE2	1:38:A:GLY:HA2	5	0.11
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB1	7	0.11
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB2	7	0.11
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB3	7	0.11
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB1	7	0.11
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB2	7	0.11
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB3	7	0.11
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB1	7	0.11
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB2	7	0.11
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB3	7	0.11
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD11	7	0.11
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD12	7	0.11
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD13	7	0.11
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD11	7	0.11
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD12	7	0.11
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD13	7	0.11
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD11	7	0.11
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD12	7	0.11
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD13	7	0.11
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	6	0.11
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	6	0.11
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	6	0.11
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	6	0.11
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	6	0.11
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	6	0.11
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	8	0.11
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD11	1	0.11
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD12	1	0.11
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD13	1	0.11
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD21	1	0.11
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD22	1	0.11
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD23	1	0.11
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD21	10	0.11
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD22	10	0.11
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD23	10	0.11
(2,2395)	1:104:A:LEU:HD21	1:63:A:GLN:HE21	10	0.11
(2,2395)	1:104:A:LEU:HD22	1:63:A:GLN:HE21	10	0.11
(2,2395)	1:104:A:LEU:HD23	1:63:A:GLN:HE21	10	0.11
(2,2305)	1:84:A:ARG:H	1:100:A:TRP:HZ3	10	0.11
(2,2304)	1:100:A:TRP:HZ3	1:84:A:ARG:H	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2131)	1:91:A:ALA:HA	1:3:A:ILE:HG13	5	0.11
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD11	9	0.11
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD12	9	0.11
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD13	9	0.11
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD11	8	0.11
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD12	8	0.11
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD13	8	0.11
(2,1566)	1:68:A:MET:HE1	1:69:A:PRO:HD2	8	0.11
(2,1566)	1:68:A:MET:HE2	1:69:A:PRO:HD2	8	0.11
(2,1566)	1:68:A:MET:HE3	1:69:A:PRO:HD2	8	0.11
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	6	0.11
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	3	0.11
(2,1030)	1:46:A:HIS:HD2	1:47:A:PRO:HD3	10	0.11
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG21	4	0.11
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG22	4	0.11
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG23	4	0.11
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	2	0.11
(2,655)	1:26:A:HIS:HD2	1:23:A:ASP:HA	6	0.11
(2,426)	1:16:A:THR:H	1:15:A:LYS:HD2	3	0.11
(2,426)	1:16:A:THR:H	1:15:A:LYS:HD2	5	0.11
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD21	3	0.1
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD22	3	0.1
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD23	3	0.1
(2,3186)	1:136:A:MET:HE1	1:87:A:LEU:HD21	1	0.1
(2,3186)	1:136:A:MET:HE1	1:87:A:LEU:HD22	1	0.1
(2,3186)	1:136:A:MET:HE1	1:87:A:LEU:HD23	1	0.1
(2,3186)	1:136:A:MET:HE2	1:87:A:LEU:HD21	1	0.1
(2,3186)	1:136:A:MET:HE2	1:87:A:LEU:HD22	1	0.1
(2,3186)	1:136:A:MET:HE2	1:87:A:LEU:HD23	1	0.1
(2,3186)	1:136:A:MET:HE3	1:87:A:LEU:HD21	1	0.1
(2,3186)	1:136:A:MET:HE3	1:87:A:LEU:HD22	1	0.1
(2,3186)	1:136:A:MET:HE3	1:87:A:LEU:HD23	1	0.1
(2,2784)	1:61:A:TYR:HE1	1:125:A:ALA:HB1	6	0.1
(2,2784)	1:61:A:TYR:HE1	1:125:A:ALA:HB2	6	0.1
(2,2784)	1:61:A:TYR:HE1	1:125:A:ALA:HB3	6	0.1
(2,2784)	1:61:A:TYR:HE2	1:125:A:ALA:HB1	6	0.1
(2,2784)	1:61:A:TYR:HE2	1:125:A:ALA:HB2	6	0.1
(2,2784)	1:61:A:TYR:HE2	1:125:A:ALA:HB3	6	0.1
(2,2767)	1:124:A:VAL:HB	1:121:A:THR:HA	10	0.1
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD11	4	0.1
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD12	4	0.1
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD13	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD11	4	0.1
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD12	4	0.1
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD13	4	0.1
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD11	4	0.1
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD12	4	0.1
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD13	4	0.1
(2,2693)	1:68:A:MET:HE1	1:122:A:GLU:HB3	9	0.1
(2,2693)	1:68:A:MET:HE2	1:122:A:GLU:HB3	9	0.1
(2,2693)	1:68:A:MET:HE3	1:122:A:GLU:HB3	9	0.1
(2,2676)	1:68:A:MET:HE1	1:121:A:THR:HG21	3	0.1
(2,2676)	1:68:A:MET:HE1	1:121:A:THR:HG22	3	0.1
(2,2676)	1:68:A:MET:HE1	1:121:A:THR:HG23	3	0.1
(2,2676)	1:68:A:MET:HE2	1:121:A:THR:HG21	3	0.1
(2,2676)	1:68:A:MET:HE2	1:121:A:THR:HG22	3	0.1
(2,2676)	1:68:A:MET:HE2	1:121:A:THR:HG23	3	0.1
(2,2676)	1:68:A:MET:HE3	1:121:A:THR:HG21	3	0.1
(2,2676)	1:68:A:MET:HE3	1:121:A:THR:HG22	3	0.1
(2,2676)	1:68:A:MET:HE3	1:121:A:THR:HG23	3	0.1
(2,2675)	1:121:A:THR:HG21	1:68:A:MET:HE1	3	0.1
(2,2675)	1:121:A:THR:HG21	1:68:A:MET:HE2	3	0.1
(2,2675)	1:121:A:THR:HG21	1:68:A:MET:HE3	3	0.1
(2,2675)	1:121:A:THR:HG22	1:68:A:MET:HE1	3	0.1
(2,2675)	1:121:A:THR:HG22	1:68:A:MET:HE2	3	0.1
(2,2675)	1:121:A:THR:HG22	1:68:A:MET:HE3	3	0.1
(2,2675)	1:121:A:THR:HG23	1:68:A:MET:HE1	3	0.1
(2,2675)	1:121:A:THR:HG23	1:68:A:MET:HE2	3	0.1
(2,2675)	1:121:A:THR:HG23	1:68:A:MET:HE3	3	0.1
(2,2389)	1:63:A:GLN:HB2	1:104:A:LEU:HD11	6	0.1
(2,2389)	1:63:A:GLN:HB2	1:104:A:LEU:HD12	6	0.1
(2,2389)	1:63:A:GLN:HB2	1:104:A:LEU:HD13	6	0.1
(2,2203)	1:94:A:LYS:HB2	1:94:A:LYS:HD2	10	0.1
(2,1566)	1:68:A:MET:HE1	1:69:A:PRO:HD2	5	0.1
(2,1566)	1:68:A:MET:HE2	1:69:A:PRO:HD2	5	0.1
(2,1566)	1:68:A:MET:HE3	1:69:A:PRO:HD2	5	0.1
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG21	8	0.1
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG22	8	0.1
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG23	8	0.1
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG21	8	0.1
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG22	8	0.1
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG23	8	0.1
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD21	9	0.1
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD22	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD23	9	0.1
(2,1014)	1:46:A:HIS:HD2	1:45:A:LEU:HB2	2	0.1
(2,1011)	1:46:A:HIS:HD2	1:42:A:ILE:HG13	1	0.1
(2,832)	1:37:A:THR:H	1:35:A:LYS:HD2	9	0.1
(2,779)	1:34:A:GLN:HG2	1:31:A:SER:HB2	8	0.1
(2,729)	1:29:A:SER:H	1:27:A:THR:HB	1	0.1
(2,467)	1:18:A:VAL:H	1:16:A:THR:HB	8	0.1
(2,224)	1:8:A:ASP:HB2	1:5:A:LYS:HB3	4	0.1

10 Dihedral-angle violation analysis [i](#)

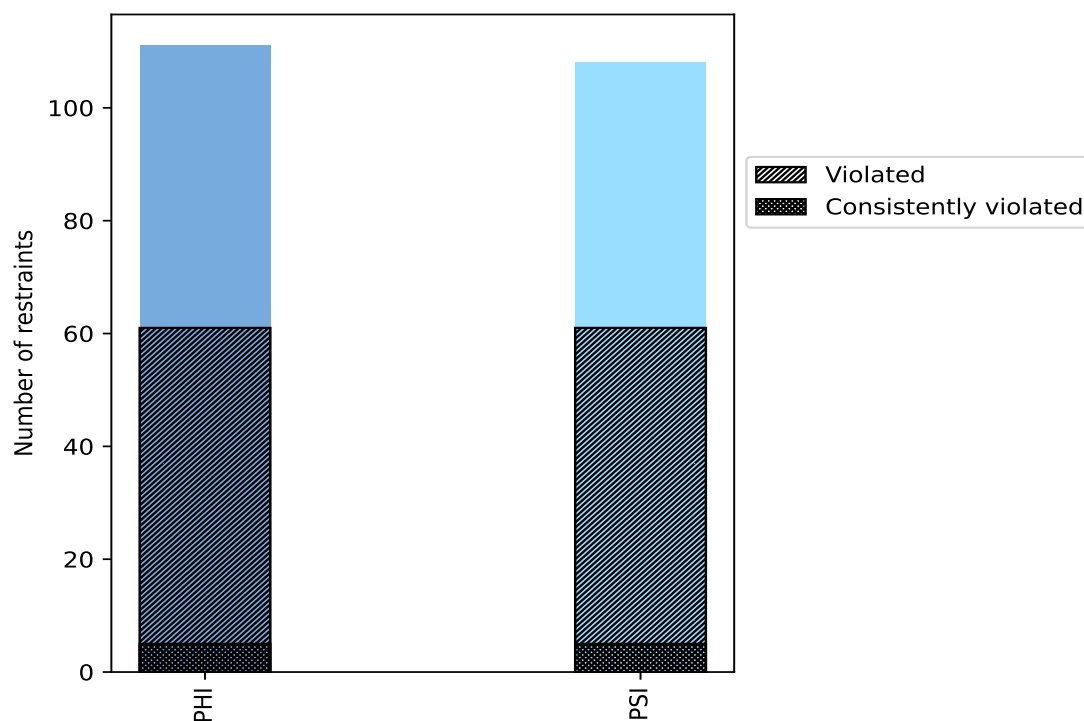
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	111	50.7	61	55.0	27.9	5	4.5	2.3
PSI	108	49.3	61	56.5	27.9	5	4.6	2.3
Total	219	100.0	122	55.7	55.7	10	4.6	4.6

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



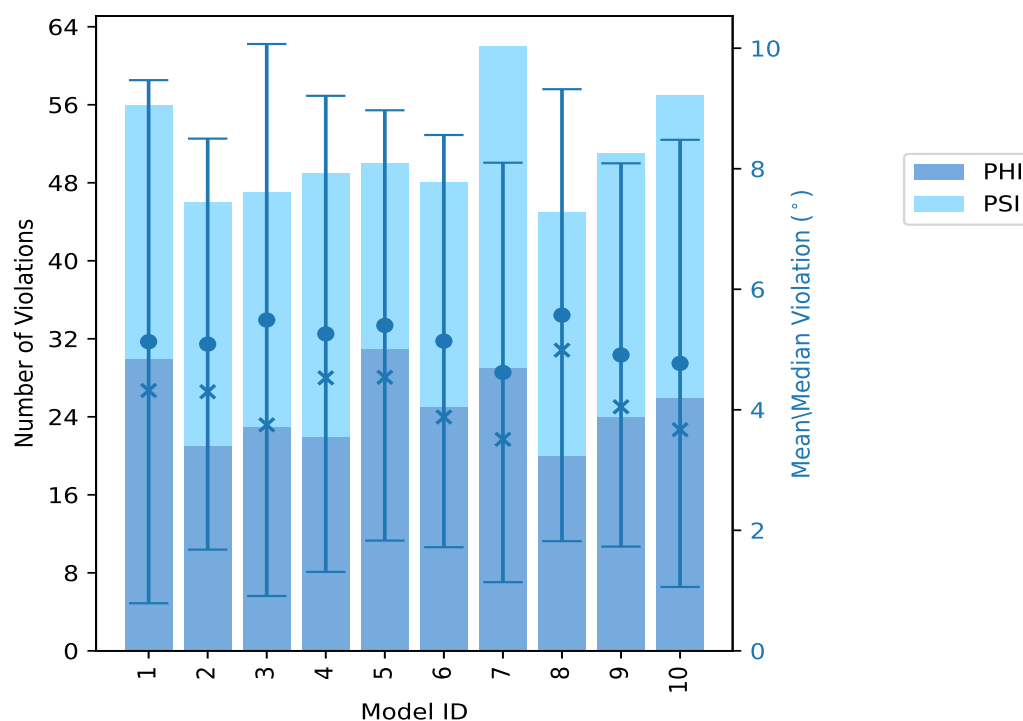
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [i](#)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	30	26	56	5.13	21.74	4.34	4.32
2	21	25	46	5.09	16.27	3.41	4.3
3	23	24	47	5.49	21.63	4.58	3.75
4	22	27	49	5.26	18.69	3.95	4.53
5	31	19	50	5.4	16.87	3.57	4.54
6	25	23	48	5.14	15.87	3.42	3.88
7	29	33	62	4.62	14.9	3.48	3.51
8	20	25	45	5.57	16.14	3.75	4.99
9	24	27	51	4.91	14.69	3.18	4.05
10	26	31	57	4.77	19.92	3.71	3.67

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

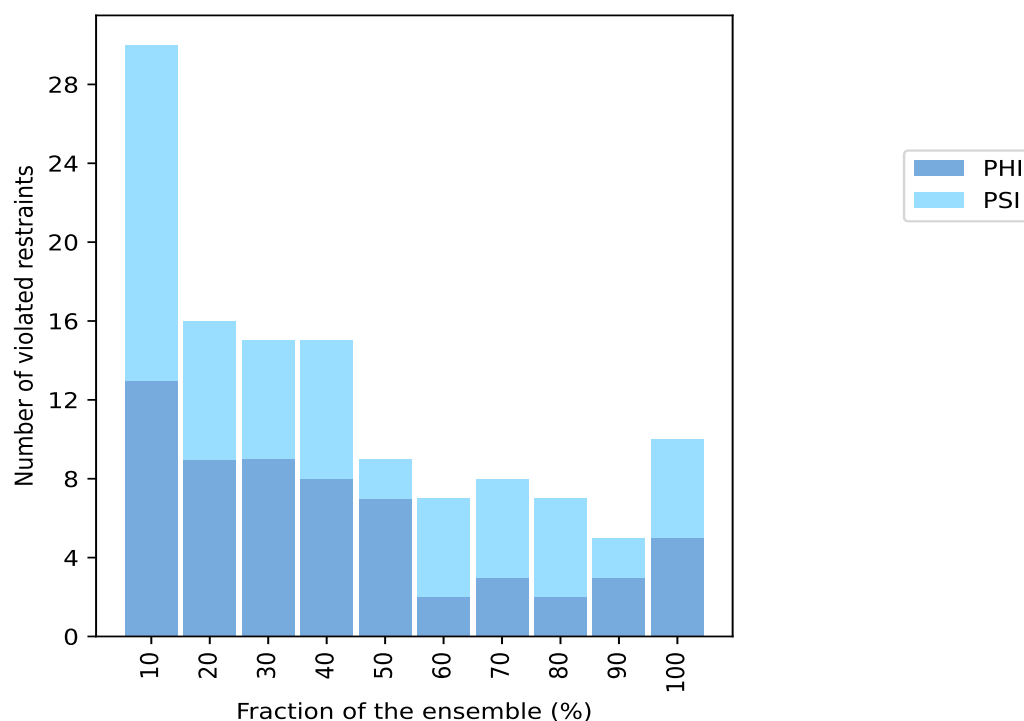
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
13	17	30	1	10.0
9	7	16	2	20.0
9	6	15	3	30.0
8	7	15	4	40.0
7	2	9	5	50.0
2	5	7	6	60.0
3	5	8	7	70.0
2	5	7	8	80.0
3	2	5	9	90.0
5	5	10	10	100.0

¹ Number of models with violations

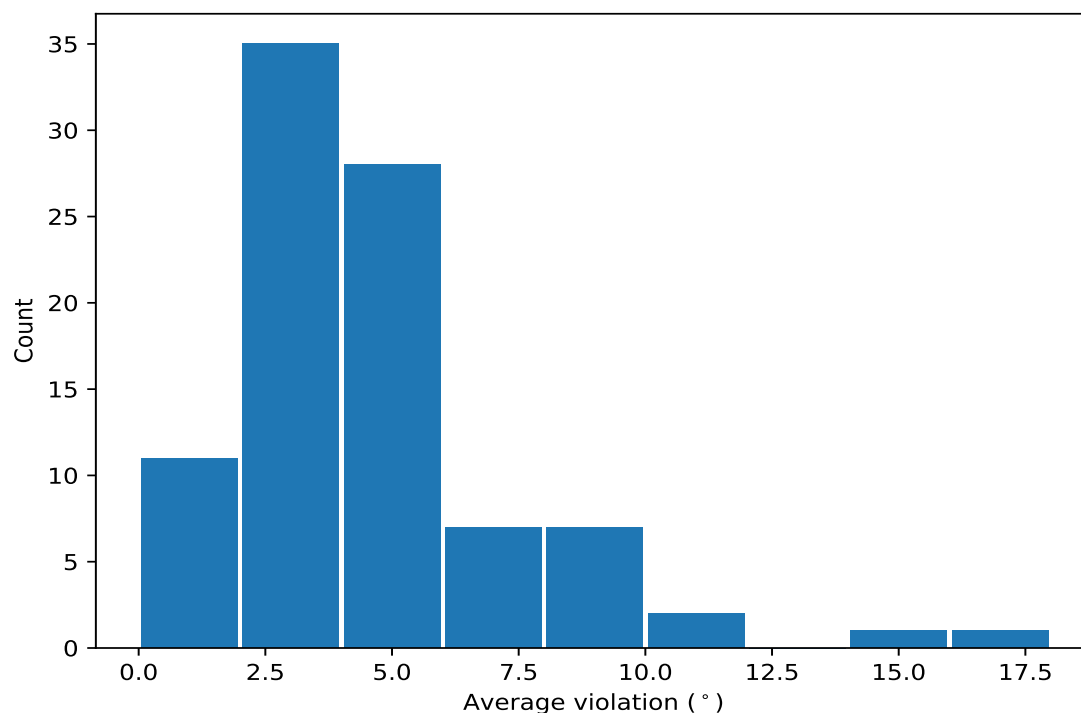
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	10	16.65	1.51	16.35
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	10	8.98	1.49	9.2
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	10	8.64	3.28	8.48
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	10	8.43	1.97	8.16
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	10	8.16	2.04	8.42
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	10	6.1	2.32	5.94
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	10	5.76	1.43	5.23
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	10	5.72	1.97	5.62
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	10	5.27	1.47	5.62
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	10	4.03	1.69	4.56
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	9	14.81	4.1	14.33
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	9	10.91	5.09	10.92
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	9	9.5	4.79	7.47

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	9	6.52	2.46	7.2
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	9	2.49	0.75	2.32
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	8	7.47	3.49	9.59
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	8	5.31	1.66	5.44
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	8	5.24	4.28	3.06
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	8	4.77	2.41	4.69
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	8	4.73	1.83	5.08
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	8	4.57	1.76	4.97
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	8	2.34	0.87	1.95
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:ILE:N	7	5.73	1.76	5.73
(1,116)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	7	5.17	2.27	4.99
(1,12)	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:ASP:N	7	5.05	1.93	4.74
(1,179)	1:122:A:GLU:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	7	4.71	1.71	4.35
(1,117)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	7	3.78	1.36	3.82
(1,154)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:PRO:N	7	3.14	1.27	3.5
(1,79)	1:58:A:LEU:C	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	7	3.09	1.07	2.84
(1,164)	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1:107:A:LEU:N	7	3.02	1.49	2.1
(1,70)	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	1:55:A:ASP:N	6	5.72	1.71	5.43
(1,96)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:MET:N	6	4.05	2.39	3.56
(1,75)	1:56:A:GLN:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	6	3.3	0.99	3.49
(1,66)	1:52:A:SER:N	1:52:A:SER:CA	1:52:A:SER:C	1:53:A:LYS:N	6	3.17	1.53	2.46
(1,40)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:ASP:N	6	3.02	2.37	2.19
(1,121)	1:81:A:GLU:C	1:82:A:ASN:N	1:82:A:ASN:CA	1:82:A:ASN:C	6	2.6	1.41	1.98
(1,34)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:ARG:N	6	2.24	0.73	2.04
(1,88)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	5	9.3	4.41	9.4
(1,53)	1:41:A:PHE:C	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	5	7.0	1.1	6.99
(1,195)	1:131:A:GLY:C	1:132:A:SER:N	1:132:A:SER:CA	1:132:A:SER:C	5	5.67	2.95	4.69
(1,9)	1:6:A:VAL:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	5	5.46	3.54	4.64
(1,115)	1:78:A:ASN:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	5	4.62	1.15	4.53
(1,111)	1:76:A:ILE:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	5	4.56	1.64	4.64
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:LYS:N	5	2.32	0.63	2.4
(1,181)	1:123:A:VAL:C	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	5	2.17	0.96	1.75
(1,183)	1:124:A:VAL:C	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	5	2.14	0.77	2.06
(1,89)	1:63:A:GLN:C	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:C	4	10.45	4.68	11.02
(1,36)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ILE:N	4	5.49	3.67	4.92
(1,103)	1:72:A:ASN:C	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	4	4.94	2.25	5.56
(1,84)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:GLN:N	4	4.42	1.38	4.83
(1,85)	1:61:A:TYR:C	1:62:A:GLN:N	1:62:A:GLN:CA	1:62:A:GLN:C	4	4.18	1.61	3.94
(1,97)	1:69:A:PRO:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	4	4.02	2.35	4.18
(1,104)	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	1:74:A:ILE:N	4	3.78	0.78	3.5
(1,178)	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1:123:A:VAL:N	4	3.72	0.96	3.45
(1,61)	1:49:A:LEU:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	4	3.43	2.08	2.9
(1,119)	1:80:A:LEU:C	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	4	3.15	1.44	3.48
(1,16)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:LYS:N	4	3.07	1.64	2.66
(1,127)	1:84:A:ARG:C	1:85:A:ASP:N	1:85:A:ASP:CA	1:85:A:ASP:C	4	2.42	1.67	1.7
(1,112)	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1:78:A:ASN:N	4	2.37	1.25	1.86
(1,199)	1:133:A:LEU:C	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	4	2.12	0.64	2.33
(1,54)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	4	1.7	0.45	1.63
(1,27)	1:15:A:LYS:C	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	3	7.36	1.52	8.07
(1,172)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:GLY:N	3	6.42	0.99	6.21
(1,60)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:THR:N	3	5.28	2.04	6.25

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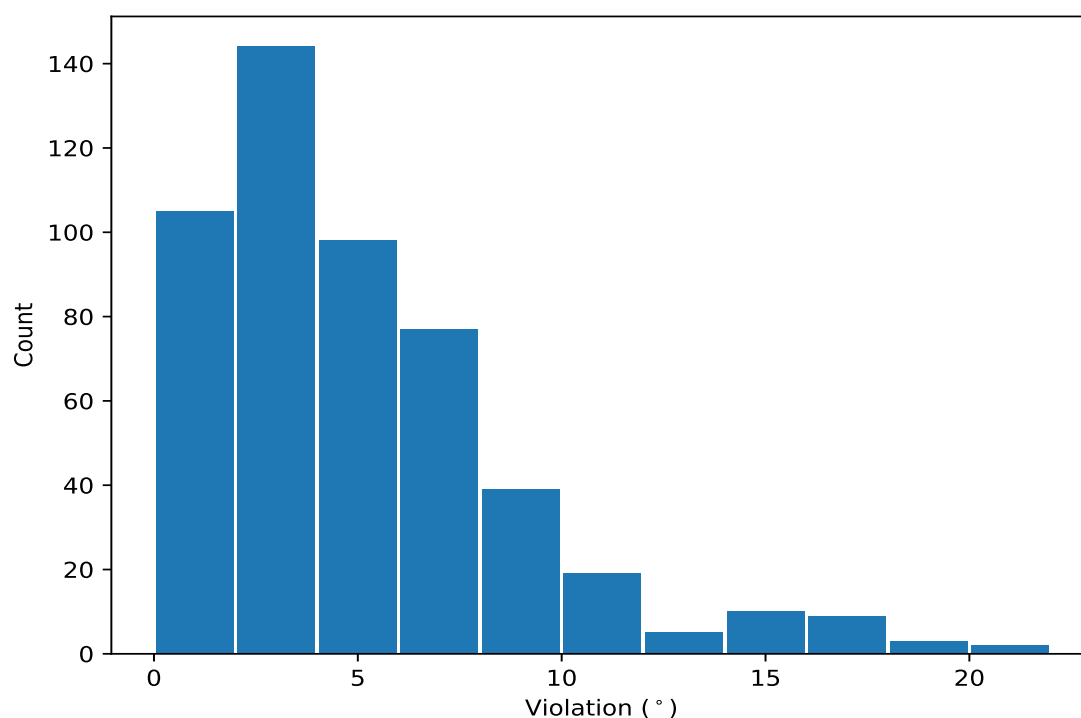
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,182)	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	1:125:A:ALA:N	3	4.21	2.46	4.53
(1,186)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:SER:N	3	4.09	1.87	5.37
(1,157)	1:101:A:ALA:C	1:102:A:SER:N	1:102:A:SER:CA	1:102:A:SER:C	3	4.0	0.83	3.75
(1,167)	1:107:A:LEU:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	3	3.14	0.61	3.19
(1,74)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:THR:N	3	3.01	0.28	3.14
(1,165)	1:106:A:THR:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	3	2.43	0.34	2.29
(1,125)	1:83:A:LEU:C	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	3	2.4	0.9	2.51
(1,81)	1:59:A:ALA:C	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	3	2.37	1.17	1.66
(1,78)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:ALA:N	3	2.3	1.02	1.64
(1,187)	1:126:A:LEU:C	1:127:A:SER:N	1:127:A:SER:CA	1:127:A:SER:C	3	2.29	0.33	2.35
(1,105)	1:73:A:VAL:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	3	1.84	0.95	1.28
(1,21)	1:12:A:THR:C	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	3	1.68	0.48	1.74
(1,59)	1:48:A:ILE:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	2	8.43	1.93	8.43
(1,118)	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1:81:A:GLU:N	2	7.89	1.41	7.89
(1,218)	1:143:A:SER:N	1:143:A:SER:CA	1:143:A:SER:C	1:144:A:PRO:N	2	2.95	1.0	2.95
(1,25)	1:14:A:ILE:C	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	2	2.7	0.1	2.7
(1,126)	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	1:85:A:ASP:N	2	2.66	0.22	2.66
(1,71)	1:54:A:MET:C	1:55:A:ASP:N	1:55:A:ASP:CA	1:55:A:ASP:C	2	2.19	0.42	2.19
(1,19)	1:11:A:LYS:C	1:12:A:THR:N	1:12:A:THR:CA	1:12:A:THR:C	2	2.15	0.06	2.15
(1,132)	1:87:A:LEU:N	1:87:A:LEU:CA	1:87:A:LEU:C	1:88:A:HIS:N	2	2.11	0.38	2.11
(1,11)	1:7:A:GLN:C	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	2	1.88	0.75	1.88
(1,17)	1:10:A:THR:C	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	2	1.84	0.34	1.84
(1,90)	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:C	1:65:A:LEU:N	2	1.78	0.46	1.78
(1,148)	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	1:96:A:CYS:N	2	1.64	0.36	1.64
(1,219)	1:145:A:GLY:C	1:146:A:CYS:N	1:146:A:CYS:CA	1:146:A:CYS:C	2	1.43	0.19	1.43
(1,87)	1:62:A:GLN:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	2	1.35	0.24	1.35
(1,82)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:TYR:N	2	1.32	0.03	1.32
(1,3)	1:3:A:ILE:C	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	2	1.06	0.03	1.06

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	1	21.74
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	3	21.63
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	10	19.92
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	3	18.97
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	4	18.69
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	4	17.65
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	5	16.87
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	1	16.73
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	3	16.43
(1,88)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	1	16.38
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	2	16.27
(1,89)	1:63:A:GLN:C	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:C	1	16.26
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	4	16.19
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	8	16.14
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	6	15.87
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	8	15.61
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	10	15.24
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	5	15.05
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	7	14.9
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	7	14.83
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	6	14.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	9	14.69
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	9	14.33
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	3	14.06
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	8	13.78
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	7	13.71
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	8	12.82
(1,89)	1:63:A:GLN:C	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:C	10	12.56
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	2	12.49
(1,9)	1:6:A:VAL:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	9	11.88
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	2	11.75
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	1	11.5
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	10	11.4
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	6	11.07
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	2	10.99
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	5	10.92
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	9	10.73
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	9	10.57
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	1	10.51
(1,36)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ILE:N	2	10.46
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	4	10.44
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	7	10.38
(1,59)	1:48:A:ILE:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	2	10.37
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	7	10.3
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	3	10.3
(1,88)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	10	10.27
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	10	10.25
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	4	10.21
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	5	9.94
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	7	9.91
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	6	9.86
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	10	9.84
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	8	9.8
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	7	9.65
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	6	9.63
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	4	9.61
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	6	9.56
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	5	9.53
(1,89)	1:63:A:GLN:C	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:C	5	9.49
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	7	9.46
(1,88)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	5	9.4
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	5	9.38
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	7	9.36
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	9	9.33
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	8	9.31
(1,118)	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1:81:A:GLU:N	2	9.3
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	5	9.18
(1,70)	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	1:55:A:ASP:N	6	9.15
(1,195)	1:131:A:GLY:C	1:132:A:SER:N	1:132:A:SER:CA	1:132:A:SER:C	8	9.0
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	8	8.93
(1,195)	1:131:A:GLY:C	1:132:A:SER:N	1:132:A:SER:CA	1:132:A:SER:C	5	8.87
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	1	8.81

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,27)	1:15:A:LYS:C	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	1	8.77
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	2	8.66
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	2	8.63
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	4	8.52
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	6	8.5
(1,53)	1:41:A:PHE:C	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	3	8.35
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	3	8.32
(1,116)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	5	8.3
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	8	8.28
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	3	8.23
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	3	8.18
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	7	8.11
(1,40)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:ASP:N	6	8.08
(1,27)	1:15:A:LYS:C	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	7	8.07
(1,42)	1:23:A:ASP:N	1:23:A:ASP:CA	1:23:A:ASP:C	1:24:A:ILE:N	3	8.0
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	6	7.98
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	10	7.95
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:ILE:N	8	7.94
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	8	7.89
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	3	7.8
(1,53)	1:41:A:PHE:C	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	9	7.76
(1,88)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	9	7.74
(1,172)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:GLY:N	3	7.72
(1,116)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	1	7.62
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	4	7.61
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	7	7.61
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:ILE:N	5	7.61
(1,179)	1:122:A:GLU:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	10	7.59
(1,12)	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:ASP:N	10	7.59
(1,36)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ILE:N	4	7.56
(1,96)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:MET:N	3	7.52
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	1	7.47
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	3	7.46
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	8	7.46
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	1	7.38
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	5	7.36
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	5	7.3
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	10	7.3
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	2	7.25
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:ILE:N	3	7.23
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	4	7.2
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	9	7.19
(1,60)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:THR:N	5	7.16
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	6	7.16
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	5	7.13
(1,103)	1:72:A:ASN:C	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	6	7.08
(1,182)	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	1:125:A:ALA:N	5	7.05
(1,53)	1:41:A:PHE:C	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	4	6.99
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	6	6.95
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	4	6.89
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	9	6.89

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	8	6.87
(1,103)	1:72:A:ASN:C	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	1	6.85
(1,53)	1:41:A:PHE:C	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	7	6.81
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	2	6.77
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	8	6.7
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	2	6.65
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	9	6.65
(1,85)	1:61:A:TYR:C	1:62:A:GLN:N	1:62:A:GLN:CA	1:62:A:GLN:C	5	6.62
(1,12)	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:ASP:N	4	6.61
(1,179)	1:122:A:GLU:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	5	6.6
(1,61)	1:49:A:LEU:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	5	6.59
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	10	6.58
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	6	6.58
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	6	6.57
(1,111)	1:76:A:ILE:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	8	6.54
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1	6.51
(1,59)	1:48:A:ILE:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	7	6.5
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	4	6.49
(1,118)	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1:81:A:GLU:N	10	6.48
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	7	6.45
(1,97)	1:69:A:PRO:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	1	6.43
(1,12)	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:ASP:N	6	6.41
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	1	6.38
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	8	6.34
(1,97)	1:69:A:PRO:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	9	6.29
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	8	6.28
(1,117)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	9	6.28
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	8	6.27
(1,96)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:MET:N	9	6.27
(1,60)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:THR:N	10	6.25
(1,172)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:GLY:N	10	6.21
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	6	6.2
(1,111)	1:76:A:ILE:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	7	6.19
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	5	6.18
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	3	6.15
(1,116)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	3	6.14
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	4	6.07
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	6	6.05
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	5	6.04
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	7	6.03
(1,115)	1:78:A:ASN:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	8	6.03
(1,70)	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	1:55:A:ASP:N	9	5.99
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	8	5.98
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	9	5.95
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	2	5.9
(1,84)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:GLN:N	7	5.87
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	10	5.85
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1	5.83
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	7	5.82
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	9	5.77
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	3	5.75

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:ILE:N	1	5.73
(1,115)	1:78:A:ASN:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	3	5.7
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	3	5.66
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	7	5.66
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	2	5.63
(1,16)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:LYS:N	10	5.63
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	6	5.6
(1,164)	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1:107:A:LEU:N	6	5.55
(1,66)	1:52:A:SER:N	1:52:A:SER:CA	1:52:A:SER:C	1:53:A:LYS:N	6	5.55
(1,70)	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	1:55:A:ASP:N	2	5.5
(1,9)	1:6:A:VAL:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	8	5.46
(1,186)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:SER:N	10	5.45
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	4	5.42
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	1	5.38
(1,186)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:SER:N	6	5.37
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	2	5.37
(1,70)	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	1:55:A:ASP:N	4	5.36
(1,172)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:GLY:N	1	5.33
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	1	5.33
(1,73)	1:55:A:ASP:C	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	10	5.31
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	3	5.3
(1,67)	1:52:A:SER:C	1:53:A:LYS:N	1:53:A:LYS:CA	1:53:A:LYS:C	4	5.28
(1,127)	1:84:A:ARG:C	1:85:A:ASP:N	1:85:A:ASP:CA	1:85:A:ASP:C	4	5.26
(1,96)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:MET:N	1	5.26
(1,27)	1:15:A:LYS:C	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	2	5.25
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	7	5.23
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	6	5.23
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	7	5.23
(1,178)	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1:123:A:VAL:N	9	5.22
(1,154)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:PRO:N	9	5.18
(1,79)	1:58:A:LEU:C	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	8	5.15
(1,157)	1:101:A:ALA:C	1:102:A:SER:N	1:102:A:SER:CA	1:102:A:SER:C	7	5.12
(1,53)	1:41:A:PHE:C	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1	5.11
(1,104)	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	1:74:A:ILE:N	1	5.08
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	5	5.05
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	9	5.04
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	1	5.03
(1,179)	1:122:A:GLU:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	4	5.01
(1,66)	1:52:A:SER:N	1:52:A:SER:CA	1:52:A:SER:C	1:53:A:LYS:N	5	5.0
(1,116)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	8	4.99
(1,26)	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	1:16:A:THR:N	7	4.97
(1,117)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	2	4.96
(1,116)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	2	4.95
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	1	4.93
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	9	4.89
(1,84)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:GLN:N	8	4.85
(1,84)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:GLN:N	4	4.81
(1,164)	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1:107:A:LEU:N	7	4.79
(1,70)	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	1:55:A:ASP:N	1	4.78
(1,12)	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:ASP:N	7	4.74
(1,121)	1:81:A:GLU:C	1:82:A:ASN:N	1:82:A:ASN:CA	1:82:A:ASN:C	10	4.71

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,195)	1:131:A:GLY:C	1:132:A:SER:N	1:132:A:SER:CA	1:132:A:SER:C	1	4.69
(1,111)	1:76:A:ILE:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	4	4.64
(1,9)	1:6:A:VAL:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	4	4.64
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	4	4.63
(1,195)	1:131:A:GLY:C	1:132:A:SER:N	1:132:A:SER:CA	1:132:A:SER:C	7	4.62
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	10	4.62
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	10	4.61
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	2	4.6
(1,119)	1:80:A:LEU:C	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	8	4.55
(1,12)	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:ASP:N	5	4.54
(1,182)	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	1:125:A:ALA:N	4	4.53
(1,115)	1:78:A:ASN:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	5	4.53
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	4	4.53
(1,112)	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1:78:A:ASN:N	10	4.49
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	2	4.45
(1,119)	1:80:A:LEU:C	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	5	4.43
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:ILE:N	9	4.4
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	2	4.39
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	7	4.37
(1,179)	1:122:A:GLU:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	9	4.35
(1,121)	1:81:A:GLU:C	1:82:A:ASN:N	1:82:A:ASN:CA	1:82:A:ASN:C	2	4.35
(1,85)	1:61:A:TYR:C	1:62:A:GLN:N	1:62:A:GLN:CA	1:62:A:GLN:C	1	4.33
(1,75)	1:56:A:GLN:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1	4.32
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	3	4.31
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	9	4.28
(1,103)	1:72:A:ASN:C	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	10	4.27
(1,75)	1:56:A:GLN:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	5	4.27
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	4	4.27
(1,152)	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	1:98:A:LEU:N	2	4.26
(1,9)	1:6:A:VAL:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	3	4.25
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	1	4.23
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	10	4.23
(1,12)	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:ASP:N	9	4.16
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	9	4.05
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	4	4.04
(1,81)	1:59:A:ALA:C	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	6	4.02
(1,154)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:PRO:N	7	4.0
(1,61)	1:49:A:LEU:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	10	3.98
(1,115)	1:78:A:ASN:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	9	3.96
(1,218)	1:143:A:SER:N	1:143:A:SER:CA	1:143:A:SER:C	1:144:A:PRO:N	10	3.95
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:ILE:N	2	3.94
(1,133)	1:87:A:LEU:C	1:88:A:HIS:N	1:88:A:HIS:CA	1:88:A:HIS:C	4	3.89
(1,117)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	4	3.89
(1,178)	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1:123:A:VAL:N	5	3.88
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	9	3.85
(1,167)	1:107:A:LEU:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1	3.85
(1,128)	1:85:A:ASP:N	1:85:A:ASP:CA	1:85:A:ASP:C	1:86:A:LEU:N	4	3.85
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	9	3.84
(1,117)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	10	3.82
(1,79)	1:58:A:LEU:C	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	4	3.77
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	8	3.76

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	9	3.75
(1,179)	1:122:A:GLU:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	6	3.75
(1,157)	1:101:A:ALA:C	1:102:A:SER:N	1:102:A:SER:CA	1:102:A:SER:C	3	3.75
(1,75)	1:56:A:GLN:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	9	3.75
(1,78)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:ALA:N	2	3.74
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	2	3.73
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	7	3.73
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	2	3.72
(1,154)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:PRO:N	10	3.67
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	9	3.64
(1,41)	1:22:A:ASN:C	1:23:A:ASP:N	1:23:A:ASP:CA	1:23:A:ASP:C	6	3.64
(1,181)	1:123:A:VAL:C	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	5	3.61
(1,212)	1:140:A:LEU:N	1:140:A:LEU:CA	1:140:A:LEU:C	1:141:A:ASP:N	10	3.6
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	5	3.58
(1,70)	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	1:55:A:ASP:N	7	3.57
(1,104)	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	1:74:A:ILE:N	10	3.56
(1,85)	1:61:A:TYR:C	1:62:A:GLN:N	1:62:A:GLN:CA	1:62:A:GLN:C	10	3.56
(1,154)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:PRO:N	1	3.5
(1,89)	1:63:A:GLN:C	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:C	9	3.48
(1,196)	1:132:A:SER:N	1:132:A:SER:CA	1:132:A:SER:C	1:133:A:LEU:N	7	3.45
(1,164)	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1:107:A:LEU:N	1	3.45
(1,125)	1:83:A:LEU:C	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	4	3.45
(1,104)	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	1:74:A:ILE:N	2	3.44
(1,34)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:ARG:N	3	3.44
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:LYS:N	10	3.42
(1,183)	1:124:A:VAL:C	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	3	3.36
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	6	3.36
(1,16)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:LYS:N	9	3.34
(1,76)	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1:58:A:LEU:N	8	3.33
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	7	3.31
(1,79)	1:58:A:LEU:C	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	7	3.31
(1,142)	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	1:93:A:SER:N	6	3.29
(1,74)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:THR:N	2	3.28
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:ILE:N	6	3.28
(1,40)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:ASP:N	8	3.27
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	3	3.26
(1,179)	1:122:A:GLU:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1	3.25
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	8	3.25
(1,75)	1:56:A:GLN:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	3	3.23
(1,167)	1:107:A:LEU:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	10	3.19
(1,86)	1:62:A:GLN:N	1:62:A:GLN:CA	1:62:A:GLN:C	1:63:A:GLN:N	8	3.19
(1,105)	1:73:A:VAL:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	3	3.17
(1,74)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:THR:N	9	3.14
(1,157)	1:101:A:ALA:C	1:102:A:SER:N	1:102:A:SER:CA	1:102:A:SER:C	5	3.12
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	9	3.09
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	8	3.04
(1,117)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	6	3.04
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	2	3.03
(1,178)	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1:123:A:VAL:N	10	3.02
(1,104)	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	1:74:A:ILE:N	9	3.02
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	4	3.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,181)	1:123:A:VAL:C	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	9	3.0
(1,34)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:ARG:N	10	2.97
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	6	2.93
(1,165)	1:106:A:THR:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	8	2.9
(1,111)	1:76:A:ILE:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1	2.89
(1,126)	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	1:85:A:ASP:N	5	2.87
(1,115)	1:78:A:ASN:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	2	2.87
(1,79)	1:58:A:LEU:C	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	10	2.84
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	3	2.83
(1,79)	1:58:A:LEU:C	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	6	2.82
(1,75)	1:56:A:GLN:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	6	2.8
(1,25)	1:14:A:ILE:C	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	5	2.8
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	1	2.78
(1,178)	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1:123:A:VAL:N	1	2.77
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	1	2.75
(1,37)	1:20:A:ARG:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	2	2.73
(1,199)	1:133:A:LEU:C	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	6	2.7
(1,88)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	6	2.69
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	7	2.67
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	3	2.66
(1,187)	1:126:A:LEU:C	1:127:A:SER:N	1:127:A:SER:CA	1:127:A:SER:C	2	2.65
(1,199)	1:133:A:LEU:C	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	2	2.64
(1,11)	1:7:A:GLN:C	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	10	2.63
(1,74)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:THR:N	8	2.62
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	10	2.62
(1,71)	1:54:A:MET:C	1:55:A:ASP:N	1:55:A:ASP:CA	1:55:A:ASP:C	9	2.61
(1,66)	1:52:A:SER:N	1:52:A:SER:CA	1:52:A:SER:C	1:53:A:LYS:N	3	2.61
(1,25)	1:14:A:ILE:C	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	9	2.59
(1,154)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:PRO:N	2	2.58
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	3	2.56
(1,183)	1:124:A:VAL:C	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	6	2.56
(1,111)	1:76:A:ILE:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	5	2.55
(1,119)	1:80:A:LEU:C	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	1	2.54
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	8	2.53
(1,116)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	6	2.52
(1,125)	1:83:A:LEU:C	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	8	2.51
(1,40)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:ASP:N	4	2.5
(1,132)	1:87:A:LEU:N	1:87:A:LEU:CA	1:87:A:LEU:C	1:88:A:HIS:N	10	2.49
(1,126)	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	1:85:A:ASP:N	8	2.44
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	5	2.44
(1,60)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:THR:N	7	2.44
(1,179)	1:122:A:GLU:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	7	2.42
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:LYS:N	6	2.4
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:LYS:N	9	2.4
(1,54)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	4	2.39
(1,167)	1:107:A:LEU:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	3	2.37
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	10	2.37
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	10	2.36
(1,187)	1:126:A:LEU:C	1:127:A:SER:N	1:127:A:SER:CA	1:127:A:SER:C	1	2.35
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	7	2.32
(1,72)	1:55:A:ASP:N	1:55:A:ASP:CA	1:55:A:ASP:C	1:56:A:GLN:N	4	2.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,66)	1:52:A:SER:N	1:52:A:SER:CA	1:52:A:SER:C	1:53:A:LYS:N	8	2.3
(1,165)	1:106:A:THR:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	5	2.29
(1,121)	1:81:A:GLU:C	1:82:A:ASN:N	1:82:A:ASN:CA	1:82:A:ASN:C	7	2.29
(1,36)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ILE:N	6	2.27
(1,117)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	7	2.26
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	2	2.25
(1,117)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	3	2.24
(1,90)	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:C	1:65:A:LEU:N	4	2.24
(1,21)	1:12:A:THR:C	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	5	2.24
(1,19)	1:11:A:LYS:C	1:12:A:THR:N	1:12:A:THR:CA	1:12:A:THR:C	10	2.21
(1,85)	1:61:A:TYR:C	1:62:A:GLN:N	1:62:A:GLN:CA	1:62:A:GLN:C	7	2.19
(1,17)	1:10:A:THR:C	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	7	2.17
(1,83)	1:60:A:VAL:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	5	2.16
(1,84)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:GLN:N	2	2.14
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	5	2.12
(1,165)	1:106:A:THR:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	3	2.11
(1,164)	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1:107:A:LEU:N	10	2.1
(1,79)	1:58:A:LEU:C	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	1	2.1
(1,19)	1:11:A:LYS:C	1:12:A:THR:N	1:12:A:THR:CA	1:12:A:THR:C	6	2.09
(1,207)	1:137:A:LEU:C	1:138:A:TRP:N	1:138:A:TRP:CA	1:138:A:TRP:C	5	2.08
(1,97)	1:69:A:PRO:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	2	2.07
(1,183)	1:124:A:VAL:C	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	7	2.06
(1,34)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:ARG:N	9	2.06
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	4	2.03
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	9	2.03
(1,199)	1:133:A:LEU:C	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	5	2.01
(1,154)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:PRO:N	3	2.01
(1,34)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:ARG:N	7	2.01
(1,148)	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	1:96:A:CYS:N	7	1.99
(1,164)	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1:107:A:LEU:N	3	1.98
(1,16)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:LYS:N	4	1.97
(1,218)	1:143:A:SER:N	1:143:A:SER:CA	1:143:A:SER:C	1:144:A:PRO:N	7	1.95
(1,66)	1:52:A:SER:N	1:52:A:SER:CA	1:52:A:SER:C	1:53:A:LYS:N	10	1.93
(1,15)	1:9:A:ASP:C	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	6	1.93
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	5	1.91
(1,112)	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1:78:A:ASN:N	6	1.88
(1,40)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:ASP:N	3	1.88
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	2	1.87
(1,187)	1:126:A:LEU:C	1:127:A:SER:N	1:127:A:SER:CA	1:127:A:SER:C	8	1.86
(1,127)	1:84:A:ARG:C	1:85:A:ASP:N	1:85:A:ASP:CA	1:85:A:ASP:C	7	1.86
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	10	1.85
(1,164)	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1:107:A:LEU:N	4	1.85
(1,112)	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1:78:A:ASN:N	9	1.85
(1,96)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:MET:N	7	1.85
(1,96)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:MET:N	4	1.82
(1,61)	1:49:A:LEU:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	8	1.81
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	10	1.78
(1,71)	1:54:A:MET:C	1:55:A:ASP:N	1:55:A:ASP:CA	1:55:A:ASP:C	5	1.77
(1,54)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	7	1.77
(1,181)	1:123:A:VAL:C	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	2	1.75
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:LYS:N	7	1.75

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,21)	1:12:A:THR:C	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	6	1.74
(1,132)	1:87:A:LEU:N	1:87:A:LEU:CA	1:87:A:LEU:C	1:88:A:HIS:N	4	1.73
(1,20)	1:12:A:THR:N	1:12:A:THR:CA	1:12:A:THR:C	1:13:A:LEU:N	10	1.73
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	1	1.72
(1,58)	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	1:49:A:LEU:N	7	1.71
(1,36)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ILE:N	7	1.68
(1,123)	1:82:A:ASN:C	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	5	1.67
(1,121)	1:81:A:GLU:C	1:82:A:ASN:N	1:82:A:ASN:CA	1:82:A:ASN:C	3	1.67
(1,116)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	7	1.67
(1,81)	1:59:A:ALA:C	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1	1.66
(1,78)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:ALA:N	9	1.64
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:LYS:N	4	1.64
(1,219)	1:145:A:GLY:C	1:146:A:CYS:N	1:146:A:CYS:CA	1:146:A:CYS:C	7	1.62
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	8	1.61
(1,79)	1:58:A:LEU:C	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	5	1.61
(1,66)	1:52:A:SER:N	1:52:A:SER:CA	1:52:A:SER:C	1:53:A:LYS:N	1	1.6
(1,96)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:MET:N	8	1.59
(1,34)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:ARG:N	8	1.59
(1,87)	1:62:A:GLN:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1	1.58
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	6	1.56
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	10	1.55
(1,127)	1:84:A:ARG:C	1:85:A:ASP:N	1:85:A:ASP:CA	1:85:A:ASP:C	5	1.55
(1,121)	1:81:A:GLU:C	1:82:A:ASN:N	1:82:A:ASN:CA	1:82:A:ASN:C	1	1.55
(1,103)	1:72:A:ASN:C	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	2	1.55
(1,183)	1:124:A:VAL:C	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	9	1.54
(1,78)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:ALA:N	3	1.53
(1,17)	1:10:A:THR:C	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	8	1.5
(1,54)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	3	1.49
(1,164)	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1:107:A:LEU:N	2	1.45
(1,186)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:SER:N	4	1.44
(1,81)	1:59:A:ALA:C	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	10	1.44
(1,75)	1:56:A:GLN:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	10	1.43
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	1	1.42
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	5	1.42
(1,34)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:ARG:N	6	1.4
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	3	1.39
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	3	1.36
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	1	1.35
(1,82)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:TYR:N	1	1.35
(1,61)	1:49:A:LEU:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	2	1.35
(1,16)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:LYS:N	7	1.35
(1,5)	1:4:A:GLN:C	1:5:A:LYS:N	1:5:A:LYS:CA	1:5:A:LYS:C	9	1.35
(1,90)	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:C	1:65:A:LEU:N	8	1.32
(1,97)	1:69:A:PRO:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	3	1.3
(1,82)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:TYR:N	10	1.29
(1,12)	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:ASP:N	1	1.29
(1,181)	1:123:A:VAL:C	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	4	1.28
(1,148)	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	1:96:A:CYS:N	1	1.28
(1,105)	1:73:A:VAL:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	7	1.28
(1,40)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:ASP:N	10	1.27
(1,125)	1:83:A:LEU:C	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	9	1.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,219)	1:145:A:GLY:C	1:146:A:CYS:N	1:146:A:CYS:CA	1:146:A:CYS:C	1	1.24
(1,112)	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1:78:A:ASN:N	2	1.24
(1,181)	1:123:A:VAL:C	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	7	1.22
(1,50)	1:27:A:THR:N	1:27:A:THR:CA	1:27:A:THR:C	1:28:A:GLN:N	7	1.21
(1,195)	1:131:A:GLY:C	1:132:A:SER:N	1:132:A:SER:CA	1:132:A:SER:C	4	1.17
(1,183)	1:124:A:VAL:C	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	10	1.16
(1,54)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	1	1.16
(1,29)	1:16:A:THR:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	7	1.16
(1,40)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:ASP:N	9	1.14
(1,11)	1:7:A:GLN:C	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	9	1.14
(1,199)	1:133:A:LEU:C	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	1	1.12
(1,204)	1:136:A:MET:N	1:136:A:MET:CA	1:136:A:MET:C	1:137:A:LEU:N	9	1.11
(1,87)	1:62:A:GLN:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	3	1.11
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	4	1.11
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	5	1.1
(1,28)	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	1:17:A:ILE:N	7	1.09
(1,3)	1:3:A:ILE:C	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	10	1.09
(1,176)	1:121:A:THR:N	1:121:A:THR:CA	1:121:A:THR:C	1:122:A:GLU:N	10	1.08
(1,10)	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	1:8:A:ASP:N	7	1.08
(1,9)	1:6:A:VAL:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	6	1.08
(1,119)	1:80:A:LEU:C	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	4	1.07
(1,197)	1:132:A:SER:C	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	7	1.06
(1,185)	1:125:A:ALA:C	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	10	1.06
(1,154)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:PRO:N	8	1.06
(1,105)	1:73:A:VAL:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	6	1.06
(1,21)	1:12:A:THR:C	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1	1.06
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	5	1.05
(1,121)	1:81:A:GLU:C	1:82:A:ASN:N	1:82:A:ASN:CA	1:82:A:ASN:C	6	1.05
(1,182)	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	1:125:A:ALA:N	2	1.04
(1,3)	1:3:A:ILE:C	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	3	1.03
(1,127)	1:84:A:ARG:C	1:85:A:ASP:N	1:85:A:ASP:CA	1:85:A:ASP:C	1	1.02