Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 03:03 AM EDT

PDB ID	:	2LGB
BMRB ID	:	17803
Title	:	Modified A22Gly-B31Arg Human Insulin
Authors	:	Bocian, W.; Kozerski, L.
Deposited on	:	2011-07-25

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

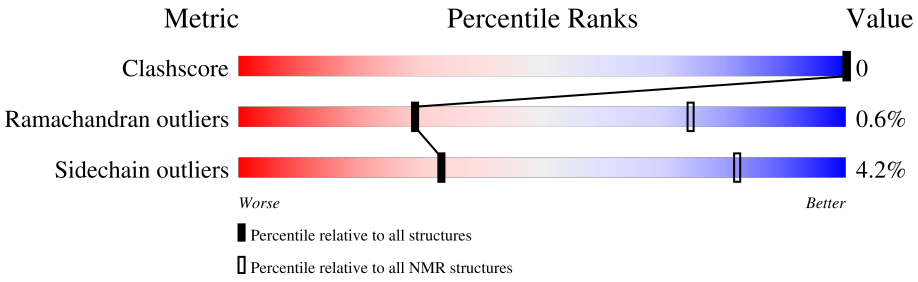
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 75%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	22	86% 14%
2	B	31	48% 52%

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 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:20, B:105-B:119 (34)	0.56	4

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

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

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 817 atoms, of which 397 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Insulin A chain.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	22	319	101	152	26	36	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	insertion	UNP P01308

- Molecule 2 is a protein called Insulin B chain.

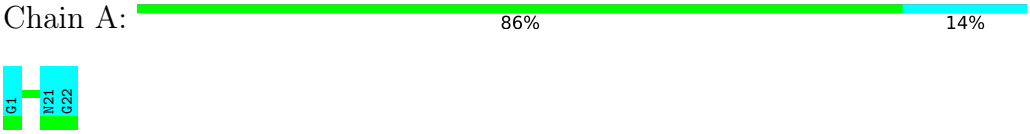
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	31	498	164	245	44	43	2	0

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: Insulin A chain



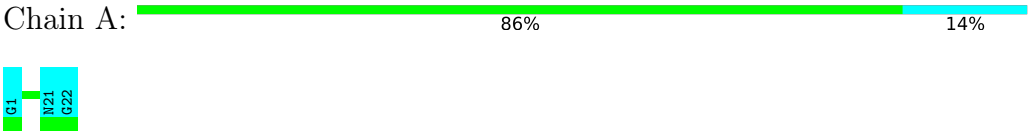
• Molecule 2: Insulin B chain

4.2 Scores per residue for each member of the ensemble

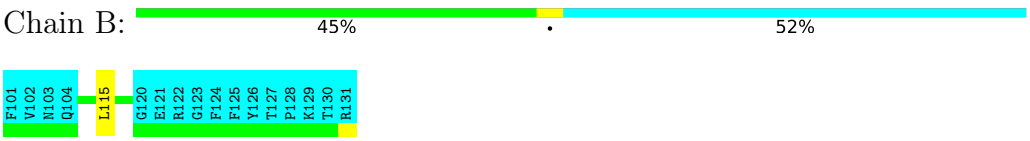
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Insulin A chain



• Molecule 2: Insulin B chain



4.2.2 Score per residue for model 2

• Molecule 1: Insulin A chain

Chain A:

• Molecule 2: Insulin B chain

Chain B:

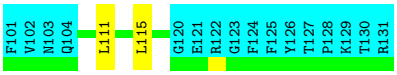
4.2.3 Score per residue for model 3

• Molecule 1: Insulin A chain

Chain A:

• Molecule 2: Insulin B chain

Chain B:



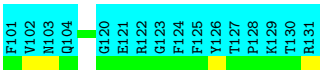
4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Insulin A chain

Chain A:

• Molecule 2: Insulin B chain

Chain B:



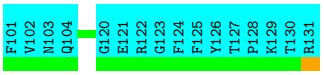
4.2.5 Score per residue for model 5

• Molecule 1: Insulin A chain

Chain A:

• Molecule 2: Insulin B chain

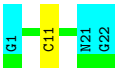
Chain B:



4.2.6 Score per residue for model 6

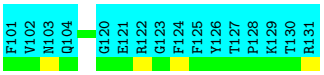
• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

Chain B:



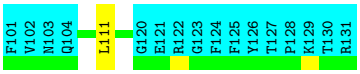
4.2.7 Score per residue for model 7

• Molecule 1: Insulin A chain

Chain A:

• Molecule 2: Insulin B chain

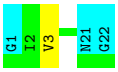
Chain B:



4.2.8 Score per residue for model 8

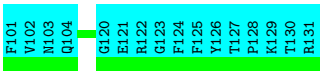
• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

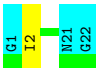
Chain B:



4.2.9 Score per residue for model 9

• Molecule 1: Insulin A chain

Chain A:



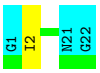
• Molecule 2: Insulin B chain

Chain B:

4.2.10 Score per residue for model 10

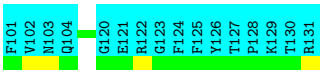
• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

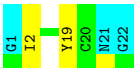
Chain B:



4.2.11 Score per residue for model 11

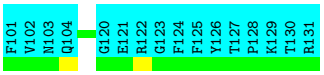
• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

Chain B:



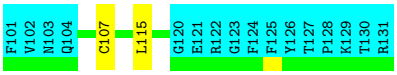
4.2.12 Score per residue for model 12

• Molecule 1: Insulin A chain

Chain A:

• Molecule 2: Insulin B chain

Chain B:



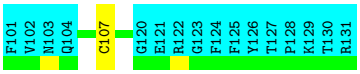
4.2.13 Score per residue for model 13

• Molecule 1: Insulin A chain

Chain A:

• Molecule 2: Insulin B chain

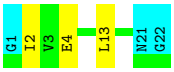
Chain B:



4.2.14 Score per residue for model 14

• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

Chain B:

4.2.15 Score per residue for model 15

• Molecule 1: Insulin A chain

Chain A:

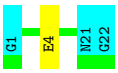
• Molecule 2: Insulin B chain

Chain B:

4.2.16 Score per residue for model 16

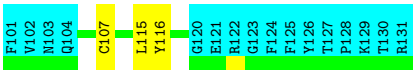
• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

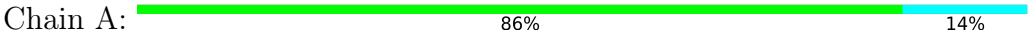
Chain B:



4.2.17 Score per residue for model 17

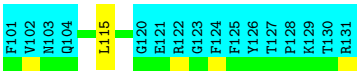
• Molecule 1: Insulin A chain

Chain A:



• Molecule 2: Insulin B chain

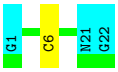
Chain B:



4.2.18 Score per residue for model 18

• Molecule 1: Insulin A chain

Chain A:



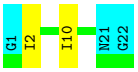
• Molecule 2: Insulin B chain

Chain B:

4.2.19 Score per residue for model 19

• Molecule 1: Insulin A chain

Chain A:



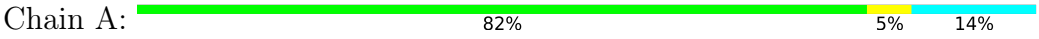
• Molecule 2: Insulin B chain

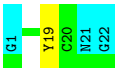
Chain B:

4.2.20 Score per residue for model 20

• Molecule 1: Insulin A chain

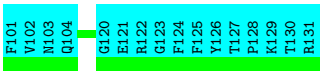
Chain A:





• Molecule 2: Insulin B chain

Chain B:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy and with the least restraint violations*.

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

Software name	Classification	Version
Amber	refinement	9
Amber	geometry optimization	9

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	509
Number of shifts mapped to atoms	509
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%

6 Model quality

6.1 Standard geometry

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	0.71±0.01	0±0/152 (0.0± 0.0%)	0.88±0.04	0±0/207 (0.0± 0.1%)
2	B	0.65±0.01	0±0/117 (0.0± 0.0%)	0.87±0.03	0±0/160 (0.0± 0.0%)
All	All	0.69	0/5380 (0.0%)	0.88	2/7340 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	19	TYR	CB-CG-CD2	-5.56	117.66	121.00	20	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	5280	5000	5000	-

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 -.

There are no clashes.

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	19/22 (86%)	18±1 (96±5%)	1±1 (3±4%)	0±0 (1±2%)	18 66
2	B	15/31 (48%)	15±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100 100
All	All	680/1060 (64%)	665 (98%)	11 (2%)	4 (1%)	29 74

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	2	ILE	4

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	19/20 (95%)	18±1 (97±4%)	0±1 (3±4%)	49 91
2	B	13/27 (48%)	12±1 (93±9%)	1±1 (7±9%)	21 69
All	All	640/940 (68%)	613 (96%)	27 (4%)	33 82

All 13 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)
2	B	115	LEU	7
2	B	107	CYS	4
1	A	4	GLU	3
1	A	13	LEU	2
2	B	116	TYR	2
2	B	111	LEU	2
2	B	118	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	11	CYS	1
1	A	3	VAL	1
1	A	2	ILE	1
2	B	105	HIS	1
1	A	6	CYS	1
1	A	10	ILE	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 monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 75% for the well-defined parts and 72% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_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	509
Number of shifts mapped to atoms	509
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	51	0.47 ± 0.20	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	43	0.26 ± 0.21	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	0	—	None (insufficient data)

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 75%, i.e. 336 atoms were assigned a chemical shift out of a possible 446. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	101/171 (59%)	69/69 (100%)	32/68 (47%)	0/34 (0%)
Sidechain	219/234 (94%)	155/156 (99%)	64/75 (85%)	0/3 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	16/41 (39%)	16/20 (80%)	0/19 (0%)	0/2 (0%)
Overall	336/446 (75%)	240/245 (98%)	96/162 (59%)	0/39 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 509 atoms were assigned a chemical shift out of a possible 705. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	159/268 (59%)	108/110 (98%)	51/106 (48%)	0/52 (0%)
Sidechain	316/357 (89%)	222/233 (95%)	94/111 (85%)	0/13 (0%)
Aromatic	34/80 (42%)	34/39 (87%)	0/39 (0%)	0/2 (0%)
Overall	509/705 (72%)	364/382 (95%)	145/256 (57%)	0/67 (0%)

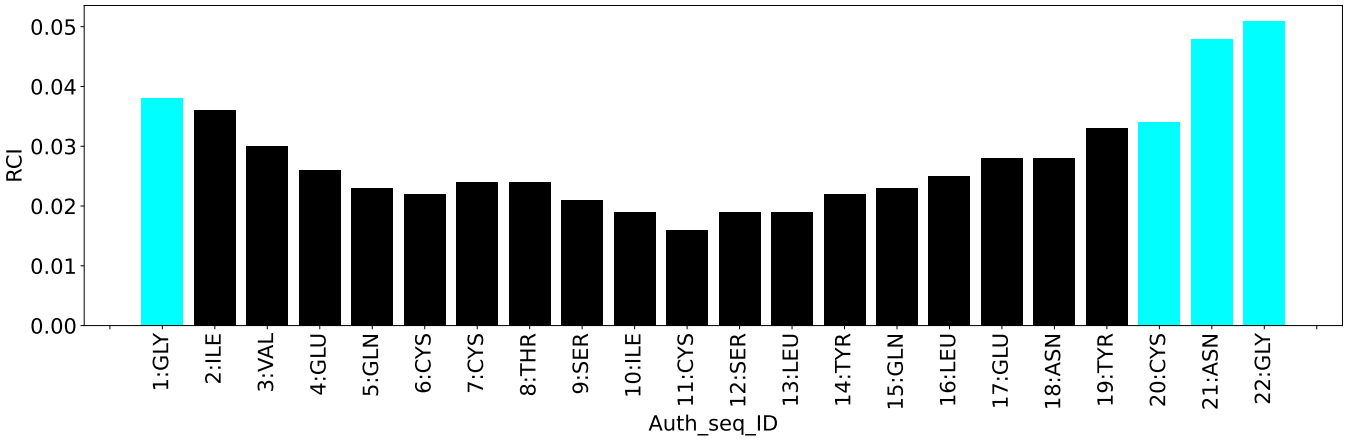
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

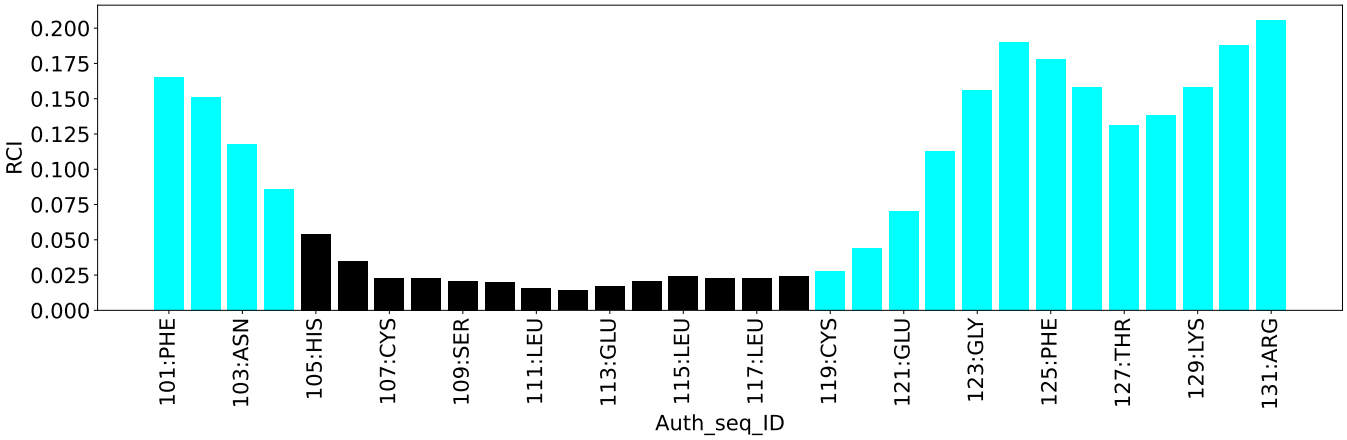
7.1.5 Random Coil Index (RCI) plots (i)

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



Random coil index (RCI) for chain B:


RCI
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
101:PHE
103:ASN
105:HIS
107:CYS
109:SER
111:LEU
113:GLU
115:LEU
117:LEU
119:CYS
121:GLU
123:GLY
125:PHE
127:THR
129:LYS
131:ARG
Auth_seq_ID

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	578
Intra-residue (|i-j|=0)	210
Sequential (|i-j|=1)	208
Medium range (|i-j|>1 and |i-j|<5)	88
Long range (|i-j|≥5)	22
Inter-chain	50
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	135
Number of unmapped restraints	0
Number of restraints per residue	13.5
Number of long range restraints per residue[1]	0.4

[1]Long 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)	0.2	0.2
0.2-0.5 (Medium)	0.6	0.37
>0.5 (Large)	None	None

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)	5.2	10.0
10.0-20.0 (Medium)	4.2	20.0
>20.0 (Large)	42.6	81.6

9 Distance violation analysis (i)

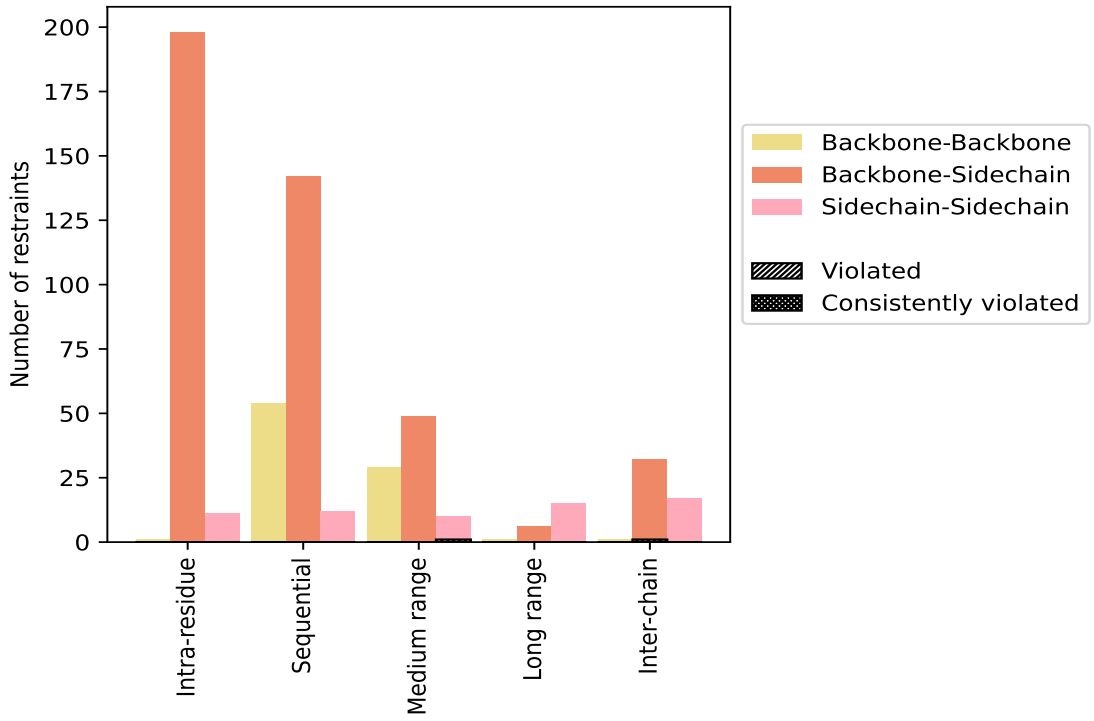
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	210	36.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	1	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	198	34.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	11	1.9	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	208	36.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	54	9.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	142	24.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	12	2.1	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	88	15.2	1	1.1	0.2	0	0.0	0.0
Backbone-Backbone	29	5.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	49	8.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	10	1.7	1	10.0	0.2	0	0.0	0.0
Long range (|i-j|≥5)	22	3.8	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	1	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	6	1.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	15	2.6	0	0.0	0.0	0	0.0	0.0
Inter-chain	50	8.7	1	2.0	0.2	0	0.0	0.0
Backbone-Backbone	1	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	32	5.5	1	3.1	0.2	0	0.0	0.0
Sidechain-Sidechain	17	2.9	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	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	578	100.0	2	0.3	0.3	0	0.0	0.0
Backbone-Backbone	86	14.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	427	73.9	1	0.2	0.2	0	0.0	0.0
Sidechain-Sidechain	65	11.2	1	1.5	0.2	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	1	1	0.29	0.29	0.0	0.29
3	0	0	0	0	1	1	0.2	0.2	0.0	0.2
4	0	0	0	0	1	1	0.18	0.18	0.0	0.18
5	0	0	0	0	1	1	0.33	0.33	0.0	0.33
6	0	0	0	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0	1	1	0.17	0.17	0.0	0.17
8	0	0	0	0	1	1	0.28	0.28	0.0	0.28
9	0	0	0	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0	1	1	0.31	0.31	0.0	0.31
11	0	0	0	0	1	1	0.33	0.33	0.0	0.33

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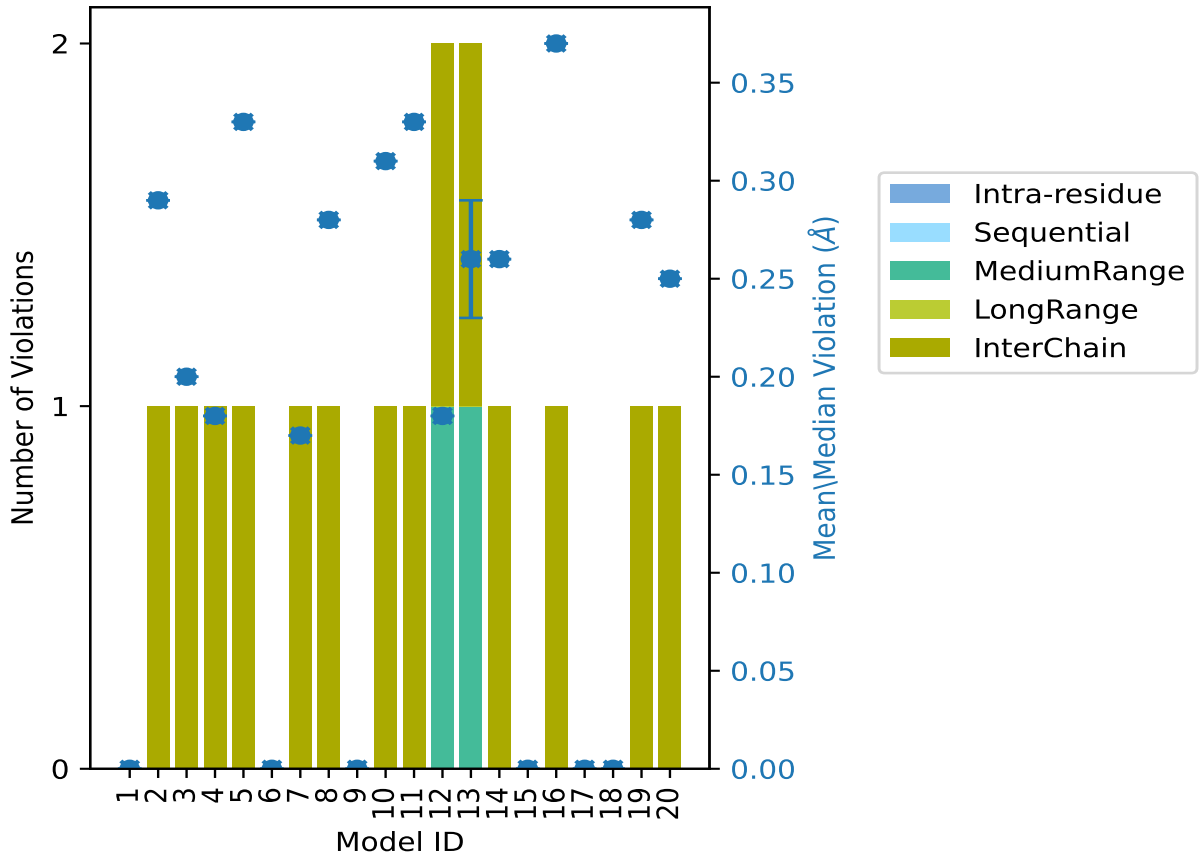
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	1	0	1	2	0.18	0.18	0.0	0.18
13	0	0	1	0	1	2	0.26	0.29	0.03	0.26
14	0	0	0	0	1	1	0.26	0.26	0.0	0.26
15	0	0	0	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0	1	1	0.37	0.37	0.0	0.37
17	0	0	0	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0	1	1	0.28	0.28	0.0	0.28
20	0	0	0	0	1	1	0.25	0.25	0.0	0.25

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

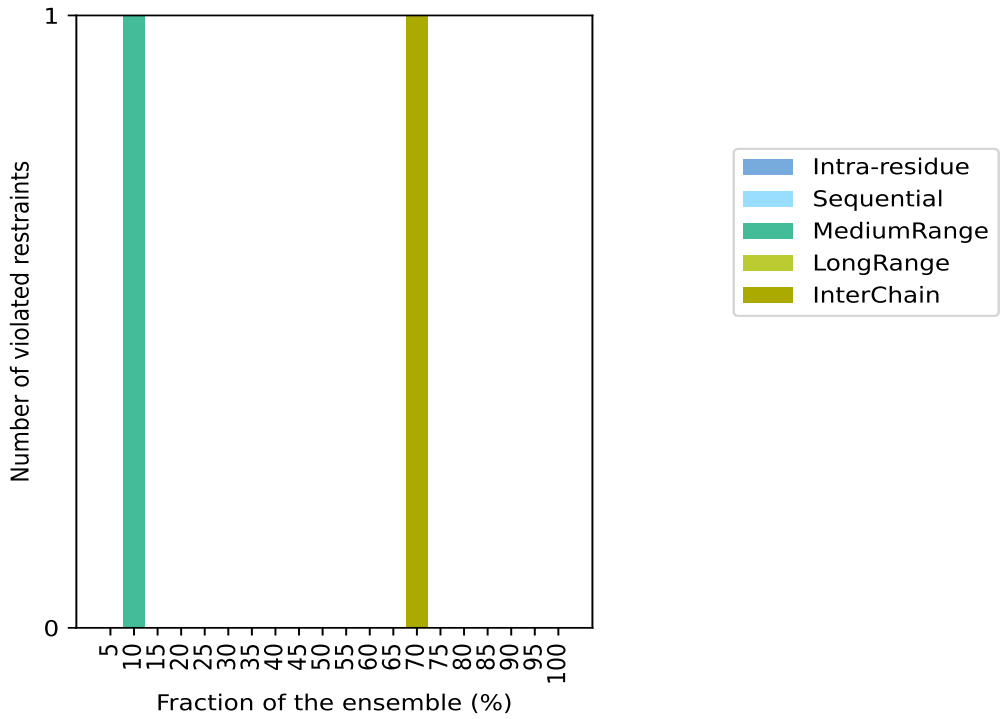
9.3 Distance violation statistics for the ensemble (i)

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, 576(IR:210, SQ:208, MR:87, LR:22, IC:49) 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]	%
0	0	0	0	0	0	1	5.0
0	0	1	0	0	1	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	1	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

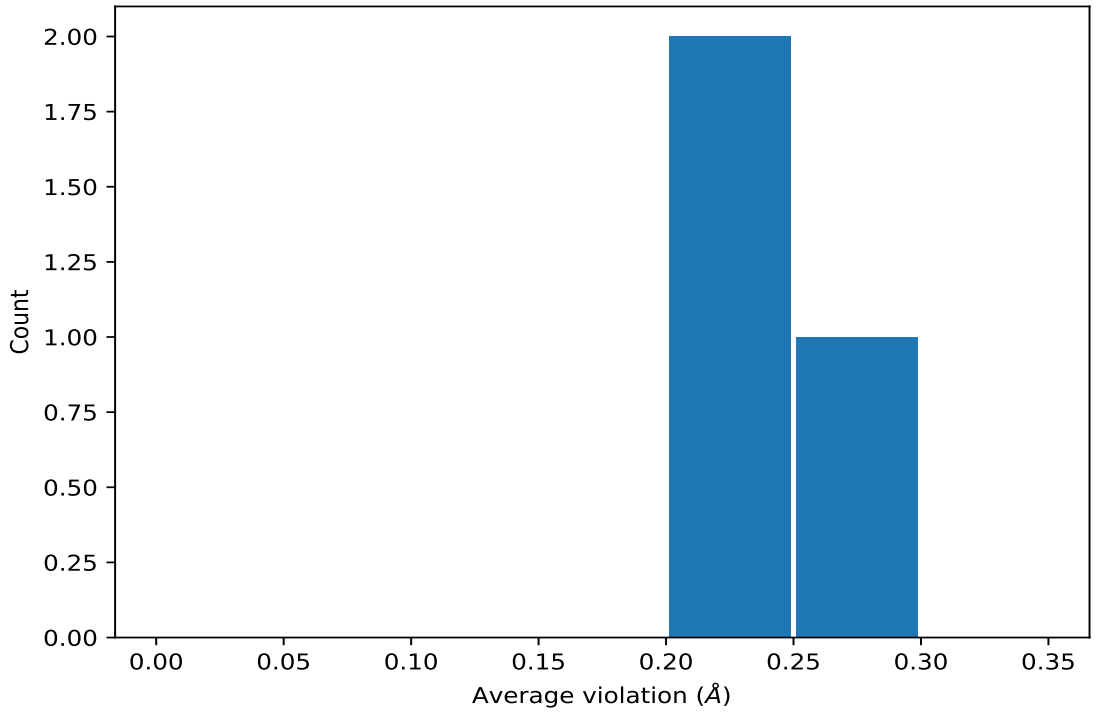
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of the 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.

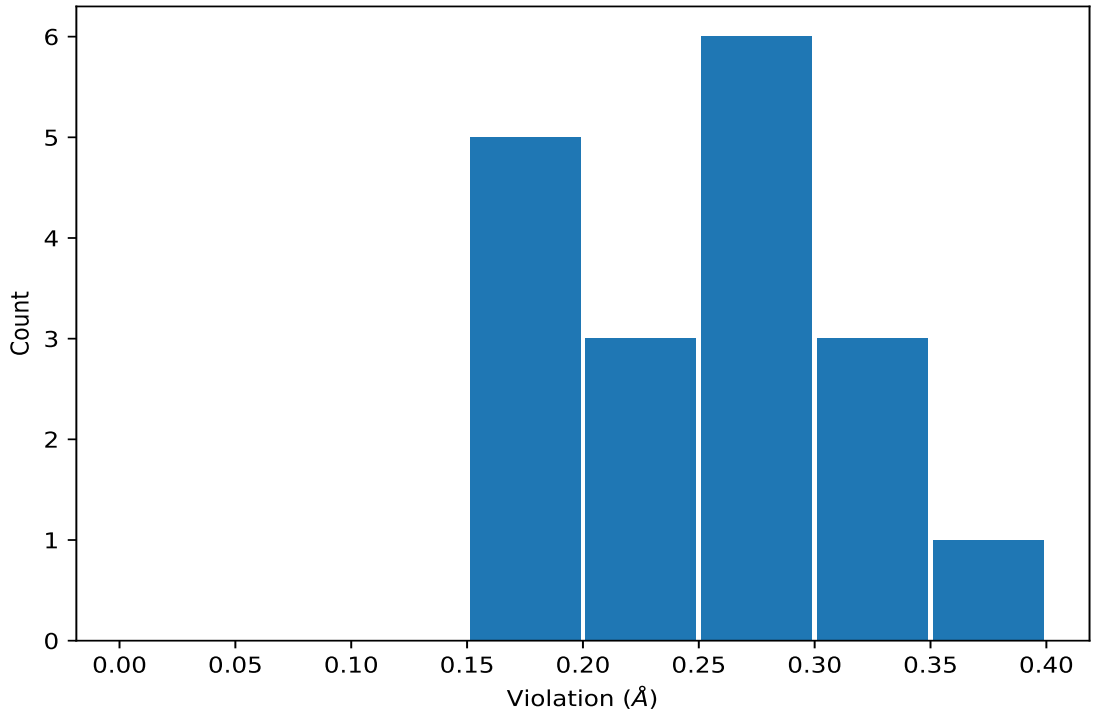
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,96)	1:A:7:CYS:HB3	2:B:108:GLY:H	14	0.26	0.06	0.28
(1,399)	1:A:4:GLU:HB2	1:A:7:CYS:HB2	2	0.2	0.02	0.2
(1,399)	1:A:4:GLU:HB3	1:A:7:CYS:HB2	2	0.2	0.02	0.2

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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



9.5.2 Table : All distance violations (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)
(1,96)	1:A:7:CYS:HB3	2:B:108:GLY:H	16	0.37
(1,96)	1:A:7:CYS:HB3	2:B:108:GLY:H	5	0.33
(1,96)	1:A:7:CYS:HB3	2:B:108:GLY:H	11	0.33
(1,96)	1:A:7:CYS:HB3	2:B:108:GLY:H	10	0.31
(1,96)	1:A:7:CYS:HB3	2:B:108:GLY:H	2	0.29
(1,96)	1:A:7:CYS:HB3	2:B:108:GLY:H	13	0.29
(1,96)	1:A:7:CYS:HB3	2:B:108:GLY:H	8	0.28
(1,96)	1:A:7:CYS:HB3	2:B:108:GLY:H	19	0.28
(1,96)	1:A:7:CYS:HB3	2:B:108:GLY:H	14	0.26
(1,96)	1:A:7:CYS:HB3	2:B:108:GLY:H	20	0.25
(1,399)	1:A:4:GLU:HB2	1:A:7:CYS:HB2	13	0.22
(1,399)	1:A:4:GLU:HB3	1:A:7:CYS:HB2	13	0.22
(1,96)	1:A:7:CYS:HB3	2:B:108:GLY:H	3	0.2
(1,96)	1:A:7:CYS:HB3	2:B:108:GLY:H	4	0.18
(1,399)	1:A:4:GLU:HB2	1:A:7:CYS:HB2	12	0.18
(1,399)	1:A:4:GLU:HB3	1:A:7:CYS:HB2	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:A:7:CYS:HB3	2:B:108:GLY:H	7	0.17
(1,96)	1:A:7:CYS:HB3	2:B:108:GLY:H	12	0.17

10 Dihedral-angle violation analysis

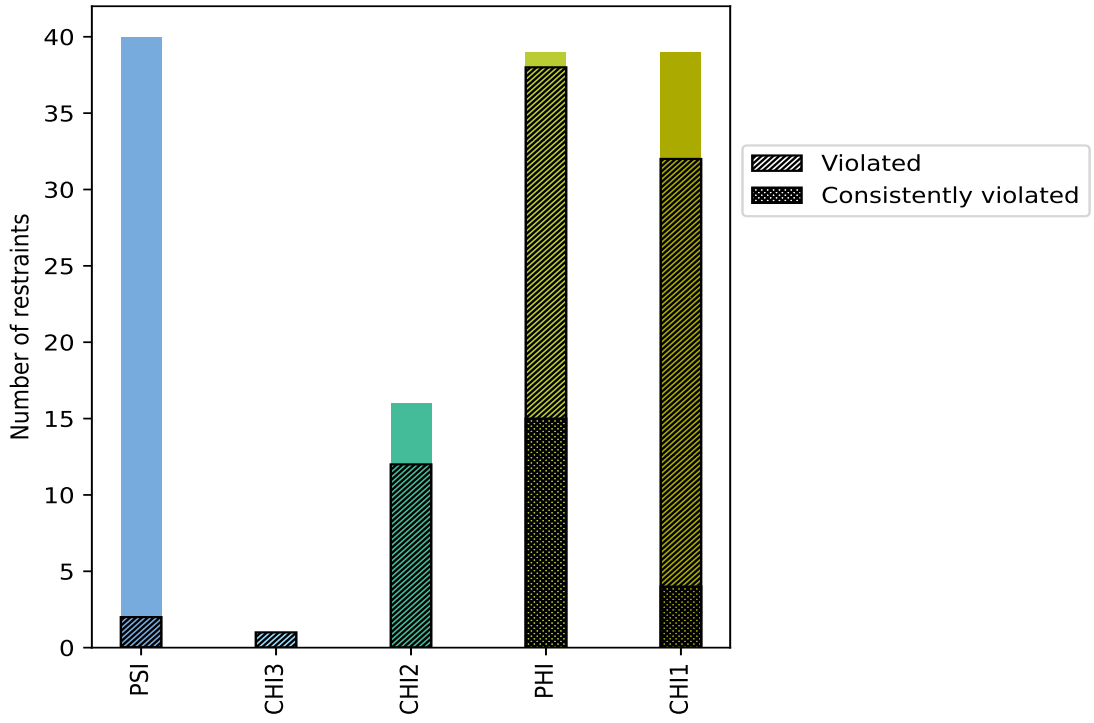
10.1 Summary of dihedral-angle violations

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]
PSI	40	29.6	2	5.0	1.5	0	0.0	0.0
CHI3	1	0.7	1	100.0	0.7	0	0.0	0.0
CHI2	16	11.9	12	75.0	8.9	0	0.0	0.0
PHI	39	28.9	38	97.4	28.1	15	38.5	11.1
CHI1	39	28.9	32	82.1	23.7	4	10.3	3.0
Total	135	100.0	85	63.0	63.0	19	14.1	14.1

[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



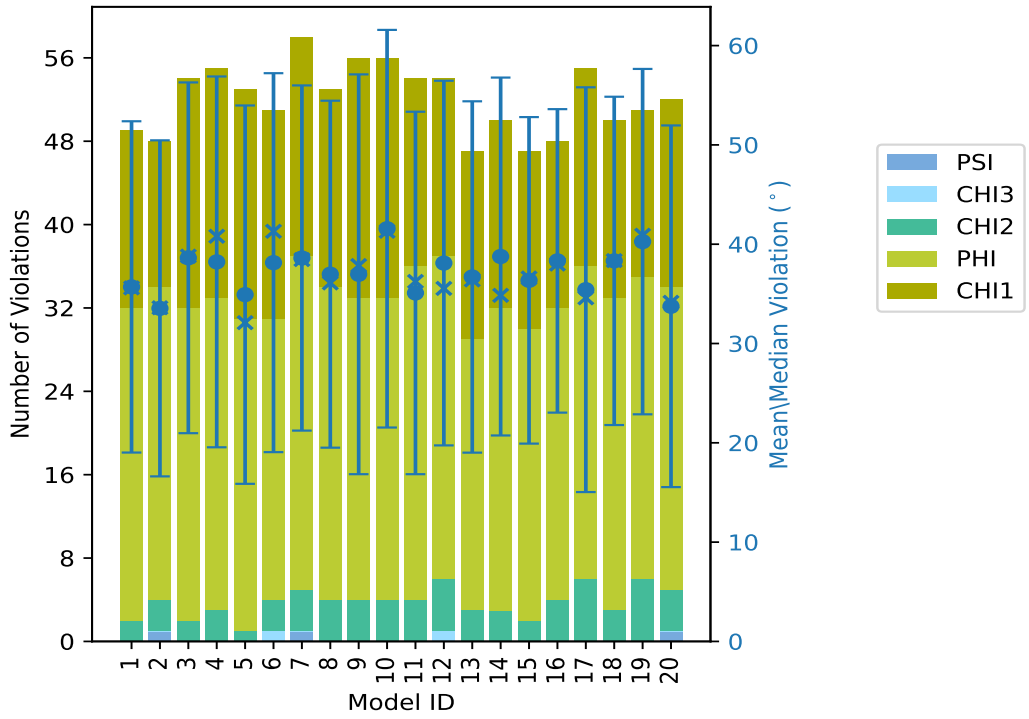
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PSI	CHI3	CHI2	PHI	CHI1	Total				
1	0	0	2	30	17	49	35.7	70.4	16.68	35.6
2	1	0	3	30	14	48	33.54	74.0	16.92	33.6
3	0	0	2	30	22	54	38.63	67.5	17.66	38.8
4	0	0	3	30	22	55	38.22	74.4	18.67	40.8
5	0	0	1	30	22	53	34.92	73.1	19.05	32.1
6	0	1	3	27	20	51	38.14	75.8	19.08	41.3
7	1	0	4	32	21	58	38.61	72.3	17.38	38.45
8	0	0	4	30	19	53	36.98	69.7	17.47	36.1
9	0	0	4	29	23	56	36.97	81.6	20.13	37.85
10	0	0	4	29	23	56	41.56	78.8	20.02	41.3
11	0	0	4	32	18	54	35.09	67.0	18.25	36.25
12	0	1	5	31	17	54	38.1	70.9	18.36	35.55
13	0	0	3	26	18	47	36.7	67.0	17.69	36.4
14	0	0	3	29	18	50	38.76	76.8	18.02	34.85
15	0	0	2	28	17	47	36.36	68.8	16.44	36.6
16	0	0	4	28	16	48	38.32	66.2	15.28	38.0
17	0	0	6	30	19	55	35.42	73.7	20.38	34.6
18	0	0	3	30	17	50	38.32	66.0	16.53	38.35
19	0	0	6	29	16	51	40.26	71.8	17.39	40.9
20	1	0	4	29	18	52	33.75	68.4	18.21	34.15

10.2.1 Bar graph : Dihedral violation statistics for each model



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

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	
PSI	CHI3	CHI2	PHI	CHI1	Total	Count[1]	%
1	0	0	3	1	5	1	5.0
1	1	0	0	1	3	2	10.0
0	0	3	2	1	6	3	15.0
0	0	3	0	0	3	4	20.0
0	0	0	0	0	0	5	25.0
0	0	1	0	3	4	6	30.0
0	0	2	0	0	2	7	35.0
0	0	1	1	3	5	8	40.0
0	0	1	0	2	3	9	45.0
0	0	0	1	3	4	10	50.0
0	0	0	1	1	2	11	55.0

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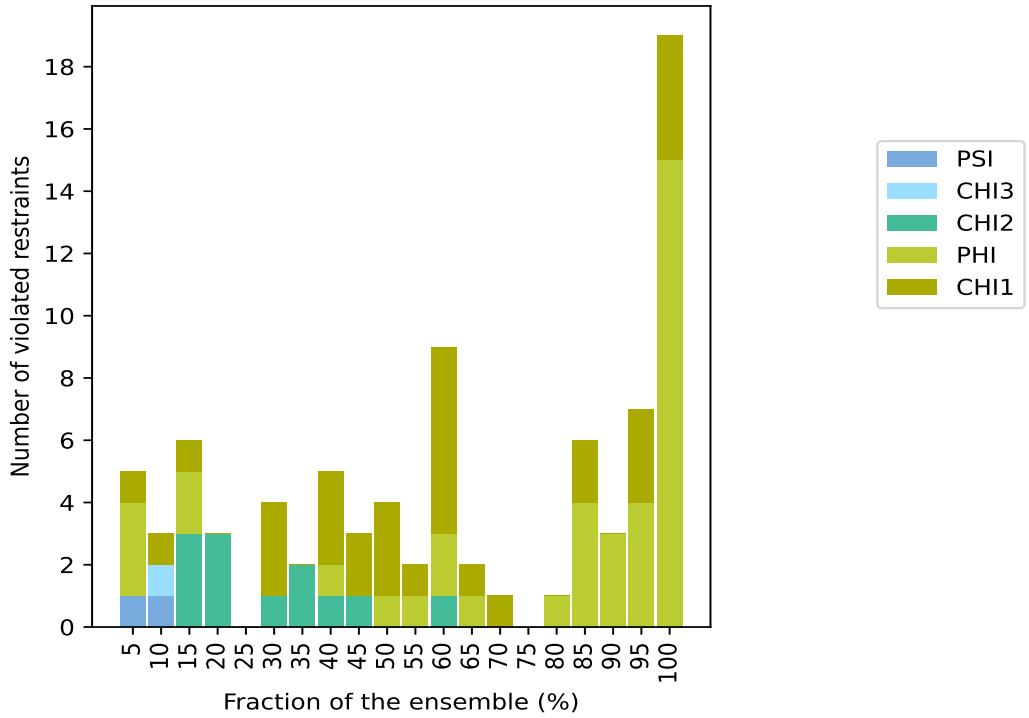
Number of violated restraints						Fraction of the ensemble	
PSI	CHI3	CHI2	PHI	CHI1	Total	Count[1]	%
0	0	1	2	6	9	12	60.0
0	0	0	1	1	2	13	65.0
0	0	0	0	1	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	1	0	1	16	80.0
0	0	0	4	2	6	17	85.0
0	0	0	3	0	3	18	90.0
0	0	0	4	3	7	19	95.0
0	0	0	15	4	19	20	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble

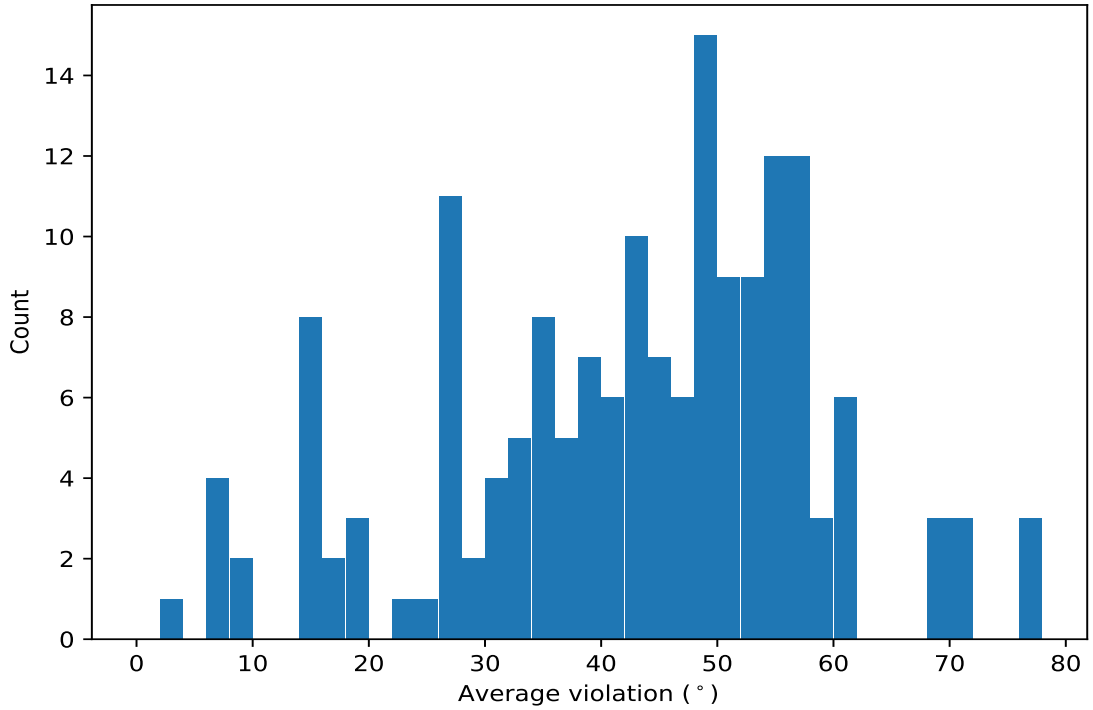


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle restraints

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]	Medi
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	20	68.06	4.96	67.4
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	20	68.06	4.96	67.4
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	20	68.06	4.96	67.4
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	20	55.92	16.56	62.3
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	20	55.92	16.56	62.3
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	20	55.92	16.56	62.3
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	20	50.67	5.12	50.7
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	20	50.67	5.12	50.7
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	20	50.67	5.12	50.7
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	20	46.34	18.34	52.0
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	20	46.34	18.34	52.0
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	20	46.34	18.34	52.0
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	20	44.86	3.71	45.0
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	20	42.4	1.48	42.5
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	20	39.56	1.74	39.0
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	20	38.24	1.67	38.6
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	20	37.25	7.97	41.1
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	20	35.32	4.91	36.4
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	20	34.51	3.99	34.4
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	20	34.45	1.66	34.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Medi
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	20	34.08	4.56	34.5
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	20	33.8	3.48	32.7
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	20	33.05	9.2	34.0
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	20	30.98	2.59	30.8
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	20	30.86	3.92	30.4
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	20	27.11	1.73	27.0
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	20	25.26	7.83	26.0
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	19	53.78	6.3	53.8
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	19	53.78	6.3	53.8
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	19	53.78	6.3	53.8
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	19	53.64	7.37	54.9
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	19	53.64	7.37	54.9
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	19	53.64	7.37	54.9
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	19	53.47	23.28	65.2
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	19	53.47	23.28	65.2
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	19	53.47	23.28	65.2
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	19	35.01	16.37	34.0
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	19	28.08	8.31	31.1
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	19	26.54	12.11	31.1
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	19	16.23	6.63	15.2
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	18	30.84	7.45	33.2
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	18	27.46	6.18	28.3
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	18	22.89	8.3	24.6
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	17	40.1	10.21	43.0
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	17	40.1	10.21	43.0
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	17	40.1	10.21	43.0
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	17	31.12	10.84	33.9
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	17	29.81	19.11	25.4
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	17	27.81	10.19	29.5
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	17	26.89	3.56	26.2
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	17	26.89	3.56	26.2
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	17	26.89	3.56	26.2
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	17	8.19	3.89	9.2
(1,78)	2:B:121:GLU:C	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:C	16	27.96	12.3	30.1
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	14	51.36	13.64	55.1
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	14	51.36	13.64	55.1
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	14	51.36	13.64	55.1
(1,1)	1:A:1:GLY:C	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:C	13	36.13	10.97	39.8
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	13	7.05	3.91	7.4
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	13	7.05	3.91	7.4
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	13	7.05	3.91	7.4
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	12	58.97	9.26	58.8
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	12	58.97	9.26	58.8
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	12	58.97	9.26	58.8
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	12	56.04	10.86	58.6
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	12	56.04	10.86	58.6
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	12	56.04	10.86	58.6
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	12	50.23	11.8	53.6
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	12	50.23	11.8	53.6
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	12	50.23	11.8	53.6
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	12	48.41	15.44	53.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Medi
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	12	48.41	15.44	53.8
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	12	48.41	15.44	53.8
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	12	45.88	16.77	51.2
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	12	45.88	16.77	51.2
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	12	45.88	16.77	51.2
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	12	39.61	25.81	51.0
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	12	39.61	25.81	51.0
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	12	39.61	25.81	51.0
(1,48)	2:B:104:GLN:C	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:C	12	17.88	6.51	19.8
(1,13)	1:A:7:CYS:C	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:C	12	14.72	7.24	14.0
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	12	14.64	17.68	8.85
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	12	14.64	17.68	8.85
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	12	14.64	17.68	8.85
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	11	43.29	27.86	60.8
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	11	43.29	27.86	60.8
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	11	43.29	27.86	60.8
(1,74)	2:B:118:VAL:C	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:C	11	14.66	10.21	10.7
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	10	56.31	9.2	60.2
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	10	56.31	9.2	60.2
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	10	56.31	9.2	60.2
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	10	48.78	30.03	65.1
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	10	48.78	30.03	65.1
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	10	48.78	30.03	65.1
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	10	42.93	10.52	45.6
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	10	42.93	10.52	45.6
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	10	42.93	10.52	45.6
(1,42)	2:B:101:PHE:C	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:C	10	38.29	13.7	32.3
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	9	60.8	6.07	58.3
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	9	60.8	6.07	58.3
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	9	60.8	6.07	58.3
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	9	54.82	4.61	53.6
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	9	54.82	4.61	53.6
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	9	54.82	4.61	53.6
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	9	47.91	18.99	58.2
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	9	47.91	18.99	58.2
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	9	47.91	18.99	58.2
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	8	61.4	4.31	60.2
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	8	61.4	4.31	60.2
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	8	61.4	4.31	60.2
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	8	57.19	4.78	56.7
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	8	57.19	4.78	56.7
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	8	57.19	4.78	56.7
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	8	56.24	7.49	55.4
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	8	56.24	7.49	55.4
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	8	56.24	7.49	55.4
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	8	41.59	20.05	50.9
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	8	41.59	20.05	50.9
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	8	41.59	20.05	50.9
(1,15)	1:A:8:THR:C	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:C	8	9.24	9.85	5.0
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	7	33.94	27.31	52.2
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	7	33.94	27.31	52.2

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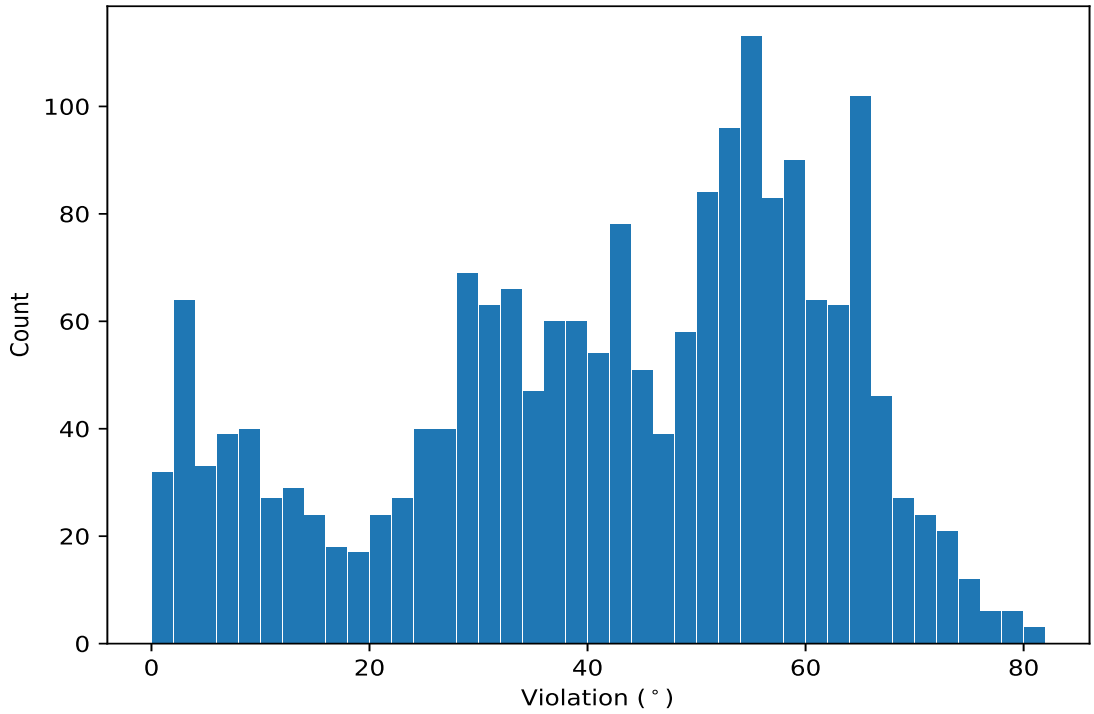
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Medi
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	7	33.94	27.31	52.2
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	7	27.87	22.18	37.9
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	7	27.87	22.18	37.9
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	7	27.87	22.18	37.9
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	6	48.22	20.26	56.7
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	6	48.22	20.26	56.7
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	6	48.22	20.26	56.7
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	6	44.33	19.14	46.4
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	6	44.33	19.14	46.4
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	6	44.33	19.14	46.4
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	6	43.95	13.06	39.0
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	6	43.95	13.06	39.0
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	6	43.95	13.06	39.0
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	6	34.97	8.6	38.4
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	6	34.97	8.6	38.4
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	6	34.97	8.6	38.4
(1,128)	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2:B:117:LEU:CD1	4	49.52	4.11	51.3
(1,128)	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2:B:117:LEU:CD1	4	49.52	4.11	51.3
(1,128)	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2:B:117:LEU:CD1	4	49.52	4.11	51.3
(1,132)	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	2:B:121:GLU:CD	4	36.6	11.09	30.4
(1,132)	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	2:B:121:GLU:CD	4	36.6	11.09	30.4
(1,132)	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	2:B:121:GLU:CD	4	36.6	11.09	30.4
(1,92)	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	1:A:10:ILE:CD1	4	15.72	23.6	2.2
(1,92)	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	1:A:10:ILE:CD1	4	15.72	23.6	2.2
(1,92)	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	1:A:10:ILE:CD1	4	15.72	23.6	2.2
(1,101)	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	1:A:16:LEU:CD1	3	71.57	10.24	75.0
(1,101)	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	1:A:16:LEU:CD1	3	71.57	10.24	75.0
(1,101)	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	1:A:16:LEU:CD1	3	71.57	10.24	75.0
(1,99)	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	1:A:15:GLN:CD	3	55.97	2.9	54.0
(1,99)	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	1:A:15:GLN:CD	3	55.97	2.9	54.0
(1,99)	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	1:A:15:GLN:CD	3	55.97	2.9	54.0
(1,115)	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	2:B:106:LEU:CD1	3	48.57	33.21	71.8
(1,115)	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	2:B:106:LEU:CD1	3	48.57	33.21	71.8
(1,115)	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	2:B:106:LEU:CD1	3	48.57	33.21	71.8
(1,46)	2:B:103:ASN:C	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:C	3	38.9	21.5	48.1
(1,108)	2:B:101:PHE:N	2:B:101:PHE:CA	2:B:101:PHE:CB	2:B:101:PHE:CG	3	19.43	20.88	7.4
(1,108)	2:B:101:PHE:N	2:B:101:PHE:CA	2:B:101:PHE:CB	2:B:101:PHE:CG	3	19.43	20.88	7.4
(1,108)	2:B:101:PHE:N	2:B:101:PHE:CA	2:B:101:PHE:CB	2:B:101:PHE:CG	3	19.43	20.88	7.4
(1,9)	1:A:5:GLN:C	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:C	3	6.4	2.19	6.9
(1,124)	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:CB	2:B:115:LEU:CG	2	77.3	1.5	77.3
(1,124)	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:CB	2:B:115:LEU:CG	2	77.3	1.5	77.3
(1,124)	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:CB	2:B:115:LEU:CG	2	77.3	1.5	77.3
(1,135)	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	2:B:122:ARG:NE	2	55.55	7.35	55.5
(1,135)	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	2:B:122:ARG:NE	2	55.55	7.35	55.5
(1,135)	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	2:B:122:ARG:NE	2	55.55	7.35	55.5
(1,40)	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	1:A:22:GLY:N	2	2.55	1.15	2.55

[1] Number of violated models, [2]Standard 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 (°)
(1,101)	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	1:A:16:LEU:CD1	9	81.6
(1,101)	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	1:A:16:LEU:CD1	9	81.6
(1,101)	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	1:A:16:LEU:CD1	9	81.6
(1,124)	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:CB	2:B:115:LEU:CG	10	78.8
(1,124)	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:CB	2:B:115:LEU:CG	10	78.8
(1,124)	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:CB	2:B:115:LEU:CG	10	78.8
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	10	78.2
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	10	78.2
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	10	78.2
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	9	77.2
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	9	77.2
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	9	77.2
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	14	76.8
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	14	76.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	14	76.8
(1,124)	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:CB	2:B:115:LEU:CG	6	75.8
(1,124)	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:CB	2:B:115:LEU:CG	6	75.8
(1,124)	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:CB	2:B:115:LEU:CG	6	75.8
(1,101)	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	1:A:16:LEU:CD1	10	75.6
(1,101)	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	1:A:16:LEU:CD1	10	75.6
(1,101)	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	1:A:16:LEU:CD1	10	75.6
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	4	74.4
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	4	74.4
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	4	74.4
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	2	74.0
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	2	74.0
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	2	74.0
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	17	73.7
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	17	73.7
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	17	73.7
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	17	73.5
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	17	73.5
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	17	73.5
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	14	73.3
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	14	73.3
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	14	73.3
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	5	73.1
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	5	73.1
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	5	73.1
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	2	72.6
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	2	72.6
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	2	72.6
(1,115)	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	2:B:106:LEU:CD1	7	72.3
(1,115)	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	2:B:106:LEU:CD1	7	72.3
(1,115)	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	2:B:106:LEU:CD1	7	72.3
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	4	72.2
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	4	72.2
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	4	72.2
(1,115)	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	2:B:106:LEU:CD1	19	71.8
(1,115)	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	2:B:106:LEU:CD1	19	71.8
(1,115)	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	2:B:106:LEU:CD1	19	71.8
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	19	71.1
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	19	71.1
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	19	71.1
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	10	71.0
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	10	71.0
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	10	71.0
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	12	70.9
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	12	70.9
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	12	70.9
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	7	70.6
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	7	70.6
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	7	70.6
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	1	70.4
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	1	70.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	1	70.4
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	10	70.3
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	10	70.3
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	10	70.3
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	14	70.1
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	14	70.1
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	14	70.1
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	8	69.7
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	8	69.7
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	8	69.7
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	14	69.5
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	14	69.5
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	14	69.5
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	8	69.4
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	8	69.4
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	8	69.4
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	19	68.8
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	19	68.8
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	19	68.8
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	15	68.8
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	15	68.8
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	15	68.8
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	4	68.7
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	4	68.7
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	4	68.7
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	20	68.4
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	20	68.4
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	20	68.4
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	12	68.3
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	12	68.3
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	12	68.3
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	12	68.1
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	12	68.1
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	12	68.1
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	4	67.6
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	4	67.6
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	4	67.6
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	3	67.5
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	3	67.5
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	3	67.5
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	5	67.2
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	5	67.2
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	5	67.2
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	13	67.0
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	13	67.0
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	13	67.0
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	11	67.0
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	11	67.0
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	11	67.0
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	10	66.8
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	10	66.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	10	66.8
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	6	66.4
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	6	66.4
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	6	66.4
(1,42)	2:B:101:PHE:C	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:C	17	66.2
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	16	66.2
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	16	66.2
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	16	66.2
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	12	66.1
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	12	66.1
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	12	66.1
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	16	66.1
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	16	66.1
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	16	66.1
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	13	66.1
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	13	66.1
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	13	66.1
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	12	66.1
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	12	66.1
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	12	66.1
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	13	66.1
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	13	66.1
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	13	66.1
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	18	66.0
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	18	66.0
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	18	66.0
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	12	66.0
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	12	66.0
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	12	66.0
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	10	65.9
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	10	65.9
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	10	65.9
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	12	65.9
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	12	65.9
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	12	65.9
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	9	65.8
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	9	65.8
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	9	65.8
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	17	65.7
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	17	65.7
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	17	65.7
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	1	65.6
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	1	65.6
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	1	65.6
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	1	65.4
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	1	65.4
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	1	65.4
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	3	65.4
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	3	65.4
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	3	65.4
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	19	65.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	19	65.4
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	19	65.4
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	9	65.3
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	9	65.3
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	9	65.3
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	11	65.3
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	11	65.3
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	11	65.3
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	8	65.2
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	8	65.2
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	8	65.2
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	6	65.2
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	6	65.2
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	6	65.2
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	17	65.1
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	17	65.1
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	17	65.1
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	14	65.1
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	14	65.1
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	14	65.1
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	8	65.1
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	8	65.1
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	8	65.1
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	7	64.9
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	7	64.9
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	7	64.9
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	19	64.9
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	19	64.9
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	19	64.9
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	5	64.9
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	5	64.9
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	5	64.9
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	15	64.9
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	15	64.9
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	15	64.9
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	18	64.9
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	18	64.9
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	18	64.9
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	3	64.8
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	3	64.8
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	3	64.8
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	11	64.8
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	11	64.8
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	11	64.8
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	18	64.7
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	18	64.7
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	18	64.7
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	12	64.7
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	12	64.7
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	12	64.7
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	3	64.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	3	64.6
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	3	64.6
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	14	64.6
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	14	64.6
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	14	64.6
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	7	64.5
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	7	64.5
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	7	64.5
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	7	64.4
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	7	64.4
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	7	64.4
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	13	64.3
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	13	64.3
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	13	64.3
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	15	64.2
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	15	64.2
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	15	64.2
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	18	64.2
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	18	64.2
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	18	64.2
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	16	64.1
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	16	64.1
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	16	64.1
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	20	64.1
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	20	64.1
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	20	64.1
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	10	64.0
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	10	64.0
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	10	64.0
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	10	63.9
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	10	63.9
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	10	63.9
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	16	63.8
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	16	63.8
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	16	63.8
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	8	63.8
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	8	63.8
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	8	63.8
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	16	63.7
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	16	63.7
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	16	63.7
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	9	63.7
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	9	63.7
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	9	63.7
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	5	63.6
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	5	63.6
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	5	63.6
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	10	63.6
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	10	63.6
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	10	63.6
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	9	63.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	9	63.5
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	9	63.5
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	6	63.4
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	6	63.4
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	6	63.4
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	14	63.4
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	14	63.4
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	14	63.4
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	18	63.3
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	18	63.3
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	18	63.3
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	6	63.3
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	6	63.3
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	6	63.3
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	5	63.2
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	5	63.2
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	5	63.2
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	10	63.0
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	10	63.0
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	10	63.0
(1,135)	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	2:B:122:ARG:NE	12	62.9
(1,135)	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	2:B:122:ARG:NE	12	62.9
(1,135)	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	2:B:122:ARG:NE	12	62.9
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	19	62.7
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	19	62.7
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	19	62.7
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	1	62.7
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	1	62.7
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	1	62.7
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	17	62.7
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	17	62.7
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	17	62.7
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	5	62.6
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	5	62.6
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	5	62.6
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	17	62.2
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	17	62.2
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	17	62.2
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	8	62.0
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	8	62.0
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	8	62.0
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	11	61.9
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	11	61.9
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	11	61.9
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	10	61.6
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	10	61.6
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	10	61.6
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	5	61.6
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	5	61.6
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	5	61.6
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	5	61.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	5	61.6
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	5	61.6
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	17	61.5
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	17	61.5
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	17	61.5
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	12	61.4
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	12	61.4
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	12	61.4
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	5	61.3
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	5	61.3
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	5	61.3
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	12	61.3
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	12	61.3
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	12	61.3
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	20	61.1
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	20	61.1
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	20	61.1
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	6	61.0
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	6	61.0
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	6	61.0
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	13	61.0
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	13	61.0
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	13	61.0
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	3	60.8
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	3	60.8
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	3	60.8
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	13	60.7
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	13	60.7
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	13	60.7
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	1	60.7
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	1	60.7
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	1	60.7
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	16	60.7
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	16	60.7
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	16	60.7
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	18	60.5
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	18	60.5
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	18	60.5
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	11	60.5
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	11	60.5
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	11	60.5
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	4	60.4
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	3	60.4
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	3	60.4
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	3	60.4
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	11	60.3
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	11	60.3
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	11	60.3
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	7	60.1
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	7	60.1
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	7	60.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,99)	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	1:A:15:GLN:CD	17	60.0
(1,99)	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	1:A:15:GLN:CD	17	60.0
(1,99)	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	1:A:15:GLN:CD	17	60.0
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	3	59.8
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	3	59.8
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	3	59.8
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	20	59.8
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	20	59.8
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	20	59.8
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	7	59.8
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	7	59.8
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	7	59.8
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	20	59.7
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	20	59.7
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	20	59.7
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	19	59.7
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	19	59.7
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	19	59.7
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	7	59.6
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	7	59.6
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	7	59.6
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	5	59.5
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	5	59.5
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	5	59.5
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	9	59.5
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	9	59.5
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	9	59.5
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	14	59.5
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	14	59.5
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	14	59.5
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	2	59.5
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	2	59.5
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	2	59.5
(1,46)	2:B:103:ASN:C	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:C	11	59.4
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	6	59.2
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	6	59.2
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	6	59.2
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	15	59.2
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	15	59.2
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	15	59.2
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	12	59.1
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	12	59.1
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	12	59.1
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	6	59.1
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	4	58.8
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	4	58.8
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	4	58.8
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	4	58.7
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	4	58.7
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	4	58.7
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	11	58.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	11	58.6
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	11	58.6
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	18	58.4
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	18	58.4
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	18	58.4
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	17	58.4
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	17	58.4
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	17	58.4
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	1	58.4
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	1	58.4
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	1	58.4
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	3	58.4
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	3	58.4
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	3	58.4
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	12	58.3
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	12	58.3
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	12	58.3
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	9	58.2
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	9	58.2
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	9	58.2
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	16	58.2
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	16	58.2
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	16	58.2
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	16	58.2
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	16	58.2
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	16	58.2
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	3	58.2
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	3	58.2
(1,105)	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:CB	1:A:19:TYR:CG	3	58.2
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	19	58.1
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	19	58.1
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	19	58.1
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	14	58.1
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	14	58.1
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	14	58.1
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	8	58.0
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	8	58.0
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	8	58.0
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	10	58.0
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	10	58.0
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	10	58.0
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	6	58.0
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	6	57.9
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	6	57.9
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	6	57.9
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	9	57.8
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	9	57.8
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	9	57.8
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	4	57.7
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	4	57.7
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	4	57.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	6	57.5
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	6	57.5
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	6	57.5
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	4	57.5
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	4	57.5
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	4	57.5
(1,101)	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	1:A:16:LEU:CD1	7	57.5
(1,101)	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	1:A:16:LEU:CD1	7	57.5
(1,101)	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	1:A:16:LEU:CD1	7	57.5
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	9	57.4
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	9	57.4
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	9	57.4
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	10	57.4
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	4	57.3
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	4	57.3
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	4	57.3
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	8	57.3
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	8	57.3
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	8	57.3
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	13	57.2
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	13	57.2
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	13	57.2
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	18	57.2
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	18	57.2
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	18	57.2
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	11	57.1
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	7	56.8
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	7	56.8
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	7	56.8
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	7	56.7
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	7	56.7
(1,83)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	7	56.7
(1,92)	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	1:A:10:ILE:CD1	19	56.6
(1,92)	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	1:A:10:ILE:CD1	19	56.6
(1,92)	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	1:A:10:ILE:CD1	19	56.6
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	19	56.6
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	19	56.6
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	19	56.6
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	4	56.6
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	4	56.6
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	4	56.6
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	19	56.5
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	19	56.5
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	19	56.5
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	9	56.4
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	20	56.4
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	20	56.4
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	20	56.4
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	11	56.4
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	11	56.4
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	11	56.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	13	56.4
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	13	56.4
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	13	56.4
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	2	56.3
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	2	56.3
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	2	56.3
(1,42)	2:B:101:PHE:C	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:C	14	56.3
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	15	56.3
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	15	56.3
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	15	56.3
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	7	56.2
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	7	56.2
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	7	56.2
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	3	56.2
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	7	56.1
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	7	56.1
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	7	56.1
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	19	56.1
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	19	56.1
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	19	56.1
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	20	56.0
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	20	56.0
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	20	56.0
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	8	55.9
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	8	55.9
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	8	55.9
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	8	55.9
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	8	55.9
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	8	55.9
(1,107)	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:CB	1:A:21:ASN:CG	10	55.9
(1,107)	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:CB	1:A:21:ASN:CG	10	55.9
(1,107)	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:CB	1:A:21:ASN:CG	10	55.9
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	3	55.8
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	3	55.8
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	3	55.8
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	10	55.8
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	10	55.8
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	10	55.8
(1,132)	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	2:B:121:GLU:CD	14	55.8
(1,132)	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	2:B:121:GLU:CD	14	55.8
(1,132)	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	2:B:121:GLU:CD	14	55.8
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	20	55.8
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	20	55.8
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	20	55.8
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	3	55.7
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	3	55.7
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	3	55.7
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	15	55.7
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	15	55.7
(1,116)	2:B:107:CYS:N	2:B:107:CYS:CA	2:B:107:CYS:CB	2:B:107:CYS:SG	15	55.7
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	18	55.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	18	55.6
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	18	55.6
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	3	55.5
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	3	55.5
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	3	55.5
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	19	55.4
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	19	55.4
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	19	55.4
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	20	55.4
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	20	55.4
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	20	55.4
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	6	55.3
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	6	55.3
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	6	55.3
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	8	55.2
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	8	55.2
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	8	55.2
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	4	55.2
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	4	55.2
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	4	55.2
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	12	55.2
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	2	55.2
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	4	55.1
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	3	55.1
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	3	55.1
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	3	55.1
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	14	55.0
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	14	55.0
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	14	55.0
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	15	55.0
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	15	55.0
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	15	55.0
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	3	55.0
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	3	55.0
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	3	55.0
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	4	55.0
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	4	55.0
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	4	55.0
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	7	54.9
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	7	54.9
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	7	54.9
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	3	54.8
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	3	54.8
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	3	54.8
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	17	54.7
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	17	54.7
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	17	54.7
(1,99)	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	1:A:15:GLN:CD	19	54.6
(1,99)	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	1:A:15:GLN:CD	19	54.6
(1,99)	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	1:A:15:GLN:CD	19	54.6
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	9	54.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	13	54.5
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	13	54.5
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	13	54.5
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	17	54.5
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	17	54.5
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	17	54.5
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	1	54.4
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	1	54.4
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	1	54.4
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	11	54.4
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	11	54.4
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	11	54.4
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	10	54.3
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	10	54.3
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	10	54.3
(1,1)	1:A:1:GLY:C	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:C	19	54.3
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	8	54.1
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	8	54.1
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	8	54.1
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	2	54.1
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	2	54.1
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	2	54.1
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	1	54.1
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	1	54.1
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	1	54.1
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	9	54.1
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	9	54.1
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	9	54.1
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	18	54.0
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	18	54.0
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	18	54.0
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	20	54.0
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	20	54.0
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	20	54.0
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	18	53.9
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	18	53.9
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	18	53.9
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	15	53.8
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	15	53.8
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	15	53.8
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	3	53.8
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	3	53.8
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	3	53.8
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	14	53.8
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	14	53.8
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	14	53.8
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	10	53.7
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	10	53.7
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	10	53.7
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	2	53.6
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	2	53.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	2	53.6
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	6	53.6
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	6	53.6
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	6	53.6
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	15	53.5
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	15	53.5
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	15	53.5
(1,99)	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	1:A:15:GLN:CD	8	53.3
(1,99)	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	1:A:15:GLN:CD	8	53.3
(1,99)	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	1:A:15:GLN:CD	8	53.3
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	16	53.3
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	16	53.3
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	16	53.3
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	12	53.1
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	12	53.1
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	12	53.1
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	18	53.0
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	18	53.0
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	18	53.0
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	15	52.9
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	15	52.9
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	15	52.9
(1,128)	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2:B:117:LEU:CD1	8	52.9
(1,128)	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2:B:117:LEU:CD1	8	52.9
(1,128)	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2:B:117:LEU:CD1	8	52.9
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	9	52.7
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	9	52.7
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	9	52.7
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	5	52.7
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	5	52.7
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	5	52.7
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	3	52.7
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	3	52.7
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	3	52.7
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	8	52.7
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	8	52.7
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	8	52.7
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	7	52.5
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	7	52.5
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	7	52.5
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	17	52.5
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	17	52.5
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	17	52.5
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1	52.5
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1	52.5
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1	52.5
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	7	52.5
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	7	52.5
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	7	52.5
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	13	52.5
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	13	52.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	13	52.5
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	2	52.5
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	2	52.5
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	2	52.5
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	1	52.4
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	1	52.4
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	1	52.4
(1,128)	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2:B:117:LEU:CD1	14	52.3
(1,128)	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2:B:117:LEU:CD1	14	52.3
(1,128)	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2:B:117:LEU:CD1	14	52.3
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	14	52.2
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	14	52.2
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	14	52.2
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	4	52.2
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	4	52.2
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	4	52.2
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	17	52.2
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	17	52.2
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	17	52.2
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	19	52.2
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	19	52.2
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	19	52.2
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	10	52.2
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	10	52.2
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	10	52.2
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	4	52.1
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	4	52.1
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	4	52.1
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	18	51.9
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	18	51.9
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	18	51.9
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	3	51.8
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	3	51.8
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	3	51.8
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	2	51.8
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	2	51.8
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	2	51.8
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	7	51.7
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	7	51.7
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	7	51.7
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	15	51.5
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	15	51.5
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	15	51.5
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	13	51.3
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	13	51.3
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	13	51.3
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	15	51.1
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	15	51.1
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	15	51.1
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	9	51.1
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	9	51.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	9	51.1
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	17	51.1
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	17	51.1
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	17	51.1
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	4	51.1
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	4	51.1
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	4	51.1
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	9	51.0
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	9	51.0
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	9	51.0
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	3	50.9
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	3	50.9
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	3	50.9
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	19	50.9
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	19	50.9
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	19	50.9
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	7	50.8
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	7	50.8
(1,109)	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:CB	2:B:102:VAL:CG1	7	50.8
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	6	50.7
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	6	50.7
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	6	50.7
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	13	50.7
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	13	50.7
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	13	50.7
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	20	50.7
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	20	50.7
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	20	50.7
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	9	50.6
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	9	50.6
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	9	50.6
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	19	50.6
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	19	50.6
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	19	50.6
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	9	50.5
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	9	50.5
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	9	50.5
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	5	50.4
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	5	50.4
(1,94)	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:CB	1:A:12:SER:OG	5	50.4
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	16	50.4
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	16	50.4
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	16	50.4
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	19	50.4
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	19	50.4
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	19	50.4
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	14	50.4
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	14	50.4
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	14	50.4
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	13	50.3
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	13	50.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	13	50.3
(1,128)	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2:B:117:LEU:CD1	16	50.3
(1,128)	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2:B:117:LEU:CD1	16	50.3
(1,128)	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2:B:117:LEU:CD1	16	50.3
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	10	50.3
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	10	50.3
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	10	50.3
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	5	50.2
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	5	50.2
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	5	50.2
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	2	49.9
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	17	49.8
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	17	49.8
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	17	49.8
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	16	49.6
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	16	49.6
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	16	49.6
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	13	49.6
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	18	49.4
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	18	49.4
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	18	49.4
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	7	49.3
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	7	49.3
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	7	49.3
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	6	49.2
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	6	49.2
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	6	49.2
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	8	49.2
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	8	49.2
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	8	49.2
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	10	48.9
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	10	48.9
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	10	48.9
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	10	48.9
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	10	48.9
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	10	48.9
(1,108)	2:B:101:PHE:N	2:B:101:PHE:CA	2:B:101:PHE:CB	2:B:101:PHE:CG	11	48.8
(1,108)	2:B:101:PHE:N	2:B:101:PHE:CA	2:B:101:PHE:CB	2:B:101:PHE:CG	11	48.8
(1,108)	2:B:101:PHE:N	2:B:101:PHE:CA	2:B:101:PHE:CB	2:B:101:PHE:CG	11	48.8
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	11	48.6
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	11	48.6
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	11	48.6
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	18	48.4
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	1	48.4
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	1	48.4
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	1	48.4
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	16	48.3
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	16	48.3
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	16	48.3
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	12	48.3
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	12	48.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	12	48.3
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	16	48.3
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	16	48.3
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	16	48.3
(1,135)	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	2:B:122:ARG:NE	6	48.2
(1,135)	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	2:B:122:ARG:NE	6	48.2
(1,135)	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	2:B:122:ARG:NE	6	48.2
(1,46)	2:B:103:ASN:C	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:C	9	48.1
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	20	48.1
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	20	48.1
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	20	48.1
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	20	48.0
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	20	48.0
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	20	48.0
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	15	48.0
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	15	48.0
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	15	48.0
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	20	47.5
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	20	47.4
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	20	47.4
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	20	47.4
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	10	47.3
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	11	47.3
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	11	47.3
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	11	47.3
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	10	47.1
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	18	47.1
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	18	47.1
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	18	47.1
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	6	46.9
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	9	46.9
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	9	46.9
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	9	46.9
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	4	46.9
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	4	46.9
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	4	46.9
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	8	46.7
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	6	46.6
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	6	46.6
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	6	46.6
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	7	46.5
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	7	46.5
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	7	46.5
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	5	46.5
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	5	46.5
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	5	46.5
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2	46.2
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2	46.2
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2	46.2
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	1	46.1
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	1	46.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	1	46.1
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2	46.1
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2	46.1
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2	46.1
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	7	46.0
(1,1)	1:A:1:GLY:C	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:C	18	45.9
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	13	45.8
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	13	45.7
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	13	45.7
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	13	45.7
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	11	45.6
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	11	45.6
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	11	45.6
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	18	45.5
(1,42)	2:B:101:PHE:C	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:C	4	45.5
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	20	45.4
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	17	45.4
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	17	45.4
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	17	45.4
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	4	45.3
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	5	45.3
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	5	45.3
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	5	45.3
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	17	45.3
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	17	45.3
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	17	45.3
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	13	45.1
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	13	45.1
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	13	45.1
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	12	44.8
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	12	44.8
(1,85)	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	12	44.8
(1,42)	2:B:101:PHE:C	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:C	10	44.8
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	12	44.8
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	6	44.7
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	6	44.7
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	6	44.7
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	11	44.7
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	11	44.7
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	11	44.7
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	14	44.7
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	1	44.7
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	1	44.7
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	1	44.7
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	8	44.5
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	19	44.5
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	19	44.5
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	19	44.5
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	18	44.4
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	19	44.2
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	3	44.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	5	44.2
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	2	44.1
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	2	44.1
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	2	44.1
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	12	44.0
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	8	43.9
(1,78)	2:B:121:GLU:C	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:C	20	43.8
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	6	43.8
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	6	43.8
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	6	43.8
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	11	43.7
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	10	43.6
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	10	43.6
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	10	43.6
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	1	43.6
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	1	43.6
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	1	43.6
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	20	43.5
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	7	43.5
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	7	43.5
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	7	43.5
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	7	43.5
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	4	43.3
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	5	43.3
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	4	43.3
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	4	43.3
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	4	43.3
(1,1)	1:A:1:GLY:C	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:C	6	43.3
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	3	43.2
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	12	43.1
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	4	43.1
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	11	43.0
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	11	43.0
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	11	43.0
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	11	43.0
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	15	43.0
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	6	42.9
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	6	42.9
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	6	42.9
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	18	42.9
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	18	42.9
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	18	42.9
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	17	42.8
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	17	42.8
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	17	42.8
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	16	42.8
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	16	42.8
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	16	42.8
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	13	42.7
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	4	42.7
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	4	42.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	4	42.7
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	2	42.6
(1,128)	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2:B:117:LEU:CD1	15	42.6
(1,128)	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2:B:117:LEU:CD1	15	42.6
(1,128)	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	2:B:117:LEU:CD1	15	42.6
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	3	42.5
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	3	42.5
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	3	42.5
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	3	42.4
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	3	42.4
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	3	42.4
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	17	42.4
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	6	42.3
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	19	42.3
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	19	42.3
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	19	42.3
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	11	42.3
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	11	42.3
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	11	42.3
(1,78)	2:B:121:GLU:C	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:C	18	42.2
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	10	42.2
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	15	42.1
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	14	42.1
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	8	42.1
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	8	42.1
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	8	42.1
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	9	42.0
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	17	42.0
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	5	42.0
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	5	42.0
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	5	42.0
(1,1)	1:A:1:GLY:C	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:C	15	42.0
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	19	41.9
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	1	41.9
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	6	41.8
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	11	41.8
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	7	41.8
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	7	41.8
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	7	41.8
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	4	41.7
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	11	41.7
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	9	41.5
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	5	41.5
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	14	41.5
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	4	41.5
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	4	41.5
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	4	41.5
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	6	41.5
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	6	41.5
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	6	41.5
(1,78)	2:B:121:GLU:C	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:C	7	41.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	14	41.4
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	10	41.4
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	10	41.4
(1,100)	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:CB	1:A:16:LEU:CG	10	41.4
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	1	41.3
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	1	41.3
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	6	41.3
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	10	41.2
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	13	41.2
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	17	41.2
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	5	41.1
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	5	41.1
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	5	41.1
(1,1)	1:A:1:GLY:C	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:C	3	41.0
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	5	40.9
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	19	40.9
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	3	40.9
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	1	40.9
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	4	40.9
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	4	40.9
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	4	40.9
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	11	40.8
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	4	40.8
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	9	40.8
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	7	40.7
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	18	40.7
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	7	40.6
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	16	40.4
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	19	40.4
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	13	40.3
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	15	40.3
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	9	40.2
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	19	40.2
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	13	40.1
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	17	40.0
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	10	39.9
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	10	39.9
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	10	39.9
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	17	39.9
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	6	39.9
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	12	39.9
(1,1)	1:A:1:GLY:C	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:C	20	39.9
(1,1)	1:A:1:GLY:C	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:C	9	39.8
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	16	39.7
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	5	39.7
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	10	39.6
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	7	39.6
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	5	39.6
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	16	39.4
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	10	39.4
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	2	39.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	2	39.3
(1,84)	1:A:4:GLU:CA	1:A:4:GLU:CB	1:A:4:GLU:CG	1:A:4:GLU:CD	2	39.3
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	14	39.3
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	11	39.2
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	20	39.2
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	16	39.2
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	17	39.1
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	15	39.1
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	15	39.0
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	3	39.0
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	7	39.0
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	8	39.0
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	10	39.0
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	6	38.9
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	15	38.9
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	18	38.9
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	18	38.9
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	18	38.9
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	18	38.9
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	4	38.8
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	13	38.8
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	5	38.7
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	18	38.6
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	1	38.6
(1,54)	2:B:108:GLY:C	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:C	16	38.6
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	3	38.6
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	6	38.5
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	9	38.5
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	16	38.4
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	8	38.4
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	13	38.4
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	2	38.3
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	16	38.3
(1,1)	1:A:1:GLY:C	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:C	8	38.3
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	16	38.2
(1,78)	2:B:121:GLU:C	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:C	9	38.1
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	10	38.1
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	18	38.1
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	16	38.1
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	20	38.1
(1,23)	1:A:12:SER:C	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:C	11	38.1
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	9	38.1
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	9	38.1
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	9	38.1
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	16	37.9
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	7	37.9
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	7	37.9
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	1	37.9
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	1	37.9
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	1	37.9
(1,78)	2:B:121:GLU:C	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:C	11	37.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	10	37.8
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	7	37.8
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	4	37.7
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	18	37.6
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	8	37.6
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	9	37.6
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	20	37.6
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	18	37.6
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	5	37.6
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	16	37.5
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	1	37.5
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	15	37.5
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	1	37.4
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	5	37.3
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	15	37.3
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	16	37.3
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	11	37.1
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	3	37.0
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	4	37.0
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	12	37.0
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	7	36.9
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	7	36.9
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	7	36.9
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	14	36.9
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	2	36.8
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	17	36.8
(1,1)	1:A:1:GLY:C	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:C	12	36.8
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	8	36.7
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	19	36.7
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	19	36.7
(1,130)	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:CB	2:B:119:CYS:SG	19	36.7
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	3	36.6
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	15	36.6
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	14	36.5
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	19	36.5
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	18	36.5
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	1	36.5
(1,62)	2:B:112:VAL:C	2:B:113:GLU:N	2:B:113:GLU:CA	2:B:113:GLU:C	12	36.4
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	12	36.4
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	13	36.4
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	8	36.3
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	9	36.3
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	1	36.3
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	2	36.3
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	20	36.2
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	12	36.2
(1,74)	2:B:118:VAL:C	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:C	16	36.1
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	8	36.1
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	17	36.0
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	17	36.0
(1,98)	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:CB	1:A:15:GLN:CG	17	36.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	12	36.0
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	4	36.0
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	18	35.9
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	2	35.8
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	8	35.8
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	6	35.7
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	9	35.7
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	8	35.6
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	1	35.6
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	13	35.5
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	2	35.4
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	16	35.4
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	11	35.4
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	11	35.4
(1,114)	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	11	35.4
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	10	35.3
(1,78)	2:B:121:GLU:C	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:C	6	35.1
(1,78)	2:B:121:GLU:C	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:C	14	35.1
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	16	35.1
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	2	35.1
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	12	35.1
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	20	35.1
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	13	35.0
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	14	35.0
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	16	34.9
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	15	34.8
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	11	34.8
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	14	34.7
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	1	34.6
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	2	34.6
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	1	34.6
(1,60)	2:B:111:LEU:C	2:B:112:VAL:N	2:B:112:VAL:CA	2:B:112:VAL:C	14	34.6
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	20	34.6
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	14	34.6
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	17	34.6
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	17	34.5
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	20	34.4
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	16	34.4
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	9	34.4
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	3	34.4
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	13	34.3
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	10	34.3
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	17	34.2
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	4	34.2
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	2	34.2
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	6	34.2
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	4	34.1
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	3	34.1
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	1	34.0
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	20	33.9
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	1	33.9

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	20	33.9
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	14	33.8
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	1	33.8
(1,74)	2:B:118:VAL:C	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:C	12	33.7
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	3	33.7
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	15	33.7
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	2	33.7
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	11	33.6
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	6	33.5
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	9	33.5
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	2	33.5
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	7	33.3
(1,42)	2:B:101:PHE:C	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:C	7	33.2
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	19	33.2
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	1	33.2
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	20	33.2
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	8	33.1
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	1	33.1
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	12	33.1
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	15	33.1
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	19	33.1
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	15	33.0
(1,15)	1:A:8:THR:C	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:C	14	33.0
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	1	32.9
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	18	32.9
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	20	32.9
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	9	32.9
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	13	32.7
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	13	32.7
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	13	32.7
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	20	32.7
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	20	32.7
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	20	32.7
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	6	32.6
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	17	32.6
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	15	32.6
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	15	32.6
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	15	32.6
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	2	32.5
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	18	32.5
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	3	32.4
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	6	32.4
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	10	32.4
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	10	32.4
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	10	32.4
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	9	32.3
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	15	32.3
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	1	32.3
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	6	32.2
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	3	32.2
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	19	32.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	12	32.2
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	19	32.2
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	19	32.2
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	19	32.2
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	4	32.1
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	5	32.1
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	10	32.1
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	7	32.1
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	15	32.1
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	17	32.0
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	5	32.0
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	9	32.0
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	13	32.0
(1,64)	2:B:113:GLU:C	2:B:114:ALA:N	2:B:114:ALA:CA	2:B:114:ALA:C	5	31.9
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	3	31.9
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	4	31.8
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	17	31.8
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	15	31.8
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	13	31.8
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	13	31.7
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	18	31.7
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	18	31.7
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	18	31.7
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	5	31.6
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	15	31.6
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	14	31.6
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	12	31.6
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	12	31.6
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	20	31.6
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	4	31.6
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	4	31.6
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	4	31.6
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	16	31.6
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	16	31.6
(1,104)	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:CB	1:A:18:ASN:CG	16	31.6
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	10	31.5
(1,42)	2:B:101:PHE:C	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:C	11	31.5
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	10	31.4
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	9	31.3
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	9	31.3
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	9	31.3
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	12	31.3
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	14	31.3
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	14	31.3
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	19	31.1
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	1	31.1
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	19	31.1
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	17	31.1
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	8	31.1
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	12	31.1
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	4	31.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	16	31.0
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	18	31.0
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	15	30.9
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1	30.8
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1	30.8
(1,80)	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1	30.8
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	19	30.8
(1,132)	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	2:B:121:GLU:CD	8	30.8
(1,132)	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	2:B:121:GLU:CD	8	30.8
(1,132)	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	2:B:121:GLU:CD	8	30.8
(1,78)	2:B:121:GLU:C	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:C	16	30.7
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	2	30.7
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	7	30.4
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	8	30.4
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	4	30.2
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	11	30.2
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	16	30.2
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	16	30.2
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	16	30.2
(1,1)	1:A:1:GLY:C	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:C	7	30.2
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	6	30.1
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	2	30.1
(1,132)	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	2:B:121:GLU:CD	12	30.1
(1,132)	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	2:B:121:GLU:CD	12	30.1
(1,132)	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	2:B:121:GLU:CD	12	30.1
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	7	29.9
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	17	29.9
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	2	29.9
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	16	29.9
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	19	29.8
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	4	29.8
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	15	29.8
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	15	29.8
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	15	29.8
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	7	29.7
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	5	29.7
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	6	29.7
(1,132)	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	2:B:121:GLU:CD	17	29.7
(1,132)	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	2:B:121:GLU:CD	17	29.7
(1,132)	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	2:B:121:GLU:CD	17	29.7
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	2	29.6
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	2	29.6
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	2	29.6
(1,78)	2:B:121:GLU:C	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:C	17	29.6
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	8	29.6
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	3	29.6
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	17	29.6
(1,42)	2:B:101:PHE:C	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:C	19	29.6
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	13	29.5
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	9	29.5
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	7	29.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,68)	2:B:115:LEU:C	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:C	11	29.4
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	8	29.3
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	9	29.3
(1,78)	2:B:121:GLU:C	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:C	2	29.2
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	13	29.2
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	2	29.2
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	4	29.2
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	8	29.1
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	8	29.1
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	8	29.1
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	14	29.1
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	20	29.1
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	13	29.1
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	15	29.0
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	8	28.9
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	2	28.9
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	14	28.9
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	6	28.9
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	11	28.8
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	14	28.8
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	9	28.7
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	9	28.7
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	9	28.7
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	3	28.7
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	15	28.7
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	14	28.6
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	9	28.6
(1,42)	2:B:101:PHE:C	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:C	3	28.6
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	10	28.5
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	7	28.5
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	5	28.4
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	11	28.3
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	20	28.3
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	11	28.2
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	12	28.1
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	3	28.1
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	20	28.1
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	7	28.1
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	14	28.1
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	14	28.1
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	14	28.1
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	20	28.0
(1,25)	1:A:13:LEU:C	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:C	5	28.0
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	7	27.9
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	11	27.8
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	5	27.8
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	2	27.7
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	14	27.6
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	14	27.6
(1,87)	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:CB	1:A:6:CYS:SG	14	27.6
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	18	27.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	14	27.6
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	12	27.6
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	18	27.6
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	18	27.6
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	18	27.6
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	9	27.3
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	11	27.3
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	16	27.3
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	16	27.2
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	4	27.1
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	11	26.9
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	9	26.9
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	16	26.9
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	7	26.7
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	8	26.5
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	14	26.5
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	5	26.5
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	20	26.4
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	4	26.4
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	9	26.4
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	12	26.3
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	10	26.3
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	5	26.3
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	5	26.3
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	5	26.3
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	20	26.2
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	6	26.2
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	6	26.2
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	6	26.2
(1,1)	1:A:1:GLY:C	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:C	4	26.2
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	8	26.1
(1,3)	1:A:2:ILE:C	1:A:3:VAL:N	1:A:3:VAL:CA	1:A:3:VAL:C	17	26.1
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	12	25.9
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	2	25.9
(1,13)	1:A:7:CYS:C	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:C	13	25.9
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	18	25.8
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	8	25.8
(1,42)	2:B:101:PHE:C	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:C	18	25.5
(1,66)	2:B:114:ALA:C	2:B:115:LEU:N	2:B:115:LEU:CA	2:B:115:LEU:C	19	25.4
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	6	25.4
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	10	25.4
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	19	25.4
(1,13)	1:A:7:CYS:C	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:C	11	25.4
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	7	25.3
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	19	25.3
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	11	25.2
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	15	25.2
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	5	25.0
(1,48)	2:B:104:GLN:C	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:C	18	25.0
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	1	24.9
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	7	24.9

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	7	24.9
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	7	24.9
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	5	24.8
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	11	24.8
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	11	24.8
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	11	24.8
(1,58)	2:B:110:HIS:C	2:B:111:LEU:N	2:B:111:LEU:CA	2:B:111:LEU:C	18	24.7
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	20	24.7
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	20	24.7
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	20	24.7
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	12	24.6
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	12	24.6
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	12	24.6
(1,48)	2:B:104:GLN:C	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:C	2	24.5
(1,48)	2:B:104:GLN:C	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:C	5	24.5
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	1	24.4
(1,56)	2:B:109:SER:C	2:B:110:HIS:N	2:B:110:HIS:CA	2:B:110:HIS:C	15	24.1
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	18	24.1
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	17	24.1
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	17	24.1
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	17	24.1
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	16	23.9
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	5	23.9
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	7	23.9
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	4	23.8
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	2	23.6
(1,48)	2:B:104:GLN:C	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:C	8	23.6
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	16	23.6
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	3	23.4
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	9	23.3
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	9	23.3
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	9	23.3
(1,78)	2:B:121:GLU:C	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:C	19	22.9
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	11	22.9
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	3	22.9
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	3	22.9
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	3	22.9
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	12	22.7
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	12	22.7
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	12	22.7
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	6	22.6
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	3	22.4
(1,13)	1:A:7:CYS:C	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:C	19	22.3
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	12	22.2
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	13	22.2
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	13	22.2
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	13	22.2
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	8	22.0
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	12	21.9
(1,13)	1:A:7:CYS:C	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:C	2	21.9
(1,5)	1:A:3:VAL:C	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	13	21.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,48)	2:B:104:GLN:C	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:C	11	21.8
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	7	21.8
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	7	21.7
(1,48)	2:B:104:GLN:C	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:C	3	21.7
(1,42)	2:B:101:PHE:C	2:B:102:VAL:N	2:B:102:VAL:CA	2:B:102:VAL:C	12	21.7
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	16	21.5
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	14	21.3
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	17	21.3
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	7	21.1
(1,1)	1:A:1:GLY:C	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:C	13	21.1
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	8	21.0
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	8	21.0
(1,126)	2:B:116:TYR:N	2:B:116:TYR:CA	2:B:116:TYR:CB	2:B:116:TYR:CG	8	21.0
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	17	20.9
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	16	20.5
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	16	20.5
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	16	20.5
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	10	20.5
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	12	20.4
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	17	20.4
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	8	20.0
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	10	19.9
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	1	19.5
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	8	19.4
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	8	19.4
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	8	19.4
(1,78)	2:B:121:GLU:C	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:C	5	19.3
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	19	19.2
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	5	18.9
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	12	18.7
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	12	18.7
(1,93)	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:CB	1:A:11:CYS:SG	12	18.7
(1,78)	2:B:121:GLU:C	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:C	12	18.5
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	20	18.5
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	18	18.4
(1,29)	1:A:15:GLN:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	3	18.3
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	3	18.2
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	1	18.2
(1,48)	2:B:104:GLN:C	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:C	1	17.9
(1,74)	2:B:118:VAL:C	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:C	1	17.8
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	2	17.8
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	14	17.7
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	14	17.7
(1,127)	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:CB	2:B:117:LEU:CG	14	17.7
(1,48)	2:B:104:GLN:C	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:C	13	17.5
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	14	17.0
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	2	16.8
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	2	16.8
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	2	16.8
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	10	16.6
(1,76)	2:B:120:GLY:C	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:C	13	16.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	17	16.3
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	15	16.2
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	15	16.2
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	15	16.2
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	12	16.0
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	11	15.9
(1,15)	1:A:8:THR:C	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:C	16	15.7
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	13	15.6
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	13	15.6
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	13	15.6
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	10	15.5
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	19	15.2
(1,13)	1:A:7:CYS:C	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:C	7	15.0
(1,74)	2:B:118:VAL:C	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:C	15	14.9
(1,21)	1:A:11:CYS:C	1:A:12:SER:N	1:A:12:SER:CA	1:A:12:SER:C	11	14.9
(1,13)	1:A:7:CYS:C	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:C	10	14.8
(1,78)	2:B:121:GLU:C	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:C	1	14.7
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	3	14.6
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	20	14.6
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	10	14.5
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	19	14.3
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	12	14.2
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	12	14.2
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	12	14.2
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	4	14.2
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	4	14.2
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	4	14.2
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	8	14.1
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	5	14.0
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	14	13.9
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	15	13.8
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	15	13.8
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	15	13.8
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	5	13.7
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	3	13.6
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	3	13.6
(1,102)	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:CB	1:A:17:GLU:CG	3	13.6
(1,48)	2:B:104:GLN:C	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:C	10	13.5
(1,35)	1:A:18:ASN:C	1:A:19:TYR:N	1:A:19:TYR:CA	1:A:19:TYR:C	3	13.5
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	7	13.4
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	4	13.4
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	12	13.4
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	12	13.4
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	12	13.4
(1,13)	1:A:7:CYS:C	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:C	8	13.3
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	8	13.2
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	15	12.9
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	8	12.7
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	17	12.6
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	10	12.4
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	14	12.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	2	12.1
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	13	12.1
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	14	12.0
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	14	12.0
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	14	12.0
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1	12.0
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	20	12.0
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	8	11.9
(1,74)	2:B:118:VAL:C	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:C	4	11.7
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	16	11.7
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	18	11.6
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	18	11.6
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	18	11.6
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	6	11.6
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	6	11.6
(1,90)	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:CB	1:A:9:SER:OG	6	11.6
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	11	11.6
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	4	11.4
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	20	11.3
(1,13)	1:A:7:CYS:C	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:C	1	11.1
(1,1)	1:A:1:GLY:C	1:A:2:ILE:N	1:A:2:ILE:CA	1:A:2:ILE:C	5	10.9
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	1	10.8
(1,74)	2:B:118:VAL:C	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:C	19	10.7
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	14	10.6
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	14	10.6
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	14	10.6
(1,74)	2:B:118:VAL:C	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:C	18	10.6
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	9	10.6
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	2	10.4
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	2	10.4
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	2	10.4
(1,44)	2:B:102:VAL:C	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	18	10.4
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	18	10.2
(1,48)	2:B:104:GLN:C	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:C	19	10.0
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	9	9.9
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	5	9.8
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	5	9.8
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	5	9.8
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	7	9.6
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	3	9.5
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	3	9.5
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	3	9.5
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	2	9.4
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	2	9.4
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	2	9.4
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	3	9.4
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	19	9.4
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	13	9.3
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	13	9.3
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	13	9.3
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	10	9.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	10	9.3
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	10	9.3
(1,13)	1:A:7:CYS:C	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:C	12	9.3
(1,46)	2:B:103:ASN:C	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:C	7	9.2
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	5	9.2
(1,9)	1:A:5:GLN:C	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:C	2	8.8
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	5	8.7
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	5	8.7
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	5	8.7
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	8	8.7
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	8	8.7
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	8	8.7
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	3	8.7
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	20	8.5
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	20	8.5
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	20	8.5
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	5	8.4
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	5	8.4
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	5	8.4
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	14	8.3
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	14	8.3
(1,95)	1:A:13:LEU:N	1:A:13:LEU:CA	1:A:13:LEU:CB	1:A:13:LEU:CG	14	8.3
(1,48)	2:B:104:GLN:C	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:C	17	8.2
(1,74)	2:B:118:VAL:C	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:C	2	7.9
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	9	7.7
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	9	7.7
(1,117)	2:B:109:SER:N	2:B:109:SER:CA	2:B:109:SER:CB	2:B:109:SER:OG	9	7.7
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	20	7.6
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	20	7.6
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	20	7.6
(1,72)	2:B:117:LEU:C	2:B:118:VAL:N	2:B:118:VAL:CA	2:B:118:VAL:C	6	7.6
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	4	7.5
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	13	7.4
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	13	7.4
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	13	7.4
(1,108)	2:B:101:PHE:N	2:B:101:PHE:CA	2:B:101:PHE:CB	2:B:101:PHE:CG	10	7.4
(1,108)	2:B:101:PHE:N	2:B:101:PHE:CA	2:B:101:PHE:CB	2:B:101:PHE:CG	10	7.4
(1,108)	2:B:101:PHE:N	2:B:101:PHE:CA	2:B:101:PHE:CB	2:B:101:PHE:CG	10	7.4
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	4	7.1
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	4	7.1
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	4	7.1
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	20	7.0
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	20	7.0
(1,113)	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:CB	2:B:105:HIS:CG	20	7.0
(1,9)	1:A:5:GLN:C	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:C	3	6.9
(1,13)	1:A:7:CYS:C	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:C	20	6.6
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	17	6.5
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	17	6.5
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	17	6.5
(1,74)	2:B:118:VAL:C	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:C	3	6.5
(1,74)	2:B:118:VAL:C	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:C	7	6.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,15)	1:A:8:THR:C	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:C	9	6.5
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	1	6.5
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	1	6.5
(1,134)	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	2:B:122:ARG:CD	1	6.5
(1,48)	2:B:104:GLN:C	2:B:105:HIS:N	2:B:105:HIS:CA	2:B:105:HIS:C	20	6.4
(1,37)	1:A:19:TYR:C	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:C	13	6.4
(1,17)	1:A:9:SER:C	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:C	6	6.4
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	14	6.3
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	20	6.0
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	20	6.0
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	20	6.0
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	9	5.9
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	9	5.9
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	9	5.9
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	6	5.5
(1,19)	1:A:10:ILE:C	1:A:11:CYS:N	1:A:11:CYS:CA	1:A:11:CYS:C	2	5.5
(1,13)	1:A:7:CYS:C	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:C	5	5.5
(1,13)	1:A:7:CYS:C	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:C	6	5.5
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	8	5.2
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	8	5.2
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	8	5.2
(1,78)	2:B:121:GLU:C	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:C	4	5.1
(1,70)	2:B:116:TYR:C	2:B:117:LEU:N	2:B:117:LEU:CA	2:B:117:LEU:C	11	5.1
(1,15)	1:A:8:THR:C	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:C	17	5.1
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	15	5.1
(1,74)	2:B:118:VAL:C	2:B:119:CYS:N	2:B:119:CYS:CA	2:B:119:CYS:C	17	4.9
(1,15)	1:A:8:THR:C	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:C	15	4.9
(1,15)	1:A:8:THR:C	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:C	5	4.8
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	18	4.4
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	18	4.4
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	18	4.4
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	17	4.4
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	17	4.4
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	17	4.4
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	6	4.4
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	11	4.4
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	11	4.4
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	11	4.4
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	2	4.2
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	2	4.2
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	2	4.2
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	9	4.1
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	9	4.1
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	9	4.1
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	6	3.9
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	6	3.9
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	6	3.9
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	4	3.9
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	4	3.9
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	4	3.9
(1,78)	2:B:121:GLU:C	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:C	10	3.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,40)	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	1:A:22:GLY:N	20	3.7
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	13	3.7
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	13	3.7
(1,120)	2:B:111:LEU:CA	2:B:111:LEU:CB	2:B:111:LEU:CG	2:B:111:LEU:CD1	13	3.7
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	9	3.6
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	9	3.6
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	9	3.6
(1,9)	1:A:5:GLN:C	1:A:6:CYS:N	1:A:6:CYS:CA	1:A:6:CYS:C	8	3.5
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	4	3.4
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	4	3.4
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	4	3.4
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	11	3.4
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	11	3.4
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	11	3.4
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	17	3.4
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	5	3.1
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	5	3.1
(1,97)	1:A:14:TYR:N	1:A:14:TYR:CA	1:A:14:TYR:CB	1:A:14:TYR:CG	5	3.1
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	6	3.1
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	6	3.1
(1,106)	1:A:20:CYS:N	1:A:20:CYS:CA	1:A:20:CYS:CB	1:A:20:CYS:SG	6	3.1
(1,39)	1:A:20:CYS:C	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	15	3.0
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	9	3.0
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	9	3.0
(1,131)	2:B:121:GLU:N	2:B:121:GLU:CA	2:B:121:GLU:CB	2:B:121:GLU:CG	9	3.0
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	9	2.9
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	9	2.9
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	9	2.9
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	9	2.9
(1,33)	1:A:17:GLU:C	1:A:18:ASN:N	1:A:18:ASN:CA	1:A:18:ASN:C	11	2.8
(1,31)	1:A:16:LEU:C	1:A:17:GLU:N	1:A:17:GLU:CA	1:A:17:GLU:C	17	2.8
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	17	2.7
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	17	2.7
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	17	2.7
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	12	2.6
(1,92)	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	1:A:10:ILE:CD1	16	2.5
(1,92)	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	1:A:10:ILE:CD1	16	2.5
(1,92)	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	1:A:10:ILE:CD1	16	2.5
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	16	2.4
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	16	2.4
(1,133)	2:B:122:ARG:N	2:B:122:ARG:CA	2:B:122:ARG:CB	2:B:122:ARG:CG	16	2.4
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	13	2.4
(1,27)	1:A:14:TYR:C	1:A:15:GLN:N	1:A:15:GLN:CA	1:A:15:GLN:C	9	2.3
(1,15)	1:A:8:THR:C	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:C	18	2.3
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	12	2.2
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	12	2.2
(1,91)	1:A:10:ILE:N	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	12	2.2
(1,7)	1:A:4:GLU:C	1:A:5:GLN:N	1:A:5:GLN:CA	1:A:5:GLN:C	10	2.2
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	6	2.1
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	6	2.1
(1,112)	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	2:B:104:GLN:CD	6	2.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,11)	1:A:6:CYS:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	17	2.1
(1,108)	2:B:101:PHE:N	2:B:101:PHE:CA	2:B:101:PHE:CB	2:B:101:PHE:CG	5	2.1
(1,108)	2:B:101:PHE:N	2:B:101:PHE:CA	2:B:101:PHE:CB	2:B:101:PHE:CG	5	2.1
(1,108)	2:B:101:PHE:N	2:B:101:PHE:CA	2:B:101:PHE:CB	2:B:101:PHE:CG	5	2.1
(1,50)	2:B:105:HIS:C	2:B:106:LEU:N	2:B:106:LEU:CA	2:B:106:LEU:C	11	2.0
(1,45)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:C	2:B:104:GLN:N	2	2.0
(1,92)	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	1:A:10:ILE:CD1	15	1.9
(1,92)	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	1:A:10:ILE:CD1	15	1.9
(1,92)	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	1:A:10:ILE:CD1	15	1.9
(1,92)	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	1:A:10:ILE:CD1	20	1.9
(1,92)	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	1:A:10:ILE:CD1	20	1.9
(1,92)	1:A:10:ILE:CA	1:A:10:ILE:CB	1:A:10:ILE:CG1	1:A:10:ILE:CD1	20	1.9
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	17	1.9
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	17	1.9
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	17	1.9
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	7	1.9
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	7	1.9
(1,110)	2:B:103:ASN:N	2:B:103:ASN:CA	2:B:103:ASN:CB	2:B:103:ASN:CG	7	1.9
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	20	1.7
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	20	1.7
(1,86)	1:A:5:GLN:CA	1:A:5:GLN:CB	1:A:5:GLN:CG	1:A:5:GLN:CD	20	1.7
(1,15)	1:A:8:THR:C	1:A:9:SER:N	1:A:9:SER:CA	1:A:9:SER:C	4	1.6
(1,115)	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	2:B:106:LEU:CD1	11	1.6
(1,115)	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	2:B:106:LEU:CD1	11	1.6
(1,115)	2:B:106:LEU:CA	2:B:106:LEU:CB	2:B:106:LEU:CG	2:B:106:LEU:CD1	11	1.6
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	1	1.5
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	1	1.5
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	1	1.5
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	11	1.4
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	11	1.4
(1,89)	1:A:8:THR:N	1:A:8:THR:CA	1:A:8:THR:CB	1:A:8:THR:OG1	11	1.4
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	19	1.4
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	19	1.4
(1,81)	1:A:2:ILE:CA	1:A:2:ILE:CB	1:A:2:ILE:CG1	1:A:2:ILE:CD1	19	1.4
(1,40)	1:A:21:ASN:N	1:A:21:ASN:CA	1:A:21:ASN:C	1:A:22:GLY:N	7	1.4
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	1	1.3
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	1	1.3
(1,111)	2:B:104:GLN:N	2:B:104:GLN:CA	2:B:104:GLN:CB	2:B:104:GLN:CG	1	1.3