



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 06:18 AM UTC

PDB ID : 2LRI / pdb_00002lri
BMRB ID : 18374
Title : NMR structure of the second PHD finger of AIRE (AIRE-PHD2)
Authors : Gaetani, M.; Chignola, F.; Mollica, L.; Quilici, G.; Mannella, V.; Spiliotopoulos, D.; Musco, G.
Deposited on : 2012-04-03

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 ⓘ symbol.

The types of validation reports are described at

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

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

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

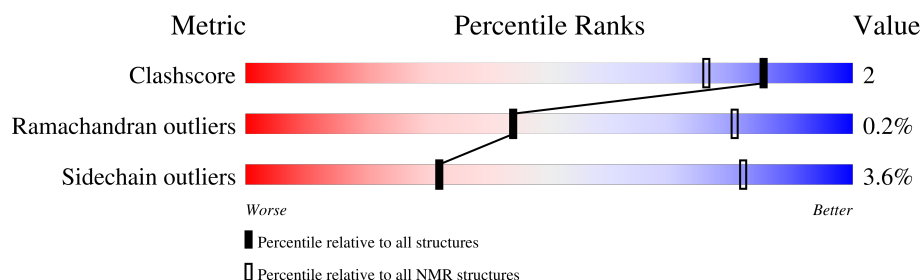
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	C	66	

2 Ensemble composition and analysis

This entry contains 50 models. Model 23 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	C:14-C:58 (45)	0.81	23

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 5 clusters and 1 single-model cluster was found.

Cluster number	Models
1	3, 5, 7, 8, 9, 11, 14, 15, 16, 18, 23, 25, 26, 27, 33, 35, 36, 37, 39, 40, 42, 43, 44, 45, 47, 48, 49, 50
2	1, 4, 20, 24, 28, 32, 34, 46
3	13, 19, 22, 29, 41
4	2, 10, 31, 38
5	6, 12, 17, 21
Single-model clusters	30

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 911 atoms, of which 438 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Autoimmune regulator.

Mol	Chain	Residues	Atoms						Trace
1	C	66	Total	C	H	N	O	S	0
			909	281	438	94	88	8	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	GLY	-	expression tag	UNP O43918
C	2	ALA	-	expression tag	UNP O43918
C	3	MET	-	expression tag	UNP O43918

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

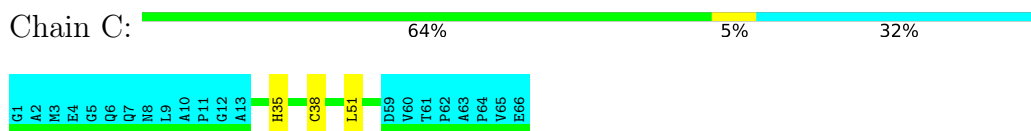
Mol	Chain	Residues	Atoms	
2	C	2	Total	Zn
			2	2

4 Residue-property plots [i](#)

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: Autoimmune regulator

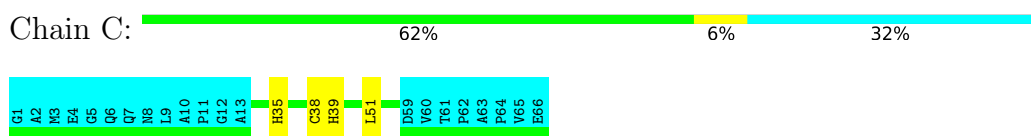


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

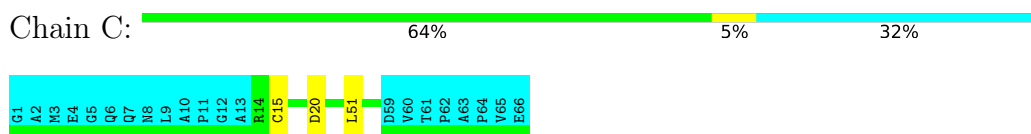
4.2.1 Score per residue for model 1

- Molecule 1: Autoimmune regulator



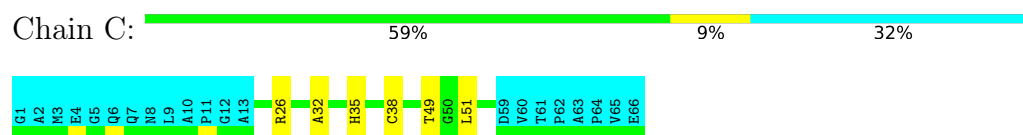
4.2.2 Score per residue for model 2

- Molecule 1: Autoimmune regulator



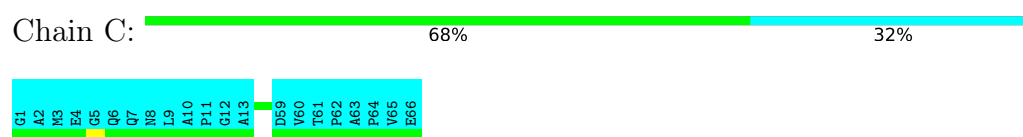
4.2.3 Score per residue for model 3

- Molecule 1: Autoimmune regulator



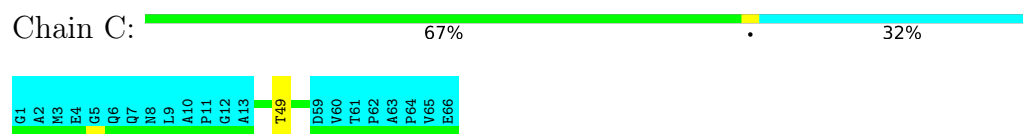
4.2.4 Score per residue for model 4

- Molecule 1: Autoimmune regulator



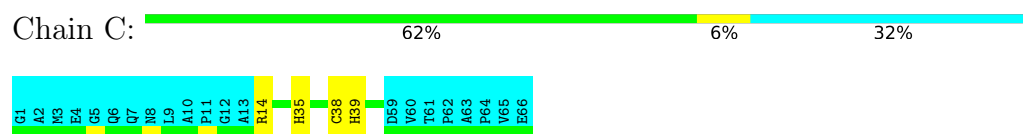
4.2.5 Score per residue for model 5

- Molecule 1: Autoimmune regulator



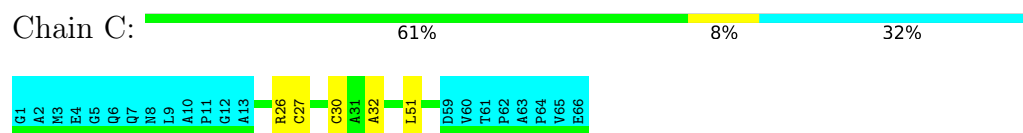
4.2.6 Score per residue for model 6

- Molecule 1: Autoimmune regulator



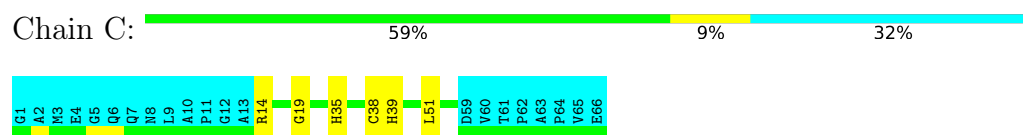
4.2.7 Score per residue for model 7

- Molecule 1: Autoimmune regulator



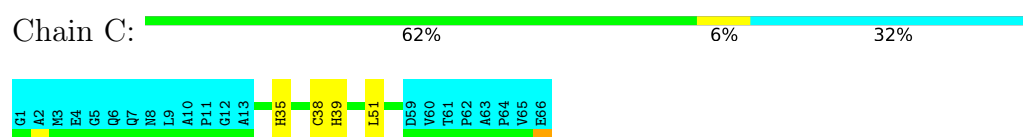
4.2.8 Score per residue for model 8

- Molecule 1: Autoimmune regulator



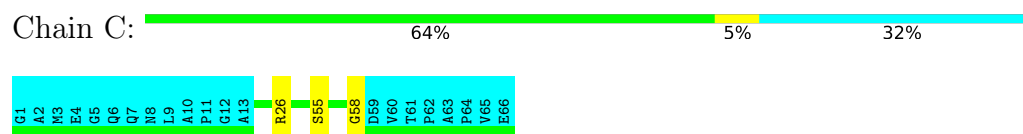
4.2.9 Score per residue for model 9

- Molecule 1: Autoimmune regulator



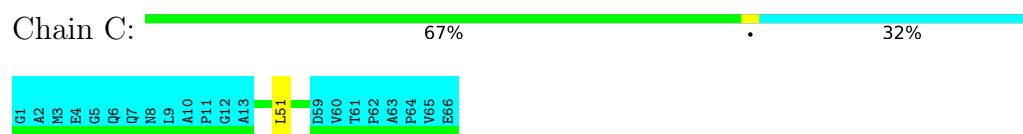
4.2.10 Score per residue for model 10

- Molecule 1: Autoimmune regulator



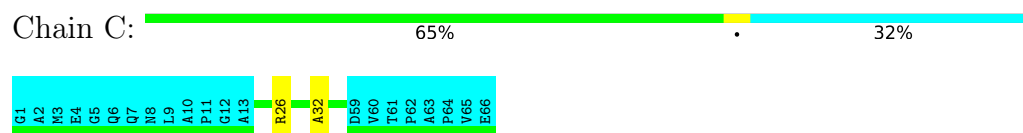
4.2.11 Score per residue for model 11

- Molecule 1: Autoimmune regulator



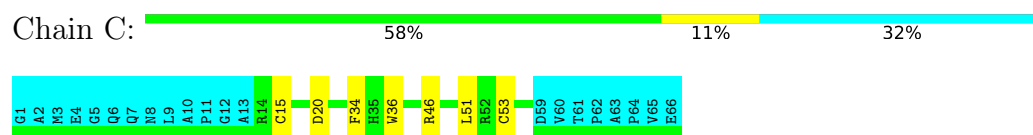
4.2.12 Score per residue for model 12

- Molecule 1: Autoimmune regulator



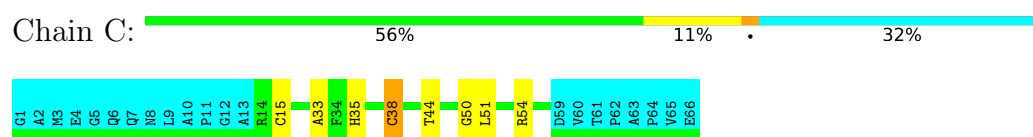
4.2.13 Score per residue for model 13

- Molecule 1: Autoimmune regulator



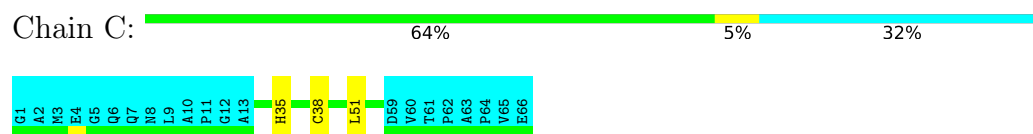
4.2.14 Score per residue for model 14

- Molecule 1: Autoimmune regulator



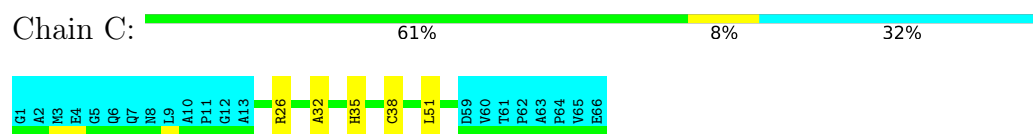
4.2.15 Score per residue for model 15

- Molecule 1: Autoimmune regulator



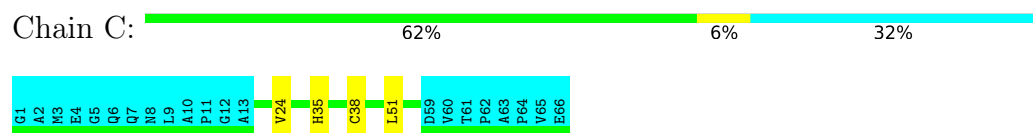
4.2.16 Score per residue for model 16

- Molecule 1: Autoimmune regulator



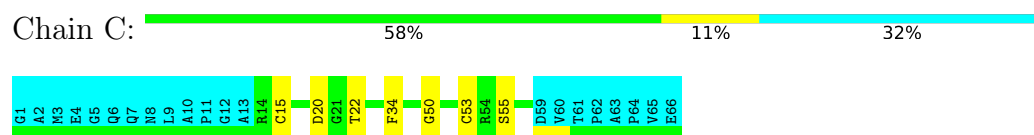
4.2.17 Score per residue for model 17

- Molecule 1: Autoimmune regulator



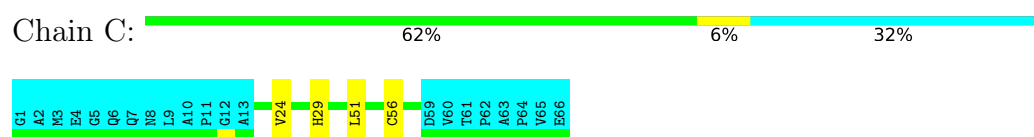
4.2.18 Score per residue for model 18

- Molecule 1: Autoimmune regulator



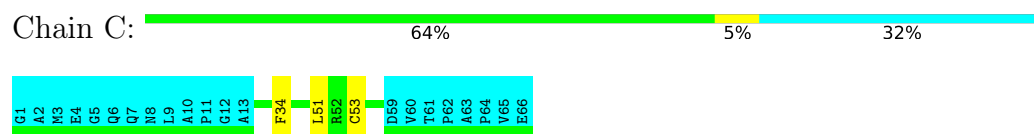
4.2.19 Score per residue for model 19

- Molecule 1: Autoimmune regulator



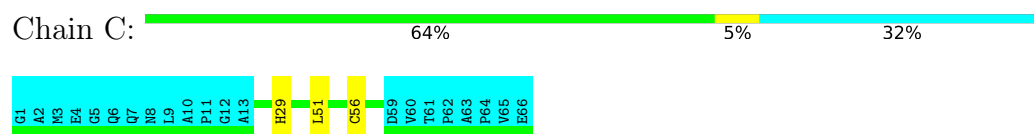
4.2.20 Score per residue for model 20

- Molecule 1: Autoimmune regulator



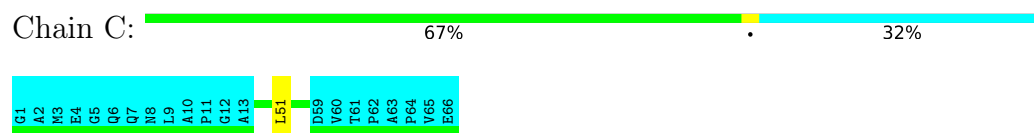
4.2.21 Score per residue for model 21

- Molecule 1: Autoimmune regulator



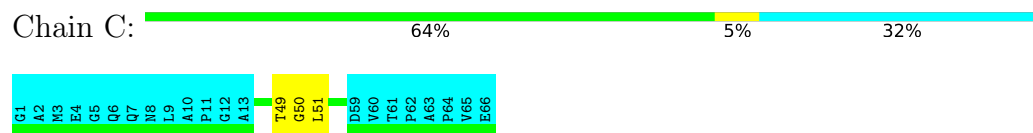
4.2.22 Score per residue for model 22

- Molecule 1: Autoimmune regulator



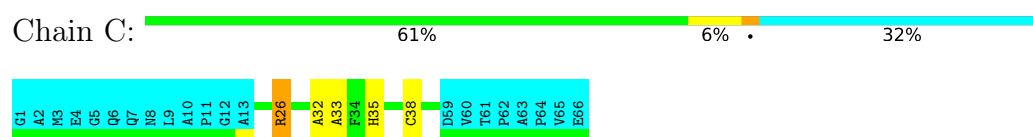
4.2.23 Score per residue for model 23 (medoid)

- Molecule 1: Autoimmune regulator



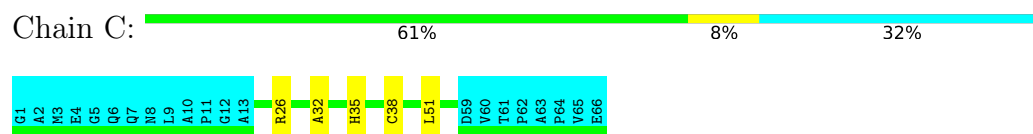
4.2.24 Score per residue for model 24

- Molecule 1: Autoimmune regulator



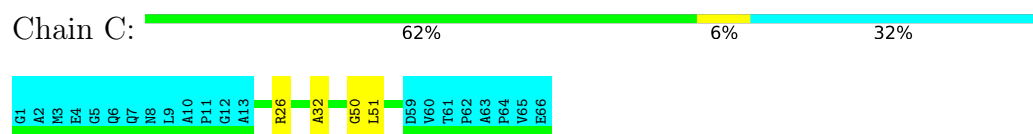
4.2.25 Score per residue for model 25

- Molecule 1: Autoimmune regulator



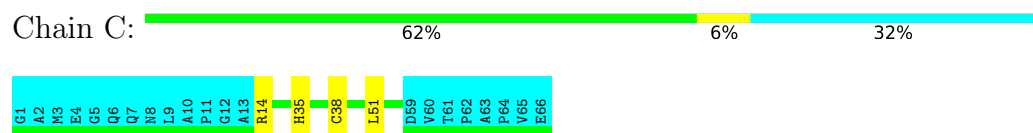
4.2.26 Score per residue for model 26

- Molecule 1: Autoimmune regulator



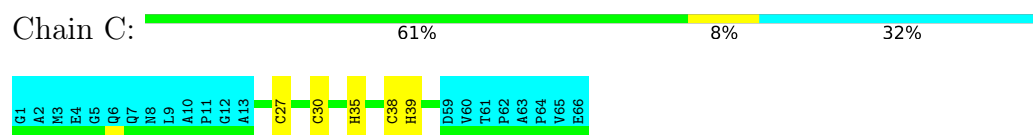
4.2.27 Score per residue for model 27

- Molecule 1: Autoimmune regulator



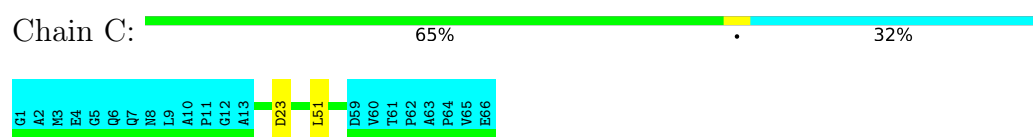
4.2.28 Score per residue for model 28

- Molecule 1: Autoimmune regulator



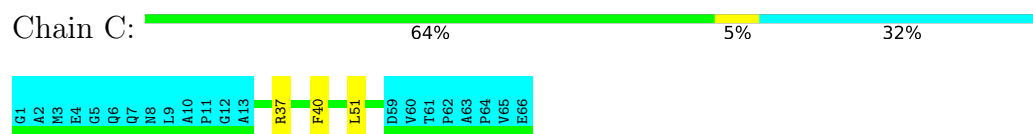
4.2.29 Score per residue for model 29

- Molecule 1: Autoimmune regulator



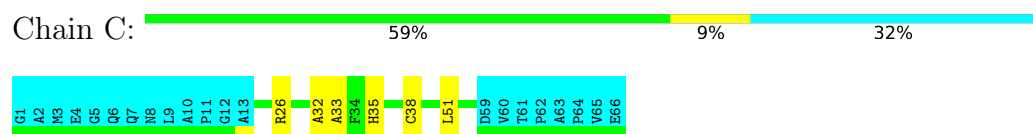
4.2.30 Score per residue for model 30

- Molecule 1: Autoimmune regulator



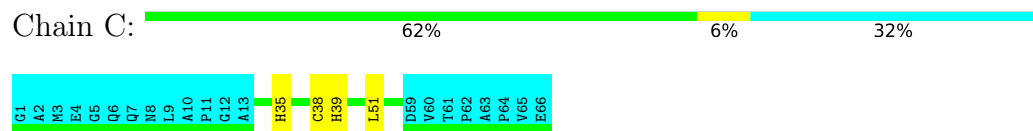
4.2.31 Score per residue for model 31

- Molecule 1: Autoimmune regulator



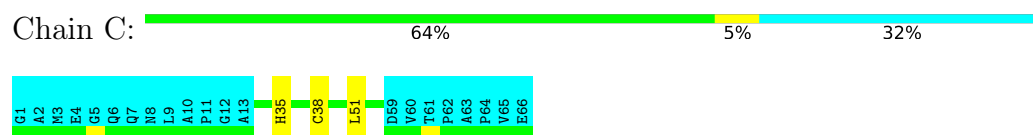
4.2.32 Score per residue for model 32

- Molecule 1: Autoimmune regulator



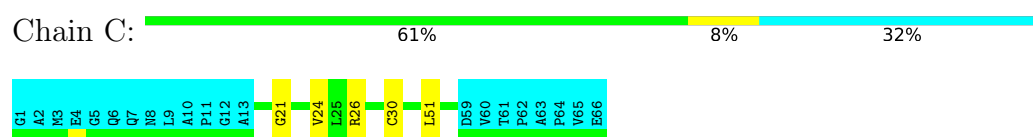
4.2.33 Score per residue for model 33

- Molecule 1: Autoimmune regulator



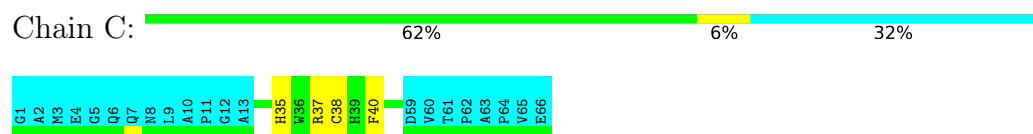
4.2.34 Score per residue for model 34

- Molecule 1: Autoimmune regulator



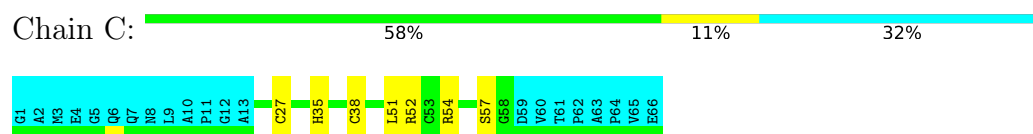
4.2.35 Score per residue for model 35

- Molecule 1: Autoimmune regulator



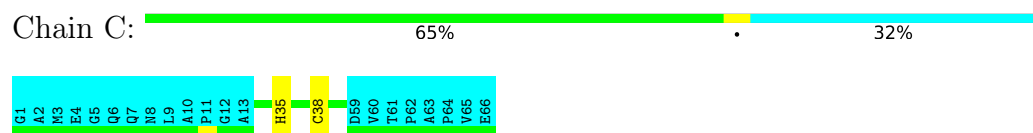
4.2.36 Score per residue for model 36

- Molecule 1: Autoimmune regulator



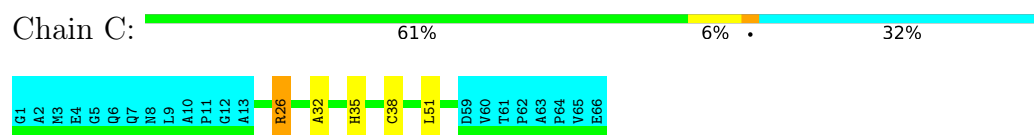
4.2.37 Score per residue for model 37

- Molecule 1: Autoimmune regulator



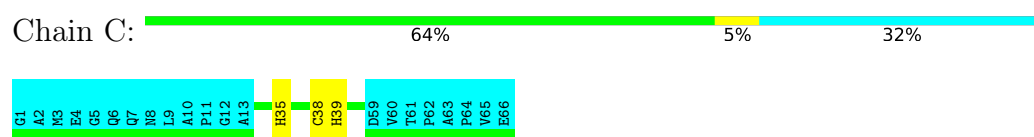
4.2.38 Score per residue for model 38

- Molecule 1: Autoimmune regulator



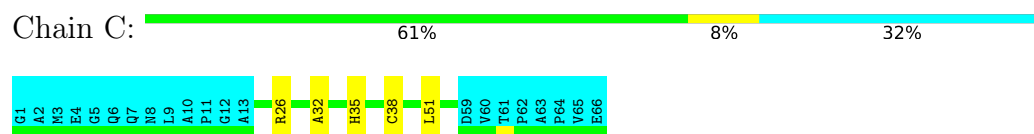
4.2.39 Score per residue for model 39

- Molecule 1: Autoimmune regulator



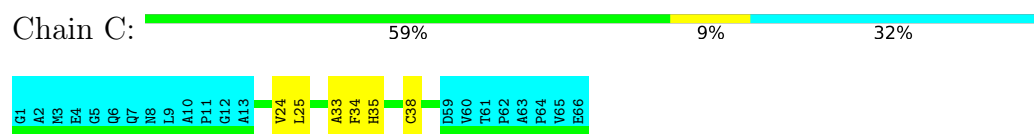
4.2.40 Score per residue for model 40

- Molecule 1: Autoimmune regulator



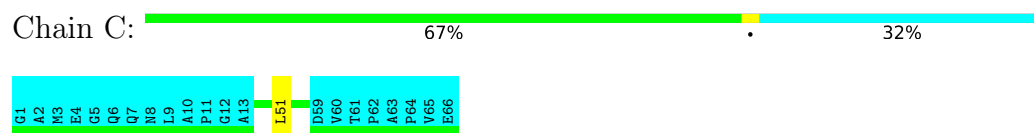
4.2.41 Score per residue for model 41

- Molecule 1: Autoimmune regulator



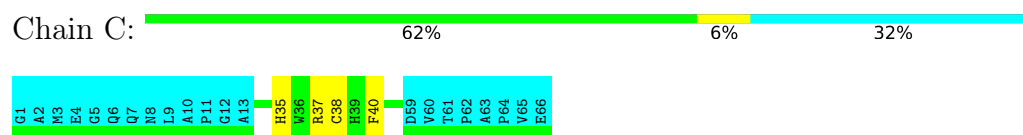
4.2.42 Score per residue for model 42

- Molecule 1: Autoimmune regulator



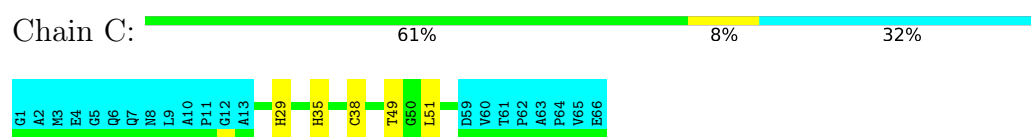
4.2.43 Score per residue for model 43

- Molecule 1: Autoimmune regulator



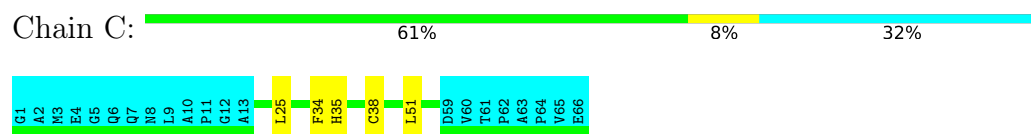
4.2.44 Score per residue for model 44

- Molecule 1: Autoimmune regulator



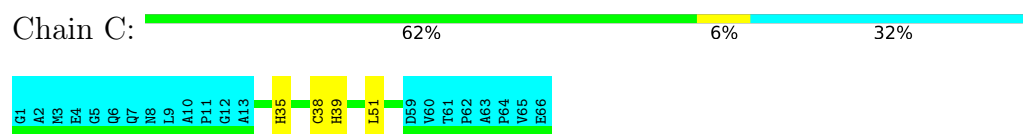
4.2.45 Score per residue for model 45

- Molecule 1: Autoimmune regulator



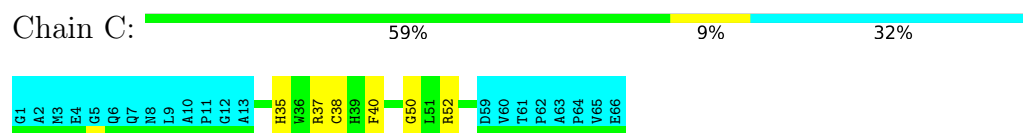
4.2.46 Score per residue for model 46

- Molecule 1: Autoimmune regulator



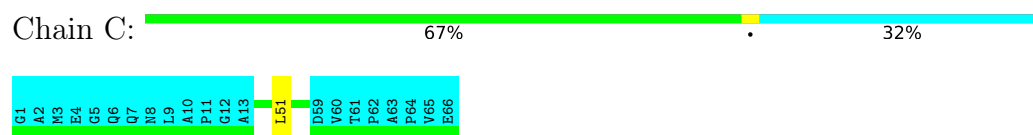
4.2.47 Score per residue for model 47

- Molecule 1: Autoimmune regulator



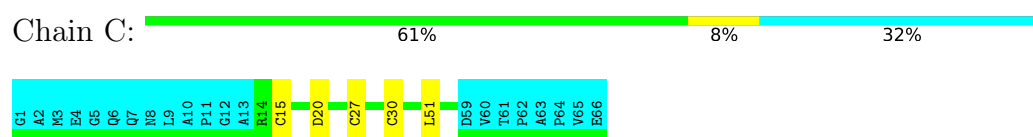
4.2.48 Score per residue for model 48

- Molecule 1: Autoimmune regulator



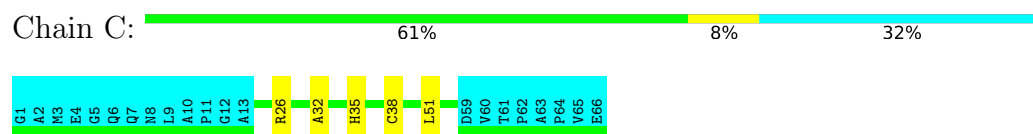
4.2.49 Score per residue for model 49

- Molecule 1: Autoimmune regulator



4.2.50 Score per residue for model 50

- Molecule 1: Autoimmune regulator



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 50 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure solution	2.3
ARIA	refinement	2.3

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	635
Number of shifts mapped to atoms	635
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	C	328	303	301	1±1
All	All	16500	15150	15050	68

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:35:HIS:HB2	1:C:38:CYS:SG	0.79	2.18	43	29
1:C:26:ARG:HA	1:C:32:ALA:O	0.57	1.99	31	10
1:C:14:ARG:HD3	1:C:19:GLY:O	0.54	2.02	8	1
1:C:29:HIS:HD2	1:C:56:CYS:SG	0.52	2.27	19	1
1:C:37:ARG:HA	1:C:40:PHE:O	0.49	2.08	30	4
1:C:36:TRP:CD1	1:C:46:ARG:HG2	0.47	2.44	13	1
1:C:29:HIS:HB2	1:C:56:CYS:SG	0.47	2.50	21	1
1:C:54:ARG:HA	1:C:57:SER:OG	0.46	2.11	36	1
1:C:27:CYS:HB3	1:C:30:CYS:O	0.46	2.11	28	3
1:C:26:ARG:HD2	1:C:32:ALA:O	0.45	2.11	16	1
1:C:27:CYS:SG	1:C:52:ARG:HA	0.44	2.52	36	1
1:C:15:CYS:HB3	1:C:20:ASP:O	0.44	2.13	49	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:55:SER:HA	1:C:58:GLY:O	0.44	2.13	10	1
1:C:25:LEU:HB2	1:C:34:PHE:O	0.43	2.12	41	2
1:C:20:ASP:OD2	1:C:22:THR:HG22	0.43	2.13	18	1
1:C:50:GLY:O	1:C:52:ARG:HG3	0.43	2.14	47	1
1:C:15:CYS:HA	1:C:33:ALA:O	0.42	2.13	14	1
1:C:34:PHE:CZ	1:C:53:CYS:HA	0.42	2.50	20	3
1:C:24:VAL:HG11	1:C:33:ALA:HB1	0.41	1.92	41	1
1:C:21:GLY:O	1:C:24:VAL:HB	0.40	2.16	34	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	45/66 (68%)	43±1 (95±3%)	2±1 (5±3%)	0±0 (0±1%)	44	80
All	All	2250/3300 (68%)	2140 (95%)	106 (5%)	4 (0%)	44	80

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	C	50	GLY	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	C	34/48 (71%)	33±1 (96±2%)	1±1 (4±2%)	32	82
All	All	1700/2400 (71%)	1638 (96%)	62 (4%)	32	82

All 12 unique residues with a non-rotameric sidechain are listed below. They are sorted by the

frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	51	LEU	36
1	C	39	HIS	8
1	C	49	THR	4
1	C	26	ARG	4
1	C	14	ARG	2
1	C	24	VAL	2
1	C	38	CYS	1
1	C	44	THR	1
1	C	54	ARG	1
1	C	23	ASP	1
1	C	30	CYS	1
1	C	29	HIS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 80% for the well-defined parts and 80% 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	635
Number of shifts mapped to atoms	635
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 $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	66	-0.26 ± 0.35	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	56	0.30 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	60	-0.80 ± 0.33	Should be applied

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 80%, i.e. 441 atoms were assigned a chemical shift out of a possible 551. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	183/228 (80%)	95/95 (100%)	45/90 (50%)	43/43 (100%)
Sidechain	212/268 (79%)	144/174 (83%)	68/76 (89%)	0/18 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	46/55 (84%)	23/28 (82%)	21/21 (100%)	2/6 (33%)
Overall	441/551 (80%)	262/297 (88%)	134/187 (72%)	45/67 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 635 atoms were assigned a chemical shift out of a possible 790. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	259/330 (78%)	133/137 (97%)	66/132 (50%)	60/61 (98%)
Sidechain	330/405 (81%)	225/264 (85%)	105/120 (88%)	0/21 (0%)
Aromatic	46/55 (84%)	23/28 (82%)	21/21 (100%)	2/6 (33%)
Overall	635/790 (80%)	381/429 (89%)	192/273 (70%)	62/88 (70%)

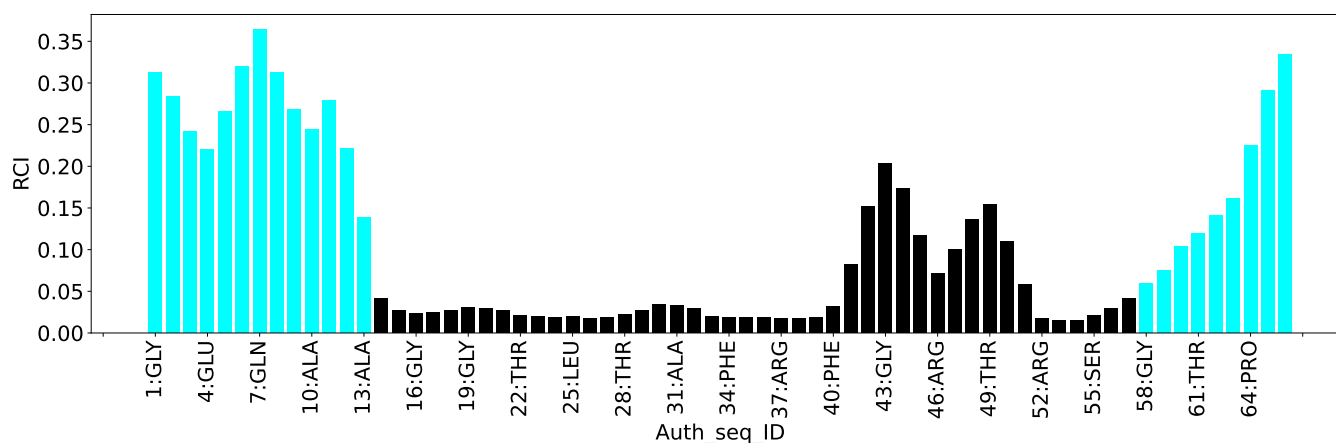
7.1.4 Statistically unusual chemical shifts [i](#)

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 C:



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	787
Intra-residue ($ i-j =0$)	365
Sequential ($ i-j =1$)	180
Medium range ($ i-j >1$ and $ i-j <5$)	61
Long range ($ i-j \geq 5$)	178
Inter-chain	0
Hydrogen bond restraints	3
Disulfide bond restraints	0
Total dihedral-angle restraints	78
Number of unmapped restraints	0
Number of restraints per residue	12.7
Number of long range restraints per residue ¹	2.7

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	10.1	0.2
0.2-0.5 (Medium)	13.9	0.5
>0.5 (Large)	28.3	3.0

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)	5.3	5.08
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

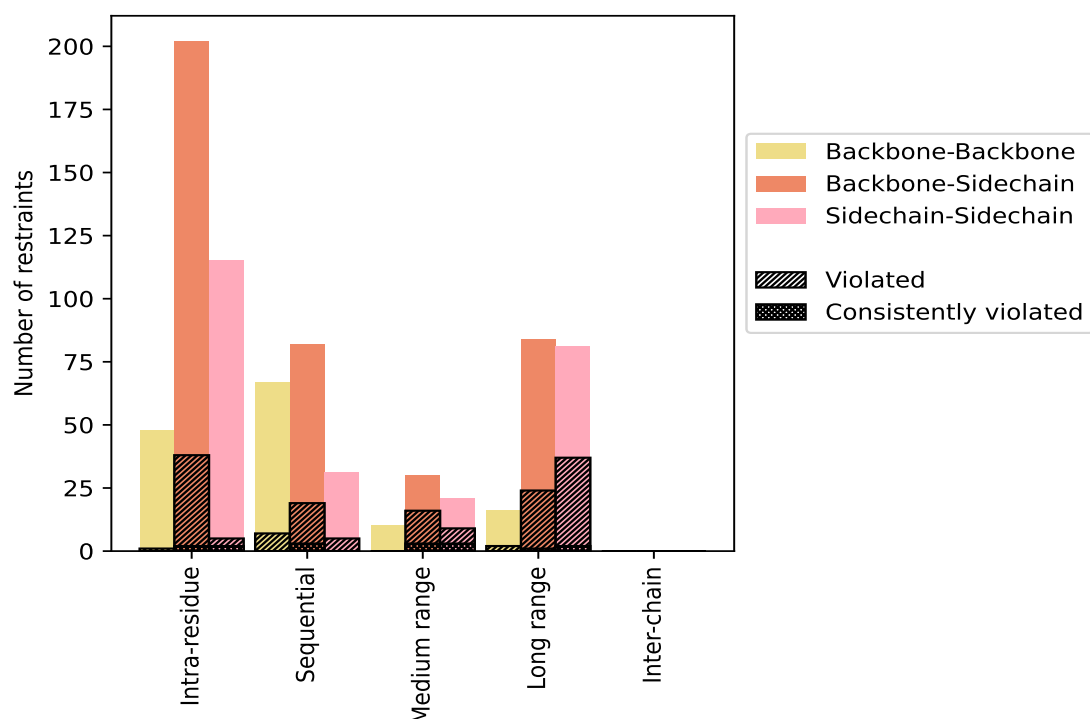
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	365	46.4	44	12.1	5.6	4	1.1	0.5
Backbone-Backbone	48	6.1	1	2.1	0.1	0	0.0	0.0
Backbone-Sidechain	202	25.7	38	18.8	4.8	2	1.0	0.3
Sidechain-Sidechain	115	14.6	5	4.3	0.6	2	1.7	0.3
Sequential ($i-j =1$)	180	22.9	31	17.2	3.9	3	1.7	0.4
Backbone-Backbone	67	8.5	7	10.4	0.9	0	0.0	0.0
Backbone-Sidechain	82	10.4	19	23.2	2.4	3	3.7	0.4
Sidechain-Sidechain	31	3.9	5	16.1	0.6	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	61	7.8	25	41.0	3.2	6	9.8	0.8
Backbone-Backbone	10	1.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	30	3.8	16	53.3	2.0	3	10.0	0.4
Sidechain-Sidechain	21	2.7	9	42.9	1.1	3	14.3	0.4
Long range ($i-j \geq 5$)	178	22.6	63	35.4	8.0	3	1.7	0.4
Backbone-Backbone	16	2.0	2	12.5	0.3	0	0.0	0.0
Backbone-Sidechain	81	10.3	24	29.6	3.0	1	1.2	0.1
Sidechain-Sidechain	81	10.3	37	45.7	4.7	2	2.5	0.3
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	3	0.4	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	787	100.0	163	20.7	20.7	16	2.0	2.0
Backbone-Backbone	141	17.9	10	7.1	1.3	0	0.0	0.0
Backbone-Sidechain	398	50.6	97	24.4	12.3	9	2.3	1.1
Sidechain-Sidechain	248	31.5	56	22.6	7.1	7	2.8	0.9

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	11	5	15	12	0	43	0.72	2.36	0.54	0.59
2	16	7	13	18	0	54	0.62	2.36	0.5	0.44
3	13	8	12	17	0	50	0.7	1.87	0.51	0.6
4	14	4	12	16	0	46	0.7	2.31	0.54	0.52
5	16	12	14	25	0	67	0.74	2.53	0.57	0.62
6	16	6	16	16	0	54	0.7	2.62	0.6	0.53
7	11	8	15	23	0	57	0.8	2.36	0.58	0.61
8	10	7	12	12	0	41	0.7	2.44	0.54	0.52
9	15	7	12	17	0	51	0.64	2.31	0.53	0.52
10	12	6	13	29	0	60	0.92	2.31	0.57	0.76

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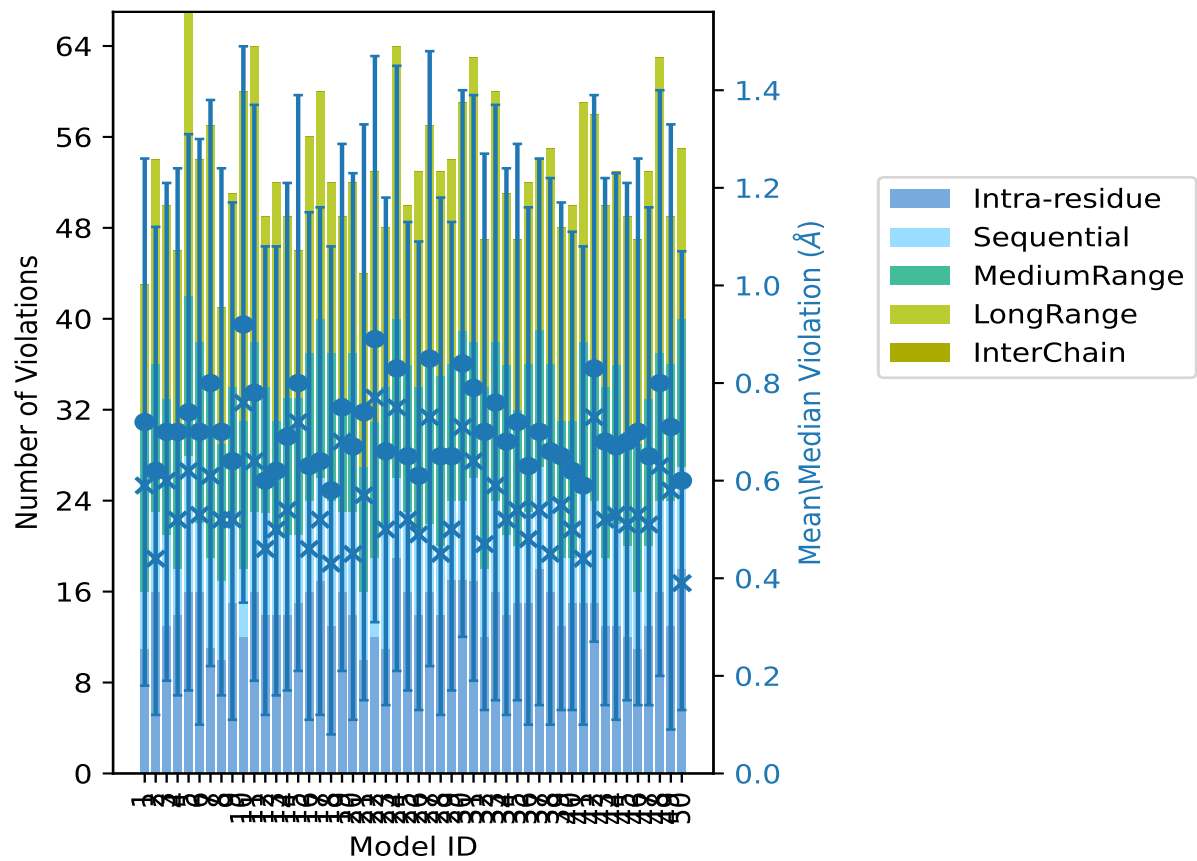
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	16	7	15	26	0	64	0.78	2.45	0.59	0.64
12	14	9	11	15	0	49	0.6	1.79	0.48	0.46
13	14	7	10	21	0	52	0.62	1.97	0.46	0.5
14	14	7	12	16	0	49	0.69	2.56	0.52	0.54
15	15	6	12	13	0	46	0.8	2.49	0.59	0.72
16	16	8	13	19	0	56	0.63	2.43	0.52	0.46
17	17	9	14	20	0	60	0.64	2.54	0.52	0.52
18	13	11	13	15	0	52	0.58	2.16	0.5	0.43
19	16	7	10	16	0	49	0.75	2.26	0.54	0.68
20	14	9	14	15	0	52	0.67	2.09	0.56	0.45
21	10	6	11	17	0	44	0.74	2.62	0.59	0.57
22	12	7	12	22	0	53	0.89	2.34	0.58	0.77
23	11	11	12	14	0	48	0.66	2.21	0.52	0.5
24	19	7	14	24	0	64	0.83	2.56	0.62	0.75
25	16	7	13	14	0	50	0.65	2.32	0.48	0.52
26	14	7	13	19	0	53	0.61	1.79	0.48	0.49
27	16	6	14	21	0	57	0.85	2.77	0.63	0.73
28	14	6	15	18	0	53	0.65	2.14	0.53	0.45
29	17	7	12	18	0	54	0.65	2.07	0.48	0.5
30	17	7	15	20	0	59	0.84	2.3	0.56	0.71
31	17	9	12	25	0	63	0.79	2.65	0.6	0.64
32	12	6	16	13	0	47	0.7	2.17	0.57	0.47
33	16	8	14	22	0	60	0.76	2.84	0.61	0.59
34	14	7	15	15	0	51	0.68	2.25	0.56	0.52
35	15	5	12	15	0	47	0.72	2.24	0.57	0.54
36	15	8	13	16	0	52	0.63	2.82	0.53	0.48
37	18	9	12	15	0	54	0.7	2.47	0.56	0.54
38	16	8	12	19	0	55	0.66	2.01	0.56	0.45
39	13	6	12	17	0	48	0.65	2.38	0.52	0.55
40	15	4	12	19	0	50	0.62	2.17	0.49	0.5
41	15	11	12	21	0	59	0.59	2.34	0.49	0.44
42	15	9	12	22	0	58	0.83	2.48	0.56	0.73
43	13	6	15	16	0	50	0.68	2.54	0.54	0.52
44	13	9	14	17	0	53	0.67	2.61	0.56	0.53
45	12	8	10	19	0	49	0.68	2.25	0.53	0.51
46	11	5	13	18	0	47	0.7	2.04	0.56	0.53
47	13	7	13	20	0	53	0.65	2.38	0.51	0.51
48	16	8	13	26	0	63	0.8	2.49	0.6	0.63
49	13	11	12	13	0	49	0.71	3.0	0.62	0.58
50	18	9	13	15	0	55	0.6	1.79	0.47	0.39

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



The mean(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 ⓘ

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, 621(IR:321, SQ:149, MR:36, LR:115, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
6	8	3	10	0	27	1	2.0
6	4	1	3	0	14	2	4.0
2	3	2	0	0	7	3	6.0
2	1	1	8	0	12	4	8.0

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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
3	1	1	2	0	7	5	10.0
1	1	0	2	0	4	6	12.0
0	1	0	2	0	3	7	14.0
2	0	2	3	0	7	8	16.0
0	0	0	2	0	2	9	18.0
2	0	0	0	0	2	10	20.0
0	2	0	2	0	4	11	22.0
2	0	2	6	0	10	12	24.0
0	1	0	2	0	3	13	26.0
1	1	1	1	0	4	14	28.0
1	0	0	1	0	2	15	30.0
2	0	0	1	0	3	16	32.0
0	0	0	1	0	1	17	34.0
0	0	1	0	0	1	18	36.0
0	0	0	0	0	0	19	38.0
0	0	0	1	0	1	20	40.0
0	1	0	0	0	1	21	42.0
0	0	0	1	0	1	22	44.0
2	0	0	1	0	3	23	46.0
1	0	0	2	0	3	24	48.0
0	0	0	1	0	1	25	50.0
0	0	0	0	0	0	26	52.0
0	1	0	1	0	2	27	54.0
1	0	0	0	0	1	28	56.0
1	0	0	1	0	2	29	58.0
0	1	0	0	0	1	30	60.0
0	0	0	0	0	0	31	62.0
0	0	0	0	0	0	32	64.0
0	0	0	0	0	0	33	66.0
0	0	0	0	0	0	34	68.0
0	0	0	1	0	1	35	70.0
0	0	0	0	0	0	36	72.0
1	1	0	0	0	2	37	74.0
0	0	1	0	0	1	38	76.0
0	0	0	0	0	0	39	78.0
0	0	0	1	0	1	40	80.0
0	0	0	0	0	0	41	82.0
1	0	1	0	0	2	42	84.0
1	1	0	1	0	3	43	86.0
0	0	0	1	0	1	44	88.0
0	0	0	0	0	0	45	90.0

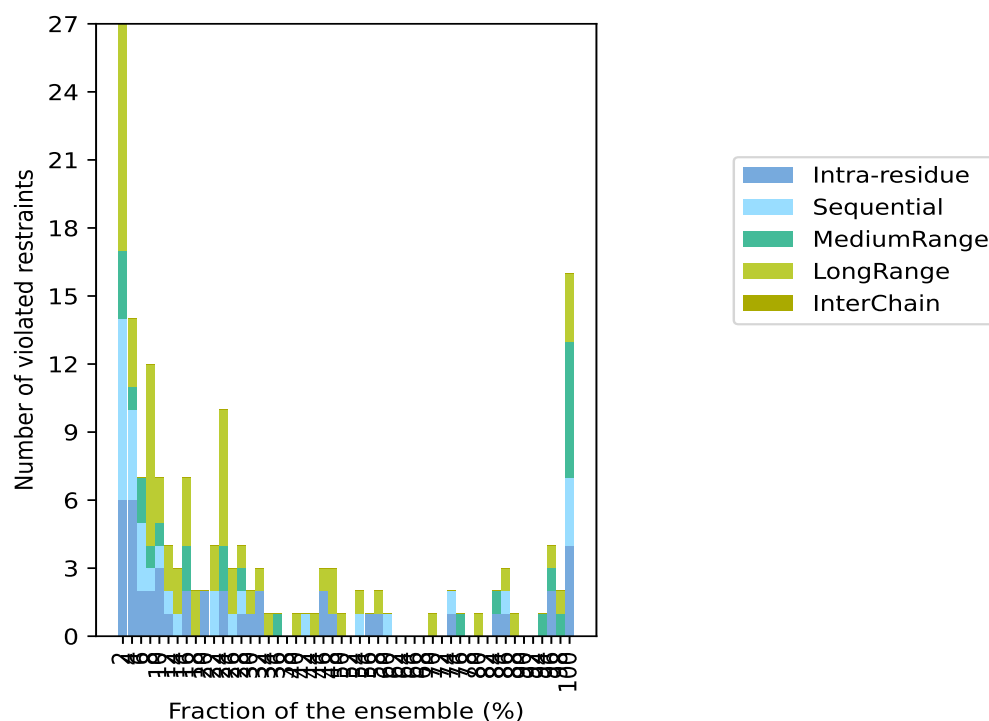
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	46	92.0
0	0	1	0	0	1	47	94.0
2	0	1	1	0	4	48	96.0
0	0	1	1	0	2	49	98.0
4	3	6	3	0	16	50	100.0

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

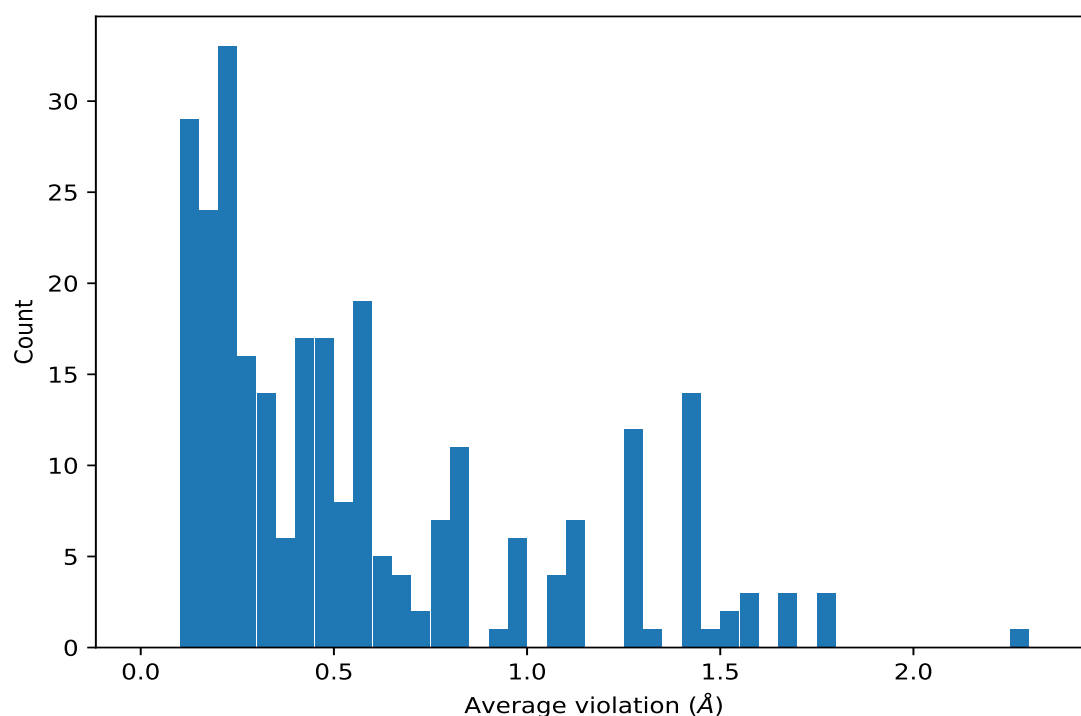
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	50	2.27	0.25	2.3
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD12	50	1.57	0.36	1.65
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	50	1.57	0.36	1.65
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD11	50	1.57	0.36	1.65
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	50	1.52	0.23	1.57
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	50	1.5	0.2	1.51
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	50	1.49	0.05	1.48
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	50	1.41	0.36	1.46
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	50	1.27	0.43	1.17
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	50	1.27	0.43	1.17
(2,176)	1:51:C:LEU:HD22	1:47:C:PRO:HD3	50	1.27	0.43	1.17
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	50	1.26	0.1	1.27
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	50	0.74	0.06	0.74
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	50	0.73	0.11	0.71
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	50	0.63	0.03	0.64
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	50	0.46	0.1	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	50	0.45	0.12	0.46
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	50	0.42	0.1	0.42
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	50	0.3	0.04	0.29
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	50	0.21	0.02	0.21
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	49	0.92	0.25	0.94
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	49	0.7	0.22	0.71
(2,233)	1:51:C:LEU:HD13	1:51:C:LEU:HB2	48	0.83	0.02	0.83
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	48	0.83	0.02	0.83
(2,233)	1:51:C:LEU:HD12	1:51:C:LEU:HB2	48	0.83	0.02	0.83
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	48	0.76	0.01	0.76
(2,188)	1:51:C:LEU:HD22	1:51:C:LEU:HB3	48	0.76	0.01	0.76
(2,188)	1:51:C:LEU:HD21	1:51:C:LEU:HB3	48	0.76	0.01	0.76
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG23	48	0.47	0.17	0.46
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	48	0.47	0.17	0.46
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG21	48	0.47	0.17	0.46
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	48	0.46	0.2	0.48
(2,634)	1:17:C:VAL:HG21	1:38:C:CYS:HB2	48	0.46	0.2	0.48
(2,634)	1:17:C:VAL:HG12	1:38:C:CYS:HB2	48	0.46	0.2	0.48
(2,634)	1:17:C:VAL:HG22	1:38:C:CYS:HB2	48	0.46	0.2	0.48
(2,634)	1:17:C:VAL:HG11	1:38:C:CYS:HB2	48	0.46	0.2	0.48
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	47	1.1	0.16	1.12
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	44	0.59	0.28	0.59
(2,704)	1:34:C:PHE:HE2	1:25:C:LEU:HB3	44	0.59	0.28	0.59
(2,704)	1:34:C:PHE:HE1	1:25:C:LEU:HB3	44	0.59	0.28	0.59
(2,252)	1:22:C:THR:HG22	1:23:C:ASP:HB3	43	0.98	0.63	1.4
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	43	0.98	0.63	1.4
(2,252)	1:22:C:THR:HG23	1:23:C:ASP:HB3	43	0.98	0.63	1.4
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	43	0.82	0.21	0.81
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	43	0.15	0.02	0.15
(2,92)	1:24:C:VAL:HG22	1:21:C:GLY:HA2	42	0.55	0.48	0.29
(2,92)	1:24:C:VAL:HG23	1:21:C:GLY:HA2	42	0.55	0.48	0.29
(2,92)	1:24:C:VAL:HG21	1:21:C:GLY:HA2	42	0.55	0.48	0.29
(2,426)	1:22:C:THR:H	1:22:C:THR:HG21	42	0.19	0.02	0.19
(2,426)	1:22:C:THR:H	1:22:C:THR:HG23	42	0.19	0.02	0.19
(2,426)	1:22:C:THR:H	1:22:C:THR:HG22	42	0.19	0.02	0.19
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	40	0.47	0.11	0.48
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB2	40	0.47	0.11	0.48
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB3	40	0.47	0.11	0.48
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG12	38	0.57	0.22	0.64
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG11	38	0.57	0.22	0.64
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG13	38	0.57	0.22	0.64
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD3	37	0.53	0.12	0.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	37	0.53	0.12	0.55
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	37	0.18	0.04	0.18
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	35	1.32	0.69	1.58
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	30	0.4	0.18	0.43
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	29	0.14	0.02	0.14
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	29	0.13	0.01	0.13
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	28	0.83	0.06	0.81
(2,702)	1:34:C:PHE:HZ	1:51:C:LEU:HD22	27	0.37	0.2	0.38
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD21	27	0.37	0.2	0.38
(2,702)	1:34:C:PHE:HZ	1:51:C:LEU:HD21	27	0.37	0.2	0.38
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD23	27	0.37	0.2	0.38
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD22	27	0.37	0.2	0.38
(2,702)	1:34:C:PHE:HZ	1:51:C:LEU:HD23	27	0.37	0.2	0.38
(2,62)	1:17:C:VAL:HG12	1:18:C:CYS:HB2	27	0.24	0.13	0.18
(2,62)	1:17:C:VAL:HG11	1:18:C:CYS:HB2	27	0.24	0.13	0.18
(2,62)	1:17:C:VAL:HG13	1:18:C:CYS:HB2	27	0.24	0.13	0.18
(2,585)	1:54:C:ARG:HG2	1:39:C:HIS:HE1	25	0.41	0.09	0.41
(2,585)	1:54:C:ARG:HG3	1:39:C:HIS:HE1	25	0.41	0.09	0.41
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	24	1.41	0.39	1.59
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	24	1.08	0.32	1.02
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	24	0.12	0.02	0.12
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	23	0.44	0.24	0.38
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	23	0.41	0.01	0.41
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD22	23	0.21	0.07	0.2
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD12	23	0.21	0.07	0.2
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD21	23	0.21	0.07	0.2
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD13	23	0.21	0.07	0.2
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD23	23	0.21	0.07	0.2
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG22	22	1.44	1.09	2.06
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG23	22	1.44	1.09	2.06
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG21	22	1.44	1.09	2.06
(2,125)	1:32:C:ALA:HB1	1:33:C:ALA:HA	21	0.18	0.06	0.17
(2,125)	1:32:C:ALA:HB3	1:33:C:ALA:HA	21	0.18	0.06	0.17
(2,125)	1:32:C:ALA:HB2	1:33:C:ALA:HA	21	0.18	0.06	0.17
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	20	0.34	0.15	0.32
(2,168)	1:44:C:THR:HG21	1:46:C:ARG:HA	18	0.28	0.09	0.27
(2,168)	1:44:C:THR:HG22	1:46:C:ARG:HA	18	0.28	0.09	0.27
(2,168)	1:44:C:THR:HG23	1:46:C:ARG:HA	18	0.28	0.09	0.27
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	17	0.77	0.37	0.8
(2,41)	1:9:C:LEU:HD11	1:9:C:LEU:HA	16	1.41	0.33	1.5
(2,41)	1:9:C:LEU:HD13	1:9:C:LEU:HA	16	1.41	0.33	1.5
(2,41)	1:9:C:LEU:HD12	1:9:C:LEU:HA	16	1.41	0.33	1.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG21	16	1.11	0.58	1.33
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG22	16	1.11	0.58	1.33
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG23	16	1.11	0.58	1.33
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG3	16	0.23	0.06	0.22
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG2	16	0.23	0.06	0.22
(2,678)	1:57:C:SER:HB3	1:52:C:ARG:HB2	15	0.31	0.14	0.3
(2,678)	1:57:C:SER:HB2	1:52:C:ARG:HB3	15	0.31	0.14	0.3
(2,678)	1:57:C:SER:HB2	1:52:C:ARG:HB2	15	0.31	0.14	0.3
(2,678)	1:57:C:SER:HB3	1:52:C:ARG:HB3	15	0.31	0.14	0.3
(2,412)	1:20:C:ASP:H	1:20:C:ASP:HB2	15	0.29	0.09	0.32
(2,610)	1:24:C:VAL:HG12	1:26:C:ARG:HD3	14	1.45	0.57	1.59
(2,610)	1:24:C:VAL:HG11	1:26:C:ARG:HD3	14	1.45	0.57	1.59
(2,610)	1:24:C:VAL:HG11	1:26:C:ARG:HD2	14	1.45	0.57	1.59
(2,610)	1:24:C:VAL:HG12	1:26:C:ARG:HD2	14	1.45	0.57	1.59
(2,610)	1:24:C:VAL:HG13	1:26:C:ARG:HD3	14	1.45	0.57	1.59
(2,610)	1:24:C:VAL:HG13	1:26:C:ARG:HD2	14	1.45	0.57	1.59
(2,73)	1:14:C:ARG:HB3	1:21:C:GLY:HA3	14	0.44	0.27	0.35
(2,145)	1:39:C:HIS:HD2	1:38:C:CYS:HB3	14	0.34	0.22	0.26
(2,715)	1:6:C:GLN:H	1:6:C:GLN:HG2	14	0.23	0.09	0.21
(2,715)	1:6:C:GLN:H	1:6:C:GLN:HG3	14	0.23	0.09	0.21
(2,367)	1:35:C:HIS:HD2	1:24:C:VAL:HG21	13	1.26	0.37	1.27
(2,367)	1:35:C:HIS:HD2	1:24:C:VAL:HG22	13	1.26	0.37	1.27
(2,367)	1:35:C:HIS:HD2	1:24:C:VAL:HG23	13	1.26	0.37	1.27
(2,419)	1:21:C:GLY:H	1:14:C:ARG:HG2	13	0.54	0.35	0.53
(2,716)	1:6:C:GLN:H	1:7:C:GLN:HB2	13	0.31	0.14	0.28
(2,716)	1:6:C:GLN:H	1:7:C:GLN:HB3	13	0.31	0.14	0.28
(2,415)	1:20:C:ASP:H	1:24:C:VAL:HG22	12	1.78	0.19	1.86
(2,415)	1:20:C:ASP:H	1:24:C:VAL:HG23	12	1.78	0.19	1.86
(2,415)	1:20:C:ASP:H	1:24:C:VAL:HG21	12	1.78	0.19	1.86
(2,56)	1:24:C:VAL:HG22	1:15:C:CYS:HB2	12	1.66	0.39	1.5
(2,56)	1:24:C:VAL:HG23	1:15:C:CYS:HB2	12	1.66	0.39	1.5
(2,56)	1:24:C:VAL:HG21	1:15:C:CYS:HB2	12	1.66	0.39	1.5
(2,55)	1:24:C:VAL:HG22	1:15:C:CYS:HB3	12	1.25	0.34	1.24
(2,55)	1:24:C:VAL:HG23	1:15:C:CYS:HB3	12	1.25	0.34	1.24
(2,55)	1:24:C:VAL:HG21	1:15:C:CYS:HB3	12	1.25	0.34	1.24
(2,90)	1:24:C:VAL:HG23	1:24:C:VAL:HA	12	1.15	0.03	1.13
(2,90)	1:24:C:VAL:HG22	1:24:C:VAL:HA	12	1.15	0.03	1.13
(2,90)	1:24:C:VAL:HG21	1:24:C:VAL:HA	12	1.15	0.03	1.13
(2,93)	1:34:C:PHE:HA	1:24:C:VAL:HG22	12	1.08	0.14	1.08
(2,93)	1:34:C:PHE:HA	1:24:C:VAL:HG23	12	1.08	0.14	1.08
(2,93)	1:34:C:PHE:HA	1:24:C:VAL:HG21	12	1.08	0.14	1.08
(2,361)	1:15:C:CYS:H	1:24:C:VAL:HG22	12	0.68	0.28	0.77

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,361)	1:15:C:CYS:H	1:24:C:VAL:HG23	12	0.68	0.28	0.77
(2,361)	1:15:C:CYS:H	1:24:C:VAL:HG21	12	0.68	0.28	0.77
(2,357)	1:34:C:PHE:H	1:24:C:VAL:HG23	12	0.62	0.25	0.68
(2,357)	1:34:C:PHE:H	1:24:C:VAL:HG21	12	0.62	0.25	0.68
(2,357)	1:34:C:PHE:H	1:24:C:VAL:HG22	12	0.62	0.25	0.68
(2,769)	1:53:C:CYS:H	1:57:C:SER:HB2	12	0.32	0.09	0.34
(2,234)	1:36:C:TRP:HZ3	1:51:C:LEU:HD23	12	0.3	0.08	0.3
(2,234)	1:36:C:TRP:HZ3	1:51:C:LEU:HD21	12	0.3	0.08	0.3
(2,556)	1:65:C:VAL:H	1:65:C:VAL:HG23	12	0.26	0.04	0.28
(2,556)	1:65:C:VAL:H	1:65:C:VAL:HG22	12	0.26	0.04	0.28
(2,556)	1:65:C:VAL:H	1:65:C:VAL:HG21	12	0.26	0.04	0.28
(2,51)	1:24:C:VAL:HG23	1:15:C:CYS:HA	11	0.82	0.41	0.82
(2,51)	1:24:C:VAL:HG21	1:15:C:CYS:HA	11	0.82	0.41	0.82
(2,51)	1:24:C:VAL:HG22	1:15:C:CYS:HA	11	0.82	0.41	0.82
(2,261)	1:25:C:LEU:H	1:24:C:VAL:HG21	11	0.48	0.12	0.47
(2,261)	1:25:C:LEU:H	1:24:C:VAL:HG22	11	0.48	0.12	0.47
(2,261)	1:25:C:LEU:H	1:24:C:VAL:HG23	11	0.48	0.12	0.47
(2,778)	1:36:C:TRP:HE1	1:46:C:ARG:HD3	11	0.4	0.23	0.35
(2,778)	1:36:C:TRP:HE1	1:46:C:ARG:HD2	11	0.4	0.23	0.35
(2,101)	1:27:C:CYS:HA	1:26:C:ARG:HB2	11	0.18	0.03	0.18
(2,181)	1:49:C:THR:HG22	1:49:C:THR:HA	10	0.6	0.02	0.6
(2,181)	1:49:C:THR:HG23	1:49:C:THR:HA	10	0.6	0.02	0.6
(2,181)	1:49:C:THR:HG21	1:49:C:THR:HA	10	0.6	0.02	0.6
(2,593)	1:6:C:GLN:HB2	1:6:C:GLN:HA	10	0.12	0.01	0.12
(2,593)	1:7:C:GLN:HB2	1:7:C:GLN:HA	10	0.12	0.01	0.12
(2,468)	1:32:C:ALA:H	1:27:C:CYS:HB2	9	0.44	0.23	0.56
(2,676)	1:57:C:SER:HA	1:52:C:ARG:HB3	9	0.21	0.07	0.18
(2,676)	1:57:C:SER:HA	1:52:C:ARG:HB2	9	0.21	0.07	0.18
(2,387)	1:12:C:GLY:H	1:10:C:ALA:HB2	8	0.56	0.12	0.6
(2,387)	1:12:C:GLY:H	1:10:C:ALA:HB3	8	0.56	0.12	0.6
(2,387)	1:12:C:GLY:H	1:10:C:ALA:HB1	8	0.56	0.12	0.6
(2,220)	1:60:C:VAL:HA	1:60:C:VAL:HG23	8	0.51	0.03	0.5
(2,220)	1:60:C:VAL:HA	1:60:C:VAL:HG21	8	0.51	0.03	0.5
(2,220)	1:60:C:VAL:HA	1:60:C:VAL:HG22	8	0.51	0.03	0.5
(2,614)	1:14:C:ARG:HG2	1:21:C:GLY:HA2	8	0.42	0.43	0.26
(2,614)	1:14:C:ARG:HB3	1:21:C:GLY:HA2	8	0.42	0.43	0.26
(2,692)	1:52:C:ARG:HG2	1:50:C:GLY:HA3	8	0.42	0.33	0.28
(2,692)	1:52:C:ARG:HG2	1:50:C:GLY:HA2	8	0.42	0.33	0.28
(2,91)	1:24:C:VAL:HG22	1:14:C:ARG:HA	8	0.31	0.13	0.28
(2,91)	1:24:C:VAL:HG23	1:14:C:ARG:HA	8	0.31	0.13	0.28
(2,91)	1:24:C:VAL:HG21	1:14:C:ARG:HA	8	0.31	0.13	0.28
(2,85)	1:24:C:VAL:HG12	1:14:C:ARG:HA	8	0.2	0.07	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,85)	1:24:C:VAL:HG13	1:14:C:ARG:HA	8	0.2	0.07	0.2
(2,85)	1:24:C:VAL:HG11	1:14:C:ARG:HA	8	0.2	0.07	0.2
(2,352)	1:34:C:PHE:HE1	1:34:C:PHE:H	8	0.16	0.03	0.18
(2,352)	1:34:C:PHE:HE2	1:34:C:PHE:H	8	0.16	0.03	0.18
(2,693)	1:49:C:THR:HG21	1:48:C:GLY:HA3	7	0.84	0.31	0.99
(2,693)	1:49:C:THR:HG22	1:48:C:GLY:HA3	7	0.84	0.31	0.99
(2,693)	1:49:C:THR:HG23	1:48:C:GLY:HA3	7	0.84	0.31	0.99
(2,68)	1:14:C:ARG:HG2	1:20:C:ASP:HA	7	0.48	0.32	0.59
(2,575)	1:36:C:TRP:HE1	1:46:C:ARG:HB2	7	0.35	0.18	0.36
(2,765)	1:61:C:THR:H	1:60:C:VAL:HG11	6	0.23	0.14	0.16
(2,765)	1:61:C:THR:H	1:60:C:VAL:HG13	6	0.23	0.14	0.16
(2,765)	1:61:C:THR:H	1:60:C:VAL:HG23	6	0.23	0.14	0.16
(2,765)	1:61:C:THR:H	1:60:C:VAL:HG21	6	0.23	0.14	0.16
(2,624)	1:33:C:ALA:HA	1:26:C:ARG:HD3	6	0.18	0.07	0.16
(2,624)	1:33:C:ALA:HA	1:26:C:ARG:HD2	6	0.18	0.07	0.16
(2,456)	1:30:C:CYS:H	1:30:C:CYS:HB3	6	0.15	0.02	0.15
(2,706)	1:34:C:PHE:HE2	1:51:C:LEU:HG	6	0.13	0.03	0.12
(2,706)	1:34:C:PHE:HZ	1:51:C:LEU:HG	6	0.13	0.03	0.12
(2,522)	1:46:C:ARG:H	1:46:C:ARG:HB3	5	0.63	0.02	0.64
(2,260)	1:39:C:HIS:HD2	1:17:C:VAL:HG22	5	0.28	0.06	0.25
(2,260)	1:39:C:HIS:HD2	1:17:C:VAL:HG23	5	0.28	0.06	0.25
(2,260)	1:39:C:HIS:HD2	1:17:C:VAL:HG21	5	0.28	0.06	0.25
(2,223)	1:61:C:THR:HG21	1:61:C:THR:HA	5	0.2	0.02	0.2
(2,223)	1:61:C:THR:HG23	1:61:C:THR:HA	5	0.2	0.02	0.2
(2,223)	1:61:C:THR:HG22	1:61:C:THR:HA	5	0.2	0.02	0.2
(2,86)	1:24:C:VAL:HG12	1:21:C:GLY:HA2	5	0.18	0.04	0.18
(2,86)	1:24:C:VAL:HG13	1:21:C:GLY:HA2	5	0.18	0.04	0.18
(2,86)	1:24:C:VAL:HG11	1:21:C:GLY:HA2	5	0.18	0.04	0.18
(2,395)	1:17:C:VAL:H	1:18:C:CYS:HB2	5	0.15	0.02	0.16
(2,448)	1:28:C:THR:H	1:51:C:LEU:HD22	5	0.13	0.02	0.13
(2,448)	1:28:C:THR:H	1:51:C:LEU:HD21	5	0.13	0.02	0.13
(2,448)	1:28:C:THR:H	1:51:C:LEU:HD23	5	0.13	0.02	0.13
(2,40)	1:9:C:LEU:HD22	1:9:C:LEU:HA	5	0.12	0.02	0.13
(2,40)	1:9:C:LEU:HD23	1:9:C:LEU:HA	5	0.12	0.02	0.13
(2,366)	1:35:C:HIS:HD2	1:24:C:VAL:HG13	4	0.55	0.13	0.52
(2,366)	1:35:C:HIS:HD2	1:24:C:VAL:HG11	4	0.55	0.13	0.52
(2,581)	1:49:C:THR:H	1:49:C:THR:HG21	4	0.54	0.1	0.5
(2,581)	1:49:C:THR:H	1:49:C:THR:HG22	4	0.54	0.1	0.5
(2,584)	1:34:C:PHE:HE1	1:39:C:HIS:HE1	4	0.42	0.24	0.42
(2,584)	1:34:C:PHE:HE2	1:39:C:HIS:HE1	4	0.42	0.24	0.42
(2,420)	1:21:C:GLY:H	1:24:C:VAL:HG22	4	0.27	0.09	0.31
(2,420)	1:21:C:GLY:H	1:24:C:VAL:HG21	4	0.27	0.09	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,126)	1:13:C:ALA:HA	1:33:C:ALA:HB1	4	0.23	0.07	0.24
(2,126)	1:13:C:ALA:HA	1:33:C:ALA:HB2	4	0.23	0.07	0.24
(2,38)	1:54:C:ARG:HG2	1:40:C:PHE:HE1	4	0.22	0.06	0.22
(2,38)	1:54:C:ARG:HG2	1:40:C:PHE:HE2	4	0.22	0.06	0.22
(2,246)	1:32:C:ALA:HB1	1:27:C:CYS:HB3	4	0.2	0.08	0.18
(2,701)	1:34:C:PHE:HE1	1:27:C:CYS:HA	4	0.19	0.06	0.16
(2,244)	1:33:C:ALA:HB1	1:24:C:VAL:HB	4	0.18	0.05	0.2
(2,244)	1:33:C:ALA:HB2	1:24:C:VAL:HB	4	0.18	0.05	0.2
(2,663)	1:57:C:SER:HB3	1:52:C:ARG:HB2	4	0.13	0.02	0.13
(2,663)	1:57:C:SER:HB3	1:52:C:ARG:HB3	4	0.13	0.02	0.13
(2,385)	1:12:C:GLY:H	1:11:C:PRO:HA	4	0.12	0.03	0.11
(2,544)	1:60:C:VAL:H	1:60:C:VAL:HB	4	0.12	0.03	0.11
(2,116)	1:28:C:THR:HG21	1:28:C:THR:HA	3	0.76	0.03	0.75
(2,116)	1:28:C:THR:HG22	1:28:C:THR:HA	3	0.76	0.03	0.75
(2,116)	1:28:C:THR:HG23	1:28:C:THR:HA	3	0.76	0.03	0.75
(2,615)	1:26:C:ARG:HD3	1:24:C:VAL:HG22	3	0.22	0.08	0.22
(2,615)	1:26:C:ARG:HD2	1:24:C:VAL:HG23	3	0.22	0.08	0.22
(2,615)	1:26:C:ARG:HD2	1:24:C:VAL:HG22	3	0.22	0.08	0.22
(2,371)	1:23:C:ASP:H	1:22:C:THR:HG21	3	0.19	0.05	0.2
(2,371)	1:23:C:ASP:H	1:22:C:THR:HG23	3	0.19	0.05	0.2
(2,524)	1:50:C:GLY:H	1:49:C:THR:HA	3	0.15	0.02	0.15
(2,543)	1:60:C:VAL:H	1:59:C:ASP:HA	3	0.13	0.03	0.13
(2,458)	1:30:C:CYS:H	1:28:C:THR:HG22	3	0.13	0.02	0.12
(2,458)	1:30:C:CYS:H	1:28:C:THR:HG21	3	0.13	0.02	0.12
(2,458)	1:30:C:CYS:H	1:28:C:THR:HG23	3	0.13	0.02	0.12
(2,190)	1:52:C:ARG:HA	1:52:C:ARG:HG3	3	0.12	0.02	0.12
(2,703)	1:34:C:PHE:HE2	1:51:C:LEU:HD12	2	1.28	0.16	1.28
(2,703)	1:34:C:PHE:HZ	1:51:C:LEU:HD13	2	1.28	0.16	1.28
(2,264)	1:52:C:ARG:H	1:51:C:LEU:HD11	2	0.99	0.09	0.99
(2,264)	1:52:C:ARG:H	1:51:C:LEU:HD12	2	0.99	0.09	0.99
(2,455)	1:30:C:CYS:H	1:29:C:HIS:HB2	2	0.98	0.04	0.98
(2,185)	1:51:C:LEU:HD11	1:51:C:LEU:HA	2	0.55	0.02	0.55
(2,185)	1:51:C:LEU:HD12	1:51:C:LEU:HA	2	0.55	0.02	0.55
(2,186)	1:51:C:LEU:HD21	1:51:C:LEU:HA	2	0.42	0.01	0.42
(2,453)	1:29:C:HIS:H	1:29:C:HIS:HD2	2	0.33	0.03	0.33
(2,757)	1:54:C:ARG:H	1:54:C:ARG:HG2	2	0.28	0.04	0.28
(2,576)	1:61:C:THR:H	1:59:C:ASP:HB2	2	0.19	0.01	0.19
(2,327)	1:36:C:TRP:HZ2	1:51:C:LEU:HD11	2	0.16	0.01	0.16
(2,327)	1:36:C:TRP:HZ2	1:51:C:LEU:HD12	2	0.16	0.01	0.16
(2,281)	1:66:C:GLU:H	1:65:C:VAL:HA	2	0.16	0.04	0.16
(2,164)	1:45:C:SER:HB3	1:44:C:THR:HG22	2	0.15	0.02	0.15
(2,727)	1:14:C:ARG:H	1:14:C:ARG:HB3	2	0.14	0.01	0.14

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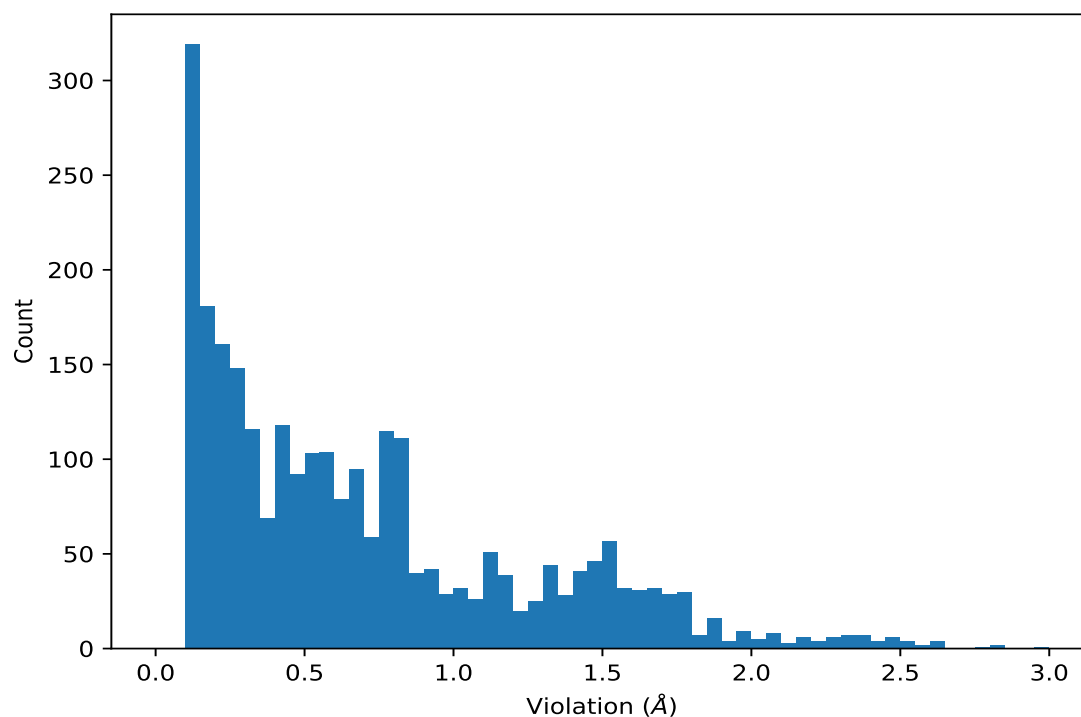
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,772)	1:57:C:SER:H	1:57:C:SER:HB3	2	0.13	0.02	0.13
(2,149)	1:38:C:CYS:HB3	1:17:C:VAL:HB	2	0.11	0.01	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	49	3.0
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG21	33	2.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	36	2.82
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG21	27	2.77
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG23	31	2.65
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	6	2.62
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	21	2.62
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	44	2.61
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG22	24	2.56
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	14	2.56
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	49	2.55
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	17	2.54
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	43	2.54
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	5	2.53
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG22	48	2.49
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	15	2.49
(2,610)	1:24:C:VAL:HG12	1:26:C:ARG:HD3	42	2.48
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	37	2.47
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	11	2.45
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	24	2.45
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	8	2.44
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	16	2.43
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG22	11	2.41
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	27	2.41
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	48	2.39
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	39	2.38
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	47	2.38
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	6	2.37
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG22	7	2.36
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	1	2.36
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	2	2.36
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	22	2.34
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	41	2.34
(2,56)	1:24:C:VAL:HG23	1:15:C:CYS:HB2	24	2.33
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	25	2.32
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG22	10	2.31
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	4	2.31
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	9	2.31
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	30	2.3
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	37	2.3
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	33	2.28
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	19	2.26
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	34	2.25
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	45	2.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	35	2.24
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG21	30	2.23
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG23	42	2.21
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	23	2.21
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG23	22	2.17
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	32	2.17
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	40	2.17
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	42	2.17
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	18	2.16
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	10	2.15
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	28	2.14
(2,56)	1:24:C:VAL:HG21	1:15:C:CYS:HB2	22	2.13
(2,56)	1:24:C:VAL:HG21	1:15:C:CYS:HB2	31	2.1
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	7	2.09
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	20	2.09
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	35	2.07
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	10	2.07
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	15	2.07
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	29	2.07
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	34	2.06
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	44	2.06
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD11	5	2.05
(2,415)	1:20:C:ASP:H	1:24:C:VAL:HG21	22	2.04
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	46	2.04
(2,56)	1:24:C:VAL:HG22	1:15:C:CYS:HB2	27	2.03
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	38	2.01
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	46	1.99
(2,415)	1:20:C:ASP:H	1:24:C:VAL:HG23	11	1.98
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD12	28	1.98
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	5	1.98
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	20	1.97
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	49	1.97
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	13	1.97
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	41	1.96
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	34	1.96
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG22	5	1.95
(2,610)	1:24:C:VAL:HG12	1:26:C:ARG:HD3	48	1.92
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD12	27	1.92
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	9	1.91
(2,415)	1:20:C:ASP:H	1:24:C:VAL:HG23	5	1.9
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD12	18	1.9
(2,415)	1:20:C:ASP:H	1:24:C:VAL:HG23	10	1.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD12	1	1.89
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	20	1.89
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD11	44	1.89
(2,415)	1:20:C:ASP:H	1:24:C:VAL:HG21	31	1.88
(2,415)	1:20:C:ASP:H	1:24:C:VAL:HG23	48	1.88
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD12	3	1.87
(2,56)	1:24:C:VAL:HG23	1:15:C:CYS:HB2	10	1.87
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD11	16	1.86
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	36	1.86
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG21	33	1.85
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	23	1.85
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	19	1.85
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD12	47	1.85
(2,415)	1:20:C:ASP:H	1:24:C:VAL:HG21	42	1.84
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD11	24	1.82
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	2	1.82
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	30	1.82
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	32	1.81
(2,55)	1:24:C:VAL:HG23	1:15:C:CYS:HB3	24	1.81
(2,415)	1:20:C:ASP:H	1:24:C:VAL:HG23	7	1.8
(2,252)	1:22:C:THR:HG23	1:23:C:ASP:HB3	21	1.79
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	31	1.79
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	12	1.79
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	26	1.79
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	50	1.79
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	28	1.79
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	35	1.79
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	45	1.79
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	7	1.78
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	11	1.78
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	12	1.78
(2,176)	1:51:C:LEU:HD22	1:47:C:PRO:HD3	38	1.78
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	32	1.78
(2,610)	1:24:C:VAL:HG13	1:26:C:ARG:HD3	30	1.77
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	38	1.77
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	41	1.77
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	38	1.77
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	47	1.77
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	6	1.77
(2,610)	1:24:C:VAL:HG13	1:26:C:ARG:HD3	11	1.76
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	4	1.76
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	17	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	24	1.76
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	3	1.76
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	45	1.76
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	46	1.75
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	37	1.75
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	12	1.75
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	32	1.75
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	4	1.75
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	23	1.74
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD11	34	1.74
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	3	1.74
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	24	1.74
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	15	1.74
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	17	1.74
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	9	1.74
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	16	1.74
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	32	1.74
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	35	1.74
(2,610)	1:24:C:VAL:HG11	1:26:C:ARG:HD3	27	1.73
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	7	1.73
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	31	1.73
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	46	1.73
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	14	1.73
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	48	1.72
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD11	26	1.72
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	3	1.72
(2,112)	1:53:C:CYS:HB2	1:27:C:CYS:HB3	31	1.72
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	19	1.72
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	33	1.72
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	30	1.71
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	32	1.71
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	10	1.71
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	18	1.71
(2,55)	1:24:C:VAL:HG21	1:15:C:CYS:HB3	31	1.71
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	8	1.71
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	27	1.71
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	40	1.71
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	43	1.7
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	22	1.7
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD11	46	1.7
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	19	1.7
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	20	1.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	38	1.7
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	13	1.7
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	28	1.7
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG22	48	1.69
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	2	1.69
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	14	1.69
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD11	21	1.69
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	29	1.69
(2,610)	1:24:C:VAL:HG12	1:26:C:ARG:HD3	33	1.68
(2,415)	1:20:C:ASP:H	1:24:C:VAL:HG22	27	1.68
(2,415)	1:20:C:ASP:H	1:24:C:VAL:HG22	30	1.68
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	20	1.68
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	45	1.68
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	19	1.68
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	1	1.68
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	17	1.67
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD12	40	1.67
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	39	1.67
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	28	1.67
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	38	1.67
(2,367)	1:35:C:HIS:HD2	1:24:C:VAL:HG22	7	1.66
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	25	1.66
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	28	1.66
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	39	1.66
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	18	1.66
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	23	1.66
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	46	1.66
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	14	1.65
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	17	1.65
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	39	1.65
(2,610)	1:24:C:VAL:HG12	1:26:C:ARG:HD2	22	1.64
(2,367)	1:35:C:HIS:HD2	1:24:C:VAL:HG22	48	1.64
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD11	50	1.64
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	50	1.64
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	26	1.64
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	8	1.63
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	10	1.63
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	1	1.63
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	1	1.63
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	42	1.63
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	5	1.63
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	34	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	3	1.62
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD11	15	1.62
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	38	1.62
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	34	1.62
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	35	1.62
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD12	48	1.61
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	14	1.61
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	6	1.61
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	31	1.61
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	48	1.61
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	41	1.61
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	15	1.6
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD12	11	1.6
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	31	1.6
(2,92)	1:24:C:VAL:HG22	1:21:C:GLY:HA2	10	1.6
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	47	1.6
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	26	1.59
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	34	1.59
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD12	6	1.59
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD11	8	1.59
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	43	1.59
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	12	1.58
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD12	2	1.58
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	11	1.58
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	4	1.58
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	12	1.58
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	37	1.57
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	6	1.57
(2,252)	1:22:C:THR:HG22	1:23:C:ASP:HB3	29	1.57
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	18	1.57
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	27	1.57
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	38	1.57
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	10	1.57
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	24	1.57
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG22	7	1.56
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG21	27	1.56
(2,252)	1:22:C:THR:HG22	1:23:C:ASP:HB3	4	1.56
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD11	42	1.56
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	21	1.56
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	6	1.56
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	45	1.56
(2,41)	1:9:C:LEU:HD12	1:9:C:LEU:HA	24	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	7	1.56
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	6	1.55
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	11	1.55
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	13	1.55
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	41	1.55
(2,41)	1:9:C:LEU:HD12	1:9:C:LEU:HA	27	1.55
(2,610)	1:24:C:VAL:HG13	1:26:C:ARG:HD2	31	1.54
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	31	1.54
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	10	1.54
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	37	1.54
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	14	1.54
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	1	1.53
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	49	1.53
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	50	1.53
(2,252)	1:22:C:THR:HG23	1:23:C:ASP:HB3	35	1.53
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	9	1.53
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	15	1.53
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	21	1.53
(2,55)	1:24:C:VAL:HG22	1:15:C:CYS:HB3	27	1.53
(2,41)	1:9:C:LEU:HD11	1:9:C:LEU:HA	15	1.53
(2,41)	1:9:C:LEU:HD11	1:9:C:LEU:HA	17	1.53
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	31	1.53
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	48	1.53
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	3	1.52
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	4	1.52
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	43	1.52
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	46	1.52
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	21	1.52
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	21	1.52
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	44	1.52
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	36	1.52
(2,41)	1:9:C:LEU:HD12	1:9:C:LEU:HA	26	1.52
(2,41)	1:9:C:LEU:HD13	1:9:C:LEU:HA	35	1.52
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	20	1.52
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	5	1.51
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	17	1.51
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	18	1.51
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	25	1.51
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	42	1.51
(2,252)	1:22:C:THR:HG23	1:23:C:ASP:HB3	9	1.51
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	19	1.51
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	39	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	2	1.51
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	7	1.51
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	8	1.51
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	30	1.51
(2,55)	1:24:C:VAL:HG23	1:15:C:CYS:HB3	10	1.51
(2,51)	1:24:C:VAL:HG21	1:15:C:CYS:HA	22	1.51
(2,41)	1:9:C:LEU:HD13	1:9:C:LEU:HA	30	1.51
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	37	1.51
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	2	1.5
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	15	1.5
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	29	1.5
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	32	1.5
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	47	1.5
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	4	1.5
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	43	1.5
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	19	1.5
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	22	1.5
(2,56)	1:24:C:VAL:HG23	1:15:C:CYS:HB2	11	1.5
(2,41)	1:9:C:LEU:HD11	1:9:C:LEU:HA	2	1.5
(2,41)	1:9:C:LEU:HD13	1:9:C:LEU:HA	38	1.5
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	11	1.5
(2,610)	1:24:C:VAL:HG12	1:26:C:ARG:HD2	7	1.49
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	22	1.49
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG22	11	1.49
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	15	1.49
(2,252)	1:22:C:THR:HG22	1:23:C:ASP:HB3	37	1.49
(2,252)	1:22:C:THR:HG23	1:23:C:ASP:HB3	44	1.49
(2,252)	1:22:C:THR:HG23	1:23:C:ASP:HB3	45	1.49
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	49	1.49
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	43	1.49
(2,56)	1:24:C:VAL:HG22	1:15:C:CYS:HB2	33	1.49
(2,41)	1:9:C:LEU:HD11	1:9:C:LEU:HA	42	1.49
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	15	1.49
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	7	1.48
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	19	1.48
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	20	1.48
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	24	1.48
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	27	1.48
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	38	1.48
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	45	1.48
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	34	1.48
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	47	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,176)	1:51:C:LEU:HD22	1:47:C:PRO:HD3	8	1.48
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	13	1.48
(2,41)	1:9:C:LEU:HD11	1:9:C:LEU:HA	20	1.48
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	9	1.47
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	28	1.47
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	36	1.47
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	39	1.47
(2,367)	1:35:C:HIS:HD2	1:24:C:VAL:HG22	11	1.47
(2,367)	1:35:C:HIS:HD2	1:24:C:VAL:HG21	30	1.47
(2,252)	1:22:C:THR:HG23	1:23:C:ASP:HB3	26	1.47
(2,41)	1:9:C:LEU:HD12	1:9:C:LEU:HA	19	1.47
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	42	1.47
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	27	1.46
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	21	1.46
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	23	1.46
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	32	1.46
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	33	1.46
(2,252)	1:22:C:THR:HG22	1:23:C:ASP:HB3	16	1.46
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	33	1.46
(2,92)	1:24:C:VAL:HG22	1:21:C:GLY:HA2	48	1.46
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	37	1.46
(2,56)	1:24:C:VAL:HG23	1:15:C:CYS:HB2	7	1.46
(2,56)	1:24:C:VAL:HG21	1:15:C:CYS:HB2	42	1.46
(2,41)	1:9:C:LEU:HD11	1:9:C:LEU:HA	33	1.46
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	25	1.46
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	5	1.45
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	31	1.45
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	30	1.45
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	35	1.45
(2,367)	1:35:C:HIS:HD2	1:24:C:VAL:HG22	10	1.45
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG21	30	1.45
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	33	1.45
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	46	1.45
(2,55)	1:24:C:VAL:HG21	1:15:C:CYS:HB3	22	1.45
(2,41)	1:9:C:LEU:HD12	1:9:C:LEU:HA	29	1.45
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	43	1.45
(2,703)	1:34:C:PHE:HE2	1:51:C:LEU:HD12	49	1.44
(2,614)	1:14:C:ARG:HG2	1:21:C:GLY:HA2	13	1.44
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	10	1.44
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	16	1.44
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	40	1.44
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	47	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,252)	1:22:C:THR:HG23	1:23:C:ASP:HB3	48	1.44
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	6	1.44
(2,176)	1:51:C:LEU:HD22	1:47:C:PRO:HD3	40	1.44
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	49	1.44
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	50	1.44
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	33	1.43
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	8	1.43
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG23	31	1.43
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	22	1.43
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	29	1.43
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	35	1.43
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	5	1.43
(2,92)	1:24:C:VAL:HG22	1:21:C:GLY:HA2	33	1.43
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	21	1.43
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	29	1.43
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	44	1.42
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	48	1.42
(2,415)	1:20:C:ASP:H	1:24:C:VAL:HG23	24	1.42
(2,415)	1:20:C:ASP:H	1:24:C:VAL:HG22	33	1.42
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	29	1.42
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	30	1.41
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	10	1.41
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	3	1.41
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	16	1.41
(2,252)	1:22:C:THR:HG22	1:23:C:ASP:HB3	41	1.4
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	10	1.4
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	9	1.4
(2,610)	1:24:C:VAL:HG11	1:26:C:ARG:HD2	5	1.39
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	40	1.39
(2,461)	1:31:C:ALA:H	1:27:C:CYS:HB2	14	1.39
(2,252)	1:22:C:THR:HG22	1:23:C:ASP:HB3	1	1.39
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	15	1.39
(2,93)	1:34:C:PHE:HA	1:24:C:VAL:HG23	24	1.39
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD12	13	1.38
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	48	1.38
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	38	1.37
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD11	25	1.37
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	23	1.37
(2,92)	1:24:C:VAL:HG23	1:21:C:GLY:HA2	11	1.37
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	3	1.37
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	22	1.37
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	6	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	11	1.36
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	50	1.36
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	45	1.36
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	42	1.35
(2,367)	1:35:C:HIS:HD2	1:24:C:VAL:HG22	5	1.35
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	11	1.35
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	46	1.35
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD12	33	1.35
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	21	1.35
(2,92)	1:24:C:VAL:HG21	1:21:C:GLY:HA2	22	1.35
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG22	24	1.34
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	22	1.34
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	16	1.34
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	39	1.34
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	42	1.34
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	50	1.34
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	20	1.34
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	25	1.34
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	27	1.34
(2,92)	1:24:C:VAL:HG23	1:21:C:GLY:HA2	5	1.34
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	36	1.34
(2,55)	1:24:C:VAL:HG22	1:15:C:CYS:HB3	33	1.34
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	7	1.33
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	25	1.33
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	36	1.33
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	5	1.33
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	23	1.33
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	32	1.33
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD12	17	1.33
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	15	1.33
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	4	1.33
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	26	1.33
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	19	1.33
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	16	1.32
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	22	1.32
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	37	1.32
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG22	10	1.32
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	17	1.32
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	24	1.32
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	12	1.31
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	24	1.31
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	29	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	30	1.31
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	7	1.31
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	49	1.31
(2,56)	1:24:C:VAL:HG23	1:15:C:CYS:HB2	48	1.31
(2,41)	1:9:C:LEU:HD12	1:9:C:LEU:HA	16	1.31
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	44	1.31
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	38	1.3
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	45	1.3
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	49	1.3
(2,252)	1:22:C:THR:HG23	1:23:C:ASP:HB3	50	1.3
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	2	1.3
(2,51)	1:24:C:VAL:HG23	1:15:C:CYS:HA	10	1.3
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	39	1.29
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	44	1.29
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	10	1.28
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	10	1.28
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	25	1.28
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	2	1.27
(2,367)	1:35:C:HIS:HD2	1:24:C:VAL:HG22	24	1.27
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	30	1.27
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	48	1.27
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	43	1.27
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	40	1.27
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	23	1.27
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	41	1.27
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	3	1.26
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	4	1.26
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	16	1.26
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	6	1.26
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	9	1.25
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	41	1.25
(2,367)	1:35:C:HIS:HD2	1:24:C:VAL:HG23	42	1.25
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	13	1.25
(2,176)	1:51:C:LEU:HD22	1:47:C:PRO:HD3	50	1.25
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	40	1.25
(2,92)	1:24:C:VAL:HG22	1:21:C:GLY:HA2	30	1.25
(2,92)	1:24:C:VAL:HG21	1:21:C:GLY:HA2	42	1.25
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	44	1.24
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG23	42	1.24
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	43	1.24
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	42	1.24
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	37	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,92)	1:24:C:VAL:HG23	1:21:C:GLY:HA2	7	1.24
(2,610)	1:24:C:VAL:HG13	1:26:C:ARG:HD3	10	1.23
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	30	1.23
(2,56)	1:24:C:VAL:HG23	1:15:C:CYS:HB2	5	1.23
(2,693)	1:49:C:THR:HG21	1:48:C:GLY:HA3	5	1.22
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	8	1.22
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	49	1.22
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	32	1.22
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	9	1.21
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	15	1.21
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	17	1.21
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	48	1.21
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	10	1.21
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	23	1.21
(2,90)	1:24:C:VAL:HG23	1:24:C:VAL:HA	33	1.21
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	27	1.2
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	13	1.2
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	20	1.2
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	35	1.2
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	20	1.2
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	4	1.2
(2,93)	1:34:C:PHE:HA	1:24:C:VAL:HG23	10	1.2
(2,93)	1:34:C:PHE:HA	1:24:C:VAL:HG22	30	1.2
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	43	1.19
(2,367)	1:35:C:HIS:HD2	1:24:C:VAL:HG23	22	1.19
(2,367)	1:35:C:HIS:HD2	1:24:C:VAL:HG23	31	1.19
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD12	45	1.19
(2,176)	1:51:C:LEU:HD22	1:47:C:PRO:HD3	22	1.19
(2,92)	1:24:C:VAL:HG21	1:21:C:GLY:HA2	31	1.19
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	1	1.18
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	14	1.18
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	18	1.18
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	28	1.18
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	28	1.18
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	20	1.18
(2,90)	1:24:C:VAL:HG21	1:24:C:VAL:HA	30	1.18
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	36	1.18
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	8	1.17
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	46	1.17
(2,367)	1:35:C:HIS:HD2	1:24:C:VAL:HG21	33	1.17
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	9	1.17
(2,176)	1:51:C:LEU:HD22	1:47:C:PRO:HD3	7	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	34	1.17
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	46	1.17
(2,704)	1:34:C:PHE:HE2	1:25:C:LEU:HB3	24	1.16
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG22	5	1.16
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	30	1.16
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	39	1.16
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	26	1.16
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	29	1.16
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	16	1.16
(2,90)	1:24:C:VAL:HG22	1:24:C:VAL:HA	10	1.16
(2,90)	1:24:C:VAL:HG22	1:24:C:VAL:HA	24	1.16
(2,90)	1:24:C:VAL:HG22	1:24:C:VAL:HA	48	1.16
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	23	1.15
(2,419)	1:21:C:GLY:H	1:14:C:ARG:HG2	47	1.15
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	12	1.15
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	30	1.15
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	19	1.14
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	21	1.14
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	37	1.14
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	47	1.14
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	19	1.14
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	36	1.14
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	24	1.14
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	7	1.14
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	39	1.14
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	44	1.14
(2,92)	1:24:C:VAL:HG23	1:21:C:GLY:HA2	24	1.14
(2,90)	1:24:C:VAL:HG21	1:24:C:VAL:HA	27	1.14
(2,55)	1:24:C:VAL:HG21	1:15:C:CYS:HB3	42	1.14
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	34	1.13
(2,367)	1:35:C:HIS:HD2	1:24:C:VAL:HG21	27	1.13
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	4	1.13
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	26	1.13
(2,93)	1:34:C:PHE:HA	1:24:C:VAL:HG23	7	1.13
(2,90)	1:24:C:VAL:HG22	1:24:C:VAL:HA	11	1.13
(2,90)	1:24:C:VAL:HG23	1:24:C:VAL:HA	31	1.13
(2,703)	1:34:C:PHE:HZ	1:51:C:LEU:HD13	37	1.12
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	24	1.12
(2,357)	1:34:C:PHE:H	1:24:C:VAL:HG21	24	1.12
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	12	1.12
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	35	1.12
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	48	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	40	1.12
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	36	1.12
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	44	1.12
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	11	1.12
(2,93)	1:34:C:PHE:HA	1:24:C:VAL:HG23	48	1.12
(2,90)	1:24:C:VAL:HG22	1:24:C:VAL:HA	7	1.12
(2,90)	1:24:C:VAL:HG23	1:24:C:VAL:HA	22	1.12
(2,90)	1:24:C:VAL:HG23	1:24:C:VAL:HA	42	1.12
(2,73)	1:14:C:ARG:HB3	1:21:C:GLY:HA3	45	1.12
(2,51)	1:24:C:VAL:HG23	1:15:C:CYS:HA	24	1.12
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	6	1.11
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	34	1.11
(2,90)	1:24:C:VAL:HG22	1:24:C:VAL:HA	5	1.11
(2,693)	1:49:C:THR:HG21	1:48:C:GLY:HA3	23	1.1
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	26	1.1
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	20	1.1
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	15	1.1
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	1	1.1
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD12	29	1.1
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	3	1.1
(2,93)	1:34:C:PHE:HA	1:24:C:VAL:HG21	31	1.1
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	46	1.09
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	36	1.09
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	47	1.09
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	45	1.09
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	12	1.09
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	40	1.09
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	29	1.09
(2,419)	1:21:C:GLY:H	1:14:C:ARG:HG2	28	1.07
(2,361)	1:15:C:CYS:H	1:24:C:VAL:HG21	31	1.07
(2,264)	1:52:C:ARG:H	1:51:C:LEU:HD11	49	1.07
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	6	1.07
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	50	1.07
(2,176)	1:51:C:LEU:HD22	1:47:C:PRO:HD3	6	1.07
(2,176)	1:51:C:LEU:HD22	1:47:C:PRO:HD3	25	1.07
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	43	1.06
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG23	22	1.06
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	3	1.06
(2,93)	1:34:C:PHE:HA	1:24:C:VAL:HG23	11	1.06
(2,55)	1:24:C:VAL:HG23	1:15:C:CYS:HB3	11	1.06
(2,693)	1:49:C:THR:HG22	1:48:C:GLY:HA3	44	1.05
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	50	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	32	1.05
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	33	1.05
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	26	1.05
(2,93)	1:34:C:PHE:HA	1:24:C:VAL:HG21	22	1.05
(2,56)	1:24:C:VAL:HG22	1:15:C:CYS:HB2	30	1.05
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	3	1.04
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	29	1.04
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	36	1.04
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	36	1.04
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	12	1.04
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	47	1.04
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	41	1.04
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	13	1.03
(2,692)	1:52:C:ARG:HG2	1:50:C:GLY:HA3	30	1.02
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	28	1.02
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	43	1.02
(2,361)	1:15:C:CYS:H	1:24:C:VAL:HG23	24	1.02
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	44	1.02
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	25	1.02
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	43	1.02
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	1	1.01
(2,479)	1:36:C:TRP:H	1:25:C:LEU:HB3	21	1.01
(2,455)	1:30:C:CYS:H	1:29:C:HIS:HB2	19	1.01
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	14	1.01
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	18	1.01
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	34	1.01
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	37	1.01
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	16	1.0
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	18	1.0
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	22	1.0
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	27	1.0
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	42	1.0
(2,176)	1:51:C:LEU:HD22	1:47:C:PRO:HD3	11	1.0
(2,166)	1:40:C:PHE:HD1	1:44:C:THR:HG21	17	1.0
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	37	1.0
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	10	1.0
(2,93)	1:34:C:PHE:HA	1:24:C:VAL:HG21	42	1.0
(2,693)	1:49:C:THR:HG21	1:48:C:GLY:HA3	3	0.99
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	5	0.99
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	21	0.99
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	24	0.99
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	14	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	30	0.99
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	44	0.99
(2,55)	1:24:C:VAL:HG23	1:15:C:CYS:HB3	7	0.99
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	25	0.98
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	37	0.98
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	6	0.98
(2,133)	1:40:C:PHE:HB3	1:36:C:TRP:HA	14	0.98
(2,51)	1:24:C:VAL:HG22	1:15:C:CYS:HA	27	0.98
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	46	0.97
(2,419)	1:21:C:GLY:H	1:14:C:ARG:HG2	27	0.97
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	50	0.97
(2,176)	1:51:C:LEU:HD22	1:47:C:PRO:HD3	10	0.97
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	13	0.97
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	3	0.97
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	4	0.97
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	28	0.97
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	49	0.97
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	5	0.97
(2,51)	1:24:C:VAL:HG21	1:15:C:CYS:HA	42	0.97
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	35	0.96
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	9	0.96
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	11	0.96
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	15	0.96
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	45	0.96
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	17	0.95
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	32	0.95
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	37	0.95
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	24	0.95
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	44	0.95
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	16	0.95
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	13	0.95
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	22	0.95
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	43	0.95
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	44	0.94
(2,610)	1:24:C:VAL:HG12	1:26:C:ARG:HD2	24	0.94
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	15	0.94
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	25	0.94
(2,455)	1:30:C:CYS:H	1:29:C:HIS:HB2	43	0.94
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	30	0.94
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	33	0.94
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	41	0.94
(2,93)	1:34:C:PHE:HA	1:24:C:VAL:HG23	5	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	32	0.93
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	3	0.93
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	30	0.92
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	49	0.92
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	38	0.92
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	38	0.92
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	47	0.92
(2,93)	1:34:C:PHE:HA	1:24:C:VAL:HG22	27	0.92
(2,92)	1:24:C:VAL:HG22	1:21:C:GLY:HA2	27	0.92
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	43	0.91
(2,702)	1:34:C:PHE:HZ	1:51:C:LEU:HD21	14	0.91
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	16	0.91
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	31	0.91
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	11	0.91
(2,361)	1:15:C:CYS:H	1:24:C:VAL:HG23	10	0.91
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	1	0.91
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	42	0.91
(2,68)	1:14:C:ARG:HG2	1:20:C:ASP:HA	28	0.91
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	15	0.9
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	25	0.9
(2,264)	1:52:C:ARG:H	1:51:C:LEU:HD12	37	0.9
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	4	0.9
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	1	0.9
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	8	0.9
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	3	0.89
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	16	0.89
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	33	0.89
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	14	0.89
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	5	0.89
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	41	0.89
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	25	0.89
(2,55)	1:24:C:VAL:HG23	1:15:C:CYS:HB3	5	0.89
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	6	0.88
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	26	0.88
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	16	0.88
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	27	0.88
(2,176)	1:51:C:LEU:HD22	1:47:C:PRO:HD3	47	0.88
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	45	0.88
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	35	0.88
(2,93)	1:34:C:PHE:HA	1:24:C:VAL:HG22	33	0.88
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	21	0.87
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	12	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	15	0.87
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	27	0.87
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG11	32	0.87
(2,233)	1:51:C:LEU:HD13	1:51:C:LEU:HB2	40	0.87
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	31	0.87
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	24	0.87
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	28	0.87
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	3	0.87
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	27	0.87
(2,55)	1:24:C:VAL:HG23	1:15:C:CYS:HB3	48	0.87
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	5	0.86
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	22	0.86
(2,233)	1:51:C:LEU:HD13	1:51:C:LEU:HB2	1	0.86
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	9	0.86
(2,233)	1:51:C:LEU:HD13	1:51:C:LEU:HB2	11	0.86
(2,233)	1:51:C:LEU:HD13	1:51:C:LEU:HB2	13	0.86
(2,233)	1:51:C:LEU:HD12	1:51:C:LEU:HB2	42	0.86
(2,233)	1:51:C:LEU:HD13	1:51:C:LEU:HB2	45	0.86
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	41	0.86
(2,176)	1:51:C:LEU:HD22	1:47:C:PRO:HD3	35	0.86
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	48	0.86
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	28	0.86
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	14	0.85
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG11	21	0.85
(2,357)	1:34:C:PHE:H	1:24:C:VAL:HG21	5	0.85
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	21	0.85
(2,233)	1:51:C:LEU:HD13	1:51:C:LEU:HB2	2	0.85
(2,233)	1:51:C:LEU:HD12	1:51:C:LEU:HB2	16	0.85
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	22	0.85
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	23	0.85
(2,233)	1:51:C:LEU:HD12	1:51:C:LEU:HB2	25	0.85
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	31	0.85
(2,233)	1:51:C:LEU:HD13	1:51:C:LEU:HB2	33	0.85
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	38	0.85
(2,233)	1:51:C:LEU:HD12	1:51:C:LEU:HB2	46	0.85
(2,233)	1:51:C:LEU:HD13	1:51:C:LEU:HB2	48	0.85
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	24	0.85
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	47	0.84
(2,634)	1:17:C:VAL:HG21	1:38:C:CYS:HB2	5	0.84
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	4	0.84
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	7	0.84
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	22	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	26	0.84
(2,233)	1:51:C:LEU:HD13	1:51:C:LEU:HB2	3	0.84
(2,233)	1:51:C:LEU:HD12	1:51:C:LEU:HB2	8	0.84
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	14	0.84
(2,233)	1:51:C:LEU:HD13	1:51:C:LEU:HB2	17	0.84
(2,233)	1:51:C:LEU:HD12	1:51:C:LEU:HB2	21	0.84
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	36	0.84
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	40	0.84
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	35	0.84
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	23	0.84
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	36	0.84
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	10	0.83
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	18	0.83
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	3	0.83
(2,419)	1:21:C:GLY:H	1:14:C:ARG:HG2	13	0.83
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	1	0.83
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	29	0.83
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	35	0.83
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	20	0.83
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	41	0.83
(2,233)	1:51:C:LEU:HD13	1:51:C:LEU:HB2	6	0.83
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	7	0.83
(2,233)	1:51:C:LEU:HD12	1:51:C:LEU:HB2	15	0.83
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	19	0.83
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	20	0.83
(2,233)	1:51:C:LEU:HD13	1:51:C:LEU:HB2	27	0.83
(2,233)	1:51:C:LEU:HD13	1:51:C:LEU:HB2	28	0.83
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	30	0.83
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	32	0.83
(2,233)	1:51:C:LEU:HD12	1:51:C:LEU:HB2	50	0.83
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	4	0.83
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	19	0.83
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	19	0.83
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	50	0.83
(2,73)	1:14:C:ARG:HB3	1:21:C:GLY:HA3	13	0.83
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	34	0.82
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	23	0.82
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	36	0.82
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	23	0.82
(2,233)	1:51:C:LEU:HD12	1:51:C:LEU:HB2	5	0.82
(2,233)	1:51:C:LEU:HD12	1:51:C:LEU:HB2	34	0.82
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	35	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	43	0.82
(2,233)	1:51:C:LEU:HD12	1:51:C:LEU:HB2	44	0.82
(2,176)	1:51:C:LEU:HD21	1:47:C:PRO:HD3	43	0.82
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	50	0.82
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	20	0.82
(2,51)	1:24:C:VAL:HG21	1:15:C:CYS:HA	31	0.82
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	50	0.81
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	7	0.81
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	8	0.81
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	37	0.81
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	48	0.81
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	9	0.81
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	19	0.81
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	46	0.81
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG13	34	0.81
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	34	0.81
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	10	0.81
(2,233)	1:51:C:LEU:HD12	1:51:C:LEU:HB2	24	0.81
(2,233)	1:51:C:LEU:HD13	1:51:C:LEU:HB2	29	0.81
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	41	0.81
(2,233)	1:51:C:LEU:HD13	1:51:C:LEU:HB2	47	0.81
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	48	0.81
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	49	0.81
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	17	0.81
(2,176)	1:51:C:LEU:HD22	1:47:C:PRO:HD3	19	0.81
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	8	0.81
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	15	0.81
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	32	0.81
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	38	0.81
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	18	0.81
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	33	0.8
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	36	0.8
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	2	0.8
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	15	0.8
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	17	0.8
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	20	0.8
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	30	0.8
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	40	0.8
(2,361)	1:15:C:CYS:H	1:24:C:VAL:HG23	11	0.8
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG21	33	0.8
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	13	0.8
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	19	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,233)	1:51:C:LEU:HD12	1:51:C:LEU:HB2	26	0.8
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	40	0.8
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	1	0.8
(2,145)	1:39:C:HIS:HD2	1:38:C:CYS:HB3	14	0.8
(2,116)	1:28:C:THR:HG23	1:28:C:THR:HA	30	0.8
(2,51)	1:24:C:VAL:HG23	1:15:C:CYS:HA	5	0.8
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	2	0.8
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	6	0.79
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	11	0.79
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	17	0.79
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	40	0.79
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	35	0.79
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	50	0.79
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	31	0.79
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	42	0.79
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	49	0.79
(2,361)	1:15:C:CYS:H	1:24:C:VAL:HG23	48	0.79
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG12	2	0.79
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG13	20	0.79
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG13	23	0.79
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	18	0.79
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	4	0.79
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	12	0.79
(2,233)	1:51:C:LEU:HD13	1:51:C:LEU:HB2	18	0.79
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	39	0.79
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	47	0.78
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	19	0.78
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	33	0.78
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	6	0.78
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	11	0.78
(2,361)	1:15:C:CYS:H	1:24:C:VAL:HG21	22	0.78
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG11	18	0.78
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG12	38	0.78
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG13	49	0.78
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	48	0.78
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	24	0.78
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	42	0.78
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	46	0.78
(2,188)	1:51:C:LEU:HD22	1:51:C:LEU:HB3	5	0.78
(2,188)	1:51:C:LEU:HD21	1:51:C:LEU:HB3	6	0.78
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	14	0.78
(2,188)	1:51:C:LEU:HD22	1:51:C:LEU:HB3	17	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	29	0.78
(2,188)	1:51:C:LEU:HD21	1:51:C:LEU:HB3	43	0.78
(2,188)	1:51:C:LEU:HD22	1:51:C:LEU:HB3	47	0.78
(2,188)	1:51:C:LEU:HD21	1:51:C:LEU:HB3	50	0.78
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	21	0.78
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	13	0.78
(2,68)	1:14:C:ARG:HG2	1:20:C:ASP:HA	17	0.78
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	48	0.77
(2,634)	1:17:C:VAL:HG21	1:38:C:CYS:HB2	40	0.77
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	20	0.77
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG13	12	0.77
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	1	0.77
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	11	0.77
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	29	0.77
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	48	0.77
(2,233)	1:51:C:LEU:HD11	1:51:C:LEU:HB2	39	0.77
(2,188)	1:51:C:LEU:HD21	1:51:C:LEU:HB3	10	0.77
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	12	0.77
(2,188)	1:51:C:LEU:HD22	1:51:C:LEU:HB3	15	0.77
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	18	0.77
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	24	0.77
(2,188)	1:51:C:LEU:HD22	1:51:C:LEU:HB3	27	0.77
(2,188)	1:51:C:LEU:HD22	1:51:C:LEU:HB3	28	0.77
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	32	0.77
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	34	0.77
(2,188)	1:51:C:LEU:HD21	1:51:C:LEU:HB3	38	0.77
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	42	0.77
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	10	0.77
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	22	0.77
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	10	0.76
(2,634)	1:17:C:VAL:HG21	1:38:C:CYS:HB2	29	0.76
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	42	0.76
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	49	0.76
(2,361)	1:15:C:CYS:H	1:24:C:VAL:HG21	42	0.76
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG12	9	0.76
(2,357)	1:34:C:PHE:H	1:24:C:VAL:HG22	31	0.76
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	12	0.76
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	32	0.76
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	50	0.76
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	1	0.76
(2,188)	1:51:C:LEU:HD22	1:51:C:LEU:HB3	3	0.76
(2,188)	1:51:C:LEU:HD21	1:51:C:LEU:HB3	4	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,188)	1:51:C:LEU:HD21	1:51:C:LEU:HB3	8	0.76
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	9	0.76
(2,188)	1:51:C:LEU:HD21	1:51:C:LEU:HB3	11	0.76
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	13	0.76
(2,188)	1:51:C:LEU:HD22	1:51:C:LEU:HB3	16	0.76
(2,188)	1:51:C:LEU:HD21	1:51:C:LEU:HB3	19	0.76
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	20	0.76
(2,188)	1:51:C:LEU:HD22	1:51:C:LEU:HB3	21	0.76
(2,188)	1:51:C:LEU:HD22	1:51:C:LEU:HB3	23	0.76
(2,188)	1:51:C:LEU:HD21	1:51:C:LEU:HB3	25	0.76
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	26	0.76
(2,188)	1:51:C:LEU:HD22	1:51:C:LEU:HB3	30	0.76
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	31	0.76
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	33	0.76
(2,188)	1:51:C:LEU:HD22	1:51:C:LEU:HB3	35	0.76
(2,188)	1:51:C:LEU:HD22	1:51:C:LEU:HB3	36	0.76
(2,188)	1:51:C:LEU:HD22	1:51:C:LEU:HB3	44	0.76
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	46	0.76
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	48	0.76
(2,145)	1:39:C:HIS:HD2	1:38:C:CYS:HB3	17	0.76
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	26	0.76
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	44	0.75
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	22	0.75
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	37	0.75
(2,357)	1:34:C:PHE:H	1:24:C:VAL:HG22	22	0.75
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	36	0.75
(2,188)	1:51:C:LEU:HD22	1:51:C:LEU:HB3	2	0.75
(2,188)	1:51:C:LEU:HD21	1:51:C:LEU:HB3	7	0.75
(2,188)	1:51:C:LEU:HD21	1:51:C:LEU:HB3	22	0.75
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	39	0.75
(2,188)	1:51:C:LEU:HD21	1:51:C:LEU:HB3	40	0.75
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	41	0.75
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	42	0.75
(2,188)	1:51:C:LEU:HD23	1:51:C:LEU:HB3	45	0.75
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	31	0.75
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	39	0.75
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	9	0.75
(2,116)	1:28:C:THR:HG22	1:28:C:THR:HA	50	0.75
(2,778)	1:36:C:TRP:HE1	1:46:C:ARG:HD3	11	0.74
(2,778)	1:36:C:TRP:HE1	1:46:C:ARG:HD2	39	0.74
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	8	0.74
(2,692)	1:52:C:ARG:HG2	1:50:C:GLY:HA3	34	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	44	0.74
(2,366)	1:35:C:HIS:HD2	1:24:C:VAL:HG13	43	0.74
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG13	14	0.74
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	25	0.74
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	28	0.74
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	15	0.74
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	5	0.74
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	9	0.74
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	27	0.74
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	32	0.73
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	11	0.73
(2,584)	1:34:C:PHE:HE1	1:39:C:HIS:HE1	4	0.73
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	24	0.73
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	29	0.73
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	13	0.73
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG12	17	0.73
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	10	0.73
(2,357)	1:34:C:PHE:H	1:24:C:VAL:HG21	7	0.73
(2,357)	1:34:C:PHE:H	1:24:C:VAL:HG21	10	0.73
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	2	0.73
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	10	0.73
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	27	0.73
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	31	0.73
(2,176)	1:51:C:LEU:HD23	1:47:C:PRO:HD3	18	0.73
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	31	0.73
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	31	0.73
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	48	0.73
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	50	0.73
(2,116)	1:28:C:THR:HG21	1:28:C:THR:HA	9	0.73
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	36	0.72
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	5	0.72
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	19	0.72
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	22	0.72
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	16	0.72
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	41	0.72
(2,381)	1:9:C:LEU:H	1:9:C:LEU:HB3	25	0.72
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG21	47	0.72
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG21	50	0.72
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	5	0.72
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	40	0.72
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	45	0.72
(2,214)	1:56:C:CYS:HB2	1:52:C:ARG:HG3	34	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD11	49	0.72
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	6	0.72
(2,71)	1:35:C:HIS:HE1	1:20:C:ASP:HB2	2	0.72
(2,634)	1:17:C:VAL:HG12	1:38:C:CYS:HB2	3	0.71
(2,581)	1:49:C:THR:H	1:49:C:THR:HG21	23	0.71
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	5	0.71
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	14	0.71
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	18	0.71
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	42	0.71
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	26	0.71
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	30	0.71
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	39	0.71
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	46	0.71
(2,693)	1:49:C:THR:HG23	1:48:C:GLY:HA3	49	0.7
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	25	0.7
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	9	0.7
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	46	0.7
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	15	0.7
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	16	0.7
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	47	0.7
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	17	0.7
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	19	0.7
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	24	0.7
(2,55)	1:24:C:VAL:HG22	1:15:C:CYS:HB3	30	0.7
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD3	16	0.69
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	9	0.69
(2,702)	1:34:C:PHE:HZ	1:51:C:LEU:HD23	39	0.69
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	49	0.69
(2,634)	1:17:C:VAL:HG21	1:38:C:CYS:HB2	10	0.69
(2,634)	1:17:C:VAL:HG22	1:38:C:CYS:HB2	44	0.69
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	19	0.69
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	3	0.69
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	8	0.69
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	43	0.69
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	14	0.69
(2,73)	1:14:C:ARG:HB3	1:21:C:GLY:HA3	43	0.69
(2,68)	1:14:C:ARG:HG2	1:20:C:ASP:HA	27	0.69
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	45	0.68
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	32	0.68
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	38	0.68
(2,468)	1:32:C:ALA:H	1:27:C:CYS:HB2	3	0.68
(2,468)	1:32:C:ALA:H	1:27:C:CYS:HB2	26	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	19	0.68
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG12	6	0.68
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG13	19	0.68
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG11	29	0.68
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG23	12	0.68
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	17	0.68
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	35	0.68
(2,51)	1:24:C:VAL:HG23	1:15:C:CYS:HA	11	0.68
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD3	39	0.67
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD3	44	0.67
(2,702)	1:34:C:PHE:HZ	1:51:C:LEU:HD23	23	0.67
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	21	0.67
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	4	0.67
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	17	0.67
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	6	0.67
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	14	0.67
(2,261)	1:25:C:LEU:H	1:24:C:VAL:HG22	22	0.67
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	38	0.67
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	32	0.67
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	17	0.67
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	33	0.67
(2,614)	1:14:C:ARG:HB3	1:21:C:GLY:HA2	47	0.66
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	1	0.66
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	27	0.66
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	28	0.66
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG13	13	0.66
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG11	26	0.66
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG23	9	0.66
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	9	0.66
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	37	0.66
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	31	0.66
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	6	0.66
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	8	0.66
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	9	0.66
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	37	0.66
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	38	0.66
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	44	0.66
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	47	0.66
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	49	0.66
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD3	14	0.65
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	30	0.65
(2,704)	1:34:C:PHE:HE2	1:25:C:LEU:HB3	26	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,692)	1:52:C:ARG:HG2	1:50:C:GLY:HA3	41	0.65
(2,634)	1:17:C:VAL:HG21	1:38:C:CYS:HB2	11	0.65
(2,634)	1:17:C:VAL:HG22	1:38:C:CYS:HB2	21	0.65
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	7	0.65
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	12	0.65
(2,522)	1:46:C:ARG:H	1:46:C:ARG:HB3	2	0.65
(2,522)	1:46:C:ARG:H	1:46:C:ARG:HB3	13	0.65
(2,387)	1:12:C:GLY:H	1:10:C:ALA:HB2	1	0.65
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG13	28	0.65
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	40	0.65
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	49	0.65
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	38	0.65
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	44	0.65
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	49	0.65
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	3	0.65
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	5	0.65
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	14	0.65
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	15	0.65
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	16	0.65
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	27	0.65
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	30	0.65
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	35	0.65
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	39	0.65
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	43	0.65
(2,778)	1:36:C:TRP:HE1	1:46:C:ARG:HD2	37	0.64
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD3	35	0.64
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD3	36	0.64
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	27	0.64
(2,716)	1:6:C:GLN:H	1:7:C:GLN:HB2	12	0.64
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	2	0.64
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	8	0.64
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	47	0.64
(2,522)	1:46:C:ARG:H	1:46:C:ARG:HB3	10	0.64
(2,468)	1:32:C:ALA:H	1:27:C:CYS:HB2	12	0.64
(2,387)	1:12:C:GLY:H	1:10:C:ALA:HB3	37	0.64
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG11	46	0.64
(2,357)	1:34:C:PHE:H	1:24:C:VAL:HG21	11	0.64
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB3	12	0.64
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB3	26	0.64
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	33	0.64
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	39	0.64
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	11	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	16	0.64
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	2	0.64
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	10	0.64
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	25	0.64
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	28	0.64
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	31	0.64
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	40	0.64
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	45	0.64
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD3	18	0.63
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	42	0.63
(2,634)	1:17:C:VAL:HG12	1:38:C:CYS:HB2	7	0.63
(2,468)	1:32:C:ALA:H	1:27:C:CYS:HB2	50	0.63
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	39	0.63
(2,387)	1:12:C:GLY:H	1:10:C:ALA:HB2	30	0.63
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG21	23	0.63
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG23	34	0.63
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	2	0.63
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	17	0.63
(2,261)	1:25:C:LEU:H	1:24:C:VAL:HG21	7	0.63
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	49	0.63
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	12	0.63
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	32	0.63
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	36	0.63
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	48	0.63
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	50	0.63
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD3	2	0.62
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	5	0.62
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	10	0.62
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	26	0.62
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	31	0.62
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	34	0.62
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	39	0.62
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	16	0.62
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	33	0.62
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	41	0.62
(2,181)	1:49:C:THR:HG22	1:49:C:THR:HA	35	0.62
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	29	0.62
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	38	0.62
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	1	0.62
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	11	0.62
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	24	0.62
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	29	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	46	0.62
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD3	13	0.61
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD3	27	0.61
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD3	43	0.61
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	30	0.61
(2,610)	1:24:C:VAL:HG11	1:26:C:ARG:HD3	36	0.61
(2,522)	1:46:C:ARG:H	1:46:C:ARG:HB3	6	0.61
(2,522)	1:46:C:ARG:H	1:46:C:ARG:HB3	33	0.61
(2,387)	1:12:C:GLY:H	1:10:C:ALA:HB3	7	0.61
(2,366)	1:35:C:HIS:HD2	1:24:C:VAL:HG11	3	0.61
(2,361)	1:15:C:CYS:H	1:24:C:VAL:HG22	27	0.61
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	44	0.61
(2,309)	1:36:C:TRP:HD1	1:36:C:TRP:HB2	6	0.61
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	2	0.61
(2,181)	1:49:C:THR:HG21	1:49:C:THR:HA	25	0.61
(2,181)	1:49:C:THR:HG23	1:49:C:THR:HA	37	0.61
(2,181)	1:49:C:THR:HG22	1:49:C:THR:HA	45	0.61
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	18	0.61
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	42	0.61
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	23	0.6
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	1	0.6
(2,387)	1:12:C:GLY:H	1:10:C:ALA:HB3	19	0.6
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	3	0.6
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	5	0.6
(2,181)	1:49:C:THR:HG22	1:49:C:THR:HA	41	0.6
(2,181)	1:49:C:THR:HG22	1:49:C:THR:HA	42	0.6
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	39	0.6
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	13	0.6
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	19	0.6
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	1	0.59
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	28	0.59
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	1	0.59
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	22	0.59
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	25	0.59
(2,634)	1:17:C:VAL:HG11	1:38:C:CYS:HB2	34	0.59
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	40	0.59
(2,387)	1:12:C:GLY:H	1:10:C:ALA:HB2	28	0.59
(2,361)	1:15:C:CYS:H	1:24:C:VAL:HG23	7	0.59
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG23	1	0.59
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	16	0.59
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	19	0.59
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB2	41	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	19	0.59
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	21	0.59
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	24	0.59
(2,261)	1:25:C:LEU:H	1:24:C:VAL:HG21	5	0.59
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	41	0.59
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	47	0.59
(2,181)	1:49:C:THR:HG23	1:49:C:THR:HA	4	0.59
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	46	0.59
(2,68)	1:14:C:ARG:HG2	1:20:C:ASP:HA	47	0.59
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	23	0.59
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	34	0.59
(2,15)	1:39:C:HIS:HE1	1:53:C:CYS:HB3	30	0.59
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD3	50	0.58
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD21	2	0.58
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	20	0.58
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	48	0.58
(2,585)	1:54:C:ARG:HG2	1:39:C:HIS:HE1	7	0.58
(2,584)	1:34:C:PHE:HE2	1:39:C:HIS:HE1	14	0.58
(2,575)	1:36:C:TRP:HE1	1:46:C:ARG:HB2	10	0.58
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	9	0.58
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	49	0.58
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG21	30	0.58
(2,181)	1:49:C:THR:HG23	1:49:C:THR:HA	40	0.58
(2,181)	1:49:C:THR:HG21	1:49:C:THR:HA	47	0.58
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	29	0.58
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	47	0.57
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	33	0.57
(2,704)	1:34:C:PHE:HE2	1:25:C:LEU:HB3	38	0.57
(2,702)	1:34:C:PHE:HZ	1:51:C:LEU:HD21	4	0.57
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	38	0.57
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	3	0.57
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	29	0.57
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	13	0.57
(2,419)	1:21:C:GLY:H	1:14:C:ARG:HG2	6	0.57
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	29	0.57
(2,187)	1:47:C:PRO:HD3	1:51:C:LEU:HD13	37	0.57
(2,181)	1:49:C:THR:HG22	1:49:C:THR:HA	49	0.57
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	10	0.57
(2,168)	1:44:C:THR:HG22	1:46:C:ARG:HA	17	0.57
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	26	0.57
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	11	0.57
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	42	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,145)	1:39:C:HIS:HD2	1:38:C:CYS:HB3	33	0.57
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	39	0.57
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	7	0.57
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	20	0.57
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	22	0.57
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	41	0.57
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD3	8	0.56
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	38	0.56
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	9	0.56
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	15	0.56
(2,716)	1:6:C:GLN:H	1:7:C:GLN:HB2	8	0.56
(2,704)	1:34:C:PHE:HE2	1:25:C:LEU:HB3	3	0.56
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	49	0.56
(2,634)	1:17:C:VAL:HG12	1:38:C:CYS:HB2	18	0.56
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	19	0.56
(2,575)	1:36:C:TRP:HE1	1:46:C:ARG:HB2	13	0.56
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	20	0.56
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	31	0.56
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	10	0.56
(2,468)	1:32:C:ALA:H	1:27:C:CYS:HB2	31	0.56
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG21	21	0.56
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB2	20	0.56
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	22	0.56
(2,220)	1:60:C:VAL:HA	1:60:C:VAL:HG22	29	0.56
(2,185)	1:51:C:LEU:HD12	1:51:C:LEU:HA	37	0.56
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	10	0.56
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	4	0.56
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	21	0.56
(2,31)	1:36:C:TRP:HE3	1:36:C:TRP:HB3	26	0.56
(2,778)	1:36:C:TRP:HE1	1:46:C:ARG:HD2	25	0.55
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD3	11	0.55
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD3	37	0.55
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	42	0.55
(2,585)	1:54:C:ARG:HG3	1:39:C:HIS:HE1	42	0.55
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	26	0.55
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	38	0.55
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	41	0.55
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	30	0.55
(2,73)	1:14:C:ARG:HB3	1:21:C:GLY:HA3	41	0.55
(2,585)	1:54:C:ARG:HG3	1:39:C:HIS:HE1	12	0.54
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	17	0.54
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	43	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	42	0.54
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	46	0.54
(2,419)	1:21:C:GLY:H	1:14:C:ARG:HG2	14	0.54
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG13	35	0.54
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG11	44	0.54
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	7	0.54
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB2	17	0.54
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	34	0.54
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	2	0.54
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	25	0.53
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	29	0.53
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	16	0.53
(2,678)	1:57:C:SER:HB3	1:52:C:ARG:HB2	17	0.53
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	39	0.53
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	4	0.53
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	44	0.53
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	45	0.53
(2,419)	1:21:C:GLY:H	1:14:C:ARG:HG2	17	0.53
(2,361)	1:15:C:CYS:H	1:24:C:VAL:HG22	33	0.53
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	22	0.53
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	7	0.53
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	31	0.53
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	46	0.53
(2,220)	1:60:C:VAL:HA	1:60:C:VAL:HG23	37	0.53
(2,185)	1:51:C:LEU:HD11	1:51:C:LEU:HA	49	0.53
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	20	0.53
(2,91)	1:24:C:VAL:HG21	1:14:C:ARG:HA	42	0.53
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	45	0.52
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	49	0.52
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	23	0.52
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD22	42	0.52
(2,702)	1:34:C:PHE:HZ	1:51:C:LEU:HD21	45	0.52
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	34	0.52
(2,585)	1:54:C:ARG:HG3	1:39:C:HIS:HE1	40	0.52
(2,535)	1:54:C:ARG:H	1:53:C:CYS:HB3	45	0.52
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	35	0.52
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	9	0.52
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	17	0.52
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG21	14	0.52
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG21	35	0.52
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	46	0.52
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	34	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	10	0.52
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	8	0.52
(2,151)	1:54:C:ARG:HB2	1:39:C:HIS:HA	25	0.52
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	45	0.51
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	7	0.51
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD23	7	0.51
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	12	0.51
(2,585)	1:54:C:ARG:HG3	1:39:C:HIS:HE1	18	0.51
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	24	0.51
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	25	0.51
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	27	0.51
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	37	0.51
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	5	0.51
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	16	0.51
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	24	0.51
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	36	0.51
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	40	0.51
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG13	39	0.51
(2,357)	1:34:C:PHE:H	1:24:C:VAL:HG22	42	0.51
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	47	0.51
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	4	0.51
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	23	0.51
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	48	0.51
(2,261)	1:25:C:LEU:H	1:24:C:VAL:HG23	30	0.51
(2,220)	1:60:C:VAL:HA	1:60:C:VAL:HG21	18	0.51
(2,220)	1:60:C:VAL:HA	1:60:C:VAL:HG22	31	0.51
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	13	0.51
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	41	0.51
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	17	0.51
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	19	0.5
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	48	0.5
(2,678)	1:57:C:SER:HB3	1:52:C:ARG:HB3	11	0.5
(2,678)	1:57:C:SER:HB3	1:52:C:ARG:HB2	26	0.5
(2,634)	1:17:C:VAL:HG22	1:38:C:CYS:HB2	4	0.5
(2,634)	1:17:C:VAL:HG22	1:38:C:CYS:HB2	13	0.5
(2,585)	1:54:C:ARG:HG2	1:39:C:HIS:HE1	47	0.5
(2,581)	1:49:C:THR:H	1:49:C:THR:HG21	5	0.5
(2,581)	1:49:C:THR:H	1:49:C:THR:HG22	44	0.5
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	1	0.5
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	8	0.5
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	32	0.5
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	36	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	40	0.5
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	44	0.5
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	47	0.5
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	50	0.5
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB2	13	0.5
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	23	0.5
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	13	0.5
(2,252)	1:22:C:THR:HG22	1:23:C:ASP:HB3	13	0.5
(2,220)	1:60:C:VAL:HA	1:60:C:VAL:HG21	5	0.5
(2,220)	1:60:C:VAL:HA	1:60:C:VAL:HG22	24	0.5
(2,220)	1:60:C:VAL:HA	1:60:C:VAL:HG23	36	0.5
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	41	0.5
(2,165)	1:36:C:TRP:HZ2	1:44:C:THR:HG22	17	0.5
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	40	0.5
(2,62)	1:17:C:VAL:HG13	1:18:C:CYS:HB2	34	0.5
(2,51)	1:24:C:VAL:HG23	1:15:C:CYS:HA	7	0.5
(2,704)	1:34:C:PHE:HE1	1:25:C:LEU:HB3	31	0.49
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	37	0.49
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	26	0.49
(2,634)	1:17:C:VAL:HG22	1:38:C:CYS:HB2	43	0.49
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	6	0.49
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	15	0.49
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	31	0.49
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	41	0.49
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	13	0.49
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	21	0.49
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	37	0.49
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	43	0.49
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG23	2	0.49
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB3	16	0.49
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB3	42	0.49
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB3	46	0.49
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	12	0.49
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	48	0.49
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	7	0.49
(2,73)	1:14:C:ARG:HB3	1:21:C:GLY:HA3	46	0.49
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	8	0.48
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	25	0.48
(2,715)	1:6:C:GLN:H	1:6:C:GLN:HG3	28	0.48
(2,704)	1:34:C:PHE:HE1	1:25:C:LEU:HB3	36	0.48
(2,634)	1:17:C:VAL:HG21	1:38:C:CYS:HB2	47	0.48
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	3	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	45	0.48
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	18	0.48
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG11	8	0.48
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG11	15	0.48
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	7	0.48
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG21	8	0.48
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	8	0.48
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB3	33	0.48
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	2	0.48
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	11	0.48
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	26	0.48
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	5	0.48
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	21	0.48
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD3	9	0.47
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	28	0.47
(2,702)	1:34:C:PHE:HZ	1:51:C:LEU:HD23	40	0.47
(2,678)	1:57:C:SER:HB3	1:52:C:ARG:HB2	4	0.47
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	20	0.47
(2,585)	1:54:C:ARG:HG3	1:39:C:HIS:HE1	23	0.47
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	15	0.47
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	47	0.47
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB2	18	0.47
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	29	0.47
(2,261)	1:25:C:LEU:H	1:24:C:VAL:HG21	10	0.47
(2,261)	1:25:C:LEU:H	1:24:C:VAL:HG23	27	0.47
(2,213)	1:52:C:ARG:HG3	1:56:C:CYS:HB3	36	0.47
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	33	0.47
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	48	0.47
(2,145)	1:39:C:HIS:HD2	1:38:C:CYS:HB3	32	0.47
(2,62)	1:17:C:VAL:HG12	1:18:C:CYS:HB2	30	0.47
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	6	0.46
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD21	21	0.46
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	41	0.46
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	13	0.46
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	4	0.46
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	46	0.46
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	28	0.46
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG12	1	0.46
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	5	0.46
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	4	0.46
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	14	0.46
(2,220)	1:60:C:VAL:HA	1:60:C:VAL:HG23	48	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	12	0.46
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	15	0.45
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	31	0.45
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	39	0.45
(2,634)	1:17:C:VAL:HG21	1:38:C:CYS:HB2	2	0.45
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	19	0.45
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	11	0.45
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	29	0.45
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG12	25	0.45
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	18	0.45
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	38	0.45
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG23	39	0.45
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG21	41	0.45
(2,357)	1:34:C:PHE:H	1:24:C:VAL:HG21	48	0.45
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	1	0.45
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB3	24	0.45
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB3	32	0.45
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	38	0.45
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB2	39	0.45
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB2	40	0.45
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	5	0.45
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	28	0.45
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	9	0.45
(2,73)	1:14:C:ARG:HB3	1:21:C:GLY:HA3	10	0.45
(2,765)	1:61:C:THR:H	1:60:C:VAL:HG21	24	0.44
(2,634)	1:17:C:VAL:HG21	1:38:C:CYS:HB2	22	0.44
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	28	0.44
(2,585)	1:54:C:ARG:HG2	1:39:C:HIS:HE1	33	0.44
(2,585)	1:54:C:ARG:HG3	1:39:C:HIS:HE1	45	0.44
(2,581)	1:49:C:THR:H	1:49:C:THR:HG21	3	0.44
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	26	0.44
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	14	0.44
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	22	0.44
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	27	0.44
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	33	0.44
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	38	0.44
(2,366)	1:35:C:HIS:HD2	1:24:C:VAL:HG13	45	0.44
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG12	16	0.44
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG12	37	0.44
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG12	41	0.44
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG23	20	0.44
(2,261)	1:25:C:LEU:H	1:24:C:VAL:HG21	24	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,261)	1:25:C:LEU:H	1:24:C:VAL:HG22	31	0.44
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	29	0.44
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	26	0.44
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	2	0.44
(2,62)	1:17:C:VAL:HG12	1:18:C:CYS:HB2	29	0.44
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	37	0.43
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	50	0.43
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	1	0.43
(2,634)	1:17:C:VAL:HG22	1:38:C:CYS:HB2	45	0.43
(2,614)	1:14:C:ARG:HG2	1:21:C:GLY:HA2	14	0.43
(2,575)	1:36:C:TRP:HE1	1:46:C:ARG:HB2	2	0.43
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	10	0.43
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	46	0.43
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	23	0.43
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	8	0.43
(2,412)	1:20:C:ASP:H	1:20:C:ASP:HB2	19	0.43
(2,412)	1:20:C:ASP:H	1:20:C:ASP:HB2	36	0.43
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG21	25	0.43
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	14	0.43
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	29	0.43
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	39	0.43
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	40	0.43
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	18	0.43
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	20	0.43
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	42	0.43
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	47	0.43
(2,186)	1:51:C:LEU:HD21	1:51:C:LEU:HA	37	0.43
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	18	0.43
(2,91)	1:24:C:VAL:HG21	1:14:C:ARG:HA	31	0.43
(2,62)	1:17:C:VAL:HG11	1:18:C:CYS:HB2	7	0.43
(2,769)	1:53:C:CYS:H	1:57:C:SER:HB2	11	0.42
(2,769)	1:53:C:CYS:H	1:57:C:SER:HB2	44	0.42
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	23	0.42
(2,678)	1:57:C:SER:HB3	1:52:C:ARG:HB2	28	0.42
(2,585)	1:54:C:ARG:HG3	1:39:C:HIS:HE1	26	0.42
(2,585)	1:54:C:ARG:HG2	1:39:C:HIS:HE1	32	0.42
(2,585)	1:54:C:ARG:HG2	1:39:C:HIS:HE1	35	0.42
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	20	0.42
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	23	0.42
(2,387)	1:12:C:GLY:H	1:10:C:ALA:HB2	44	0.42
(2,366)	1:35:C:HIS:HD2	1:24:C:VAL:HG13	41	0.42
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG23	4	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB2	9	0.42
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	2	0.42
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	10	0.42
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	16	0.42
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	20	0.42
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	25	0.42
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	35	0.42
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	25	0.42
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	41	0.42
(2,261)	1:25:C:LEU:H	1:24:C:VAL:HG21	11	0.42
(2,234)	1:36:C:TRP:HZ3	1:51:C:LEU:HD23	41	0.42
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	34	0.42
(2,203)	1:54:C:ARG:HD3	1:54:C:ARG:HB3	22	0.42
(2,778)	1:36:C:TRP:HE1	1:46:C:ARG:HD2	5	0.41
(2,769)	1:53:C:CYS:H	1:57:C:SER:HB2	43	0.41
(2,765)	1:61:C:THR:H	1:60:C:VAL:HG21	31	0.41
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	41	0.41
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	43	0.41
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD23	11	0.41
(2,702)	1:34:C:PHE:HZ	1:51:C:LEU:HD21	13	0.41
(2,702)	1:34:C:PHE:HZ	1:51:C:LEU:HD23	41	0.41
(2,693)	1:49:C:THR:HG22	1:48:C:GLY:HA3	25	0.41
(2,693)	1:49:C:THR:HG23	1:48:C:GLY:HA3	45	0.41
(2,585)	1:54:C:ARG:HG3	1:39:C:HIS:HE1	2	0.41
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	18	0.41
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	42	0.41
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	25	0.41
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB3	28	0.41
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	4	0.41
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	13	0.41
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	23	0.41
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	24	0.41
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	37	0.41
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	41	0.41
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	42	0.41
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	32	0.41
(2,260)	1:39:C:HIS:HD2	1:17:C:VAL:HG22	17	0.41
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	1	0.41
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	26	0.4
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	14	0.4
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	18	0.4
(2,692)	1:52:C:ARG:HG2	1:50:C:GLY:HA3	36	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,585)	1:54:C:ARG:HG2	1:39:C:HIS:HE1	5	0.4
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	42	0.4
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	2	0.4
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	28	0.4
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG13	36	0.4
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG23	3	0.4
(2,357)	1:34:C:PHE:H	1:24:C:VAL:HG23	30	0.4
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	6	0.4
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	15	0.4
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	18	0.4
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	30	0.4
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	34	0.4
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	30	0.4
(2,234)	1:36:C:TRP:HZ3	1:51:C:LEU:HD21	29	0.4
(2,186)	1:51:C:LEU:HD21	1:51:C:LEU:HA	49	0.4
(2,62)	1:17:C:VAL:HG12	1:18:C:CYS:HB2	48	0.4
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG2	12	0.39
(2,716)	1:6:C:GLN:H	1:7:C:GLN:HB2	39	0.39
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	48	0.39
(2,614)	1:14:C:ARG:HG2	1:21:C:GLY:HA2	45	0.39
(2,585)	1:54:C:ARG:HG2	1:39:C:HIS:HE1	17	0.39
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	11	0.39
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	22	0.39
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	30	0.39
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	49	0.39
(2,412)	1:20:C:ASP:H	1:20:C:ASP:HB2	37	0.39
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	11	0.39
(2,292)	1:55:C:SER:H	1:55:C:SER:HB3	11	0.39
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	28	0.39
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	50	0.39
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	7	0.39
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	23	0.39
(2,92)	1:24:C:VAL:HG22	1:21:C:GLY:HA2	34	0.39
(2,91)	1:24:C:VAL:HG23	1:14:C:ARG:HA	10	0.39
(2,702)	1:34:C:PHE:HZ	1:51:C:LEU:HD21	29	0.38
(2,636)	1:17:C:VAL:HG21	1:39:C:HIS:HA	40	0.38
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	4	0.38
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG21	15	0.38
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG23	29	0.38
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB2	27	0.38
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB2	35	0.38
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB3	48	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	38	0.38
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	43	0.38
(2,252)	1:22:C:THR:HG22	1:23:C:ASP:HB3	17	0.38
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	33	0.38
(2,769)	1:53:C:CYS:H	1:57:C:SER:HB2	6	0.37
(2,746)	1:46:C:ARG:H	1:45:C:SER:HB3	17	0.37
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	3	0.37
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	35	0.37
(2,678)	1:57:C:SER:HB3	1:52:C:ARG:HB2	32	0.37
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	29	0.37
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	34	0.37
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	2	0.37
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	35	0.37
(2,357)	1:34:C:PHE:H	1:24:C:VAL:HG23	27	0.37
(2,313)	1:34:C:PHE:HE2	1:39:C:HIS:HB3	29	0.37
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	1	0.37
(2,252)	1:22:C:THR:HG22	1:23:C:ASP:HB3	14	0.37
(2,92)	1:24:C:VAL:HG22	1:21:C:GLY:HA2	2	0.37
(2,92)	1:24:C:VAL:HG22	1:21:C:GLY:HA2	20	0.37
(2,769)	1:53:C:CYS:H	1:57:C:SER:HB2	17	0.36
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	44	0.36
(2,678)	1:57:C:SER:HB3	1:52:C:ARG:HB2	47	0.36
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	13	0.36
(2,634)	1:17:C:VAL:HG22	1:38:C:CYS:HB2	36	0.36
(2,634)	1:17:C:VAL:HG21	1:38:C:CYS:HB2	37	0.36
(2,585)	1:54:C:ARG:HG2	1:39:C:HIS:HE1	16	0.36
(2,585)	1:54:C:ARG:HG2	1:39:C:HIS:HE1	22	0.36
(2,575)	1:36:C:TRP:HE1	1:46:C:ARG:HB2	33	0.36
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	20	0.36
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	26	0.36
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	48	0.36
(2,468)	1:32:C:ALA:H	1:27:C:CYS:HB2	34	0.36
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	7	0.36
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	30	0.36
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	32	0.36
(2,453)	1:29:C:HIS:H	1:29:C:HIS:HD2	43	0.36
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	8	0.36
(2,252)	1:22:C:THR:HG23	1:23:C:ASP:HB3	25	0.36
(2,234)	1:36:C:TRP:HZ3	1:51:C:LEU:HD23	12	0.36
(2,234)	1:36:C:TRP:HZ3	1:51:C:LEU:HD23	39	0.36
(2,234)	1:36:C:TRP:HZ3	1:51:C:LEU:HD21	45	0.36
(2,92)	1:24:C:VAL:HG21	1:21:C:GLY:HA2	18	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,62)	1:17:C:VAL:HG13	1:18:C:CYS:HB2	44	0.36
(2,778)	1:36:C:TRP:HE1	1:46:C:ARG:HD3	4	0.35
(2,769)	1:53:C:CYS:H	1:57:C:SER:HB2	4	0.35
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	22	0.35
(2,675)	1:57:C:SER:HA	1:52:C:ARG:HD3	43	0.35
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	21	0.35
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	48	0.35
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	5	0.35
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	7	0.35
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	10	0.35
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	13	0.35
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	48	0.35
(2,420)	1:21:C:GLY:H	1:24:C:VAL:HG22	48	0.35
(2,419)	1:21:C:GLY:H	1:14:C:ARG:HG2	31	0.35
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG22	47	0.35
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG11	50	0.35
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	35	0.35
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	45	0.35
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	13	0.35
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	34	0.35
(2,139)	1:35:C:HIS:HB2	1:37:C:ARG:HG3	33	0.35
(2,73)	1:14:C:ARG:HB3	1:21:C:GLY:HA3	29	0.35
(2,73)	1:14:C:ARG:HB3	1:21:C:GLY:HA3	47	0.35
(2,769)	1:53:C:CYS:H	1:57:C:SER:HB2	2	0.34
(2,715)	1:6:C:GLN:H	1:6:C:GLN:HG2	48	0.34
(2,654)	1:34:C:PHE:HZ	1:51:C:LEU:HB2	23	0.34
(2,624)	1:33:C:ALA:HA	1:26:C:ARG:HD3	5	0.34
(2,585)	1:54:C:ARG:HG2	1:39:C:HIS:HE1	1	0.34
(2,585)	1:54:C:ARG:HG2	1:39:C:HIS:HE1	4	0.34
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	11	0.34
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	14	0.34
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	31	0.34
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	34	0.34
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	50	0.34
(2,412)	1:20:C:ASP:H	1:20:C:ASP:HB2	16	0.34
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG22	50	0.34
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	45	0.34
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	16	0.34
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	36	0.34
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	25	0.34
(2,168)	1:44:C:THR:HG21	1:46:C:ARG:HA	24	0.34
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,145)	1:39:C:HIS:HD2	1:38:C:CYS:HB3	9	0.34
(2,125)	1:32:C:ALA:HB3	1:33:C:ALA:HA	50	0.34
(2,73)	1:14:C:ARG:HB3	1:21:C:GLY:HA3	21	0.34
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD13	38	0.33
(2,716)	1:6:C:GLN:H	1:7:C:GLN:HB2	13	0.33
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	42	0.33
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD23	25	0.33
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	40	0.33
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	16	0.33
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	39	0.33
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	41	0.33
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	46	0.33
(2,412)	1:20:C:ASP:H	1:20:C:ASP:HB2	3	0.33
(2,412)	1:20:C:ASP:H	1:20:C:ASP:HB2	45	0.33
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG21	35	0.33
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	15	0.33
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	40	0.33
(2,261)	1:25:C:LEU:H	1:24:C:VAL:HG21	48	0.33
(2,168)	1:44:C:THR:HG21	1:46:C:ARG:HA	14	0.33
(2,778)	1:36:C:TRP:HE1	1:46:C:ARG:HD3	29	0.32
(2,769)	1:53:C:CYS:H	1:57:C:SER:HB2	28	0.32
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD13	45	0.32
(2,615)	1:26:C:ARG:HD3	1:24:C:VAL:HG22	36	0.32
(2,556)	1:65:C:VAL:H	1:65:C:VAL:HG22	28	0.32
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	28	0.32
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	34	0.32
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	3	0.32
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	17	0.32
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	32	0.32
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	38	0.32
(2,420)	1:21:C:GLY:H	1:24:C:VAL:HG22	10	0.32
(2,412)	1:20:C:ASP:H	1:20:C:ASP:HB2	17	0.32
(2,412)	1:20:C:ASP:H	1:20:C:ASP:HB2	32	0.32
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG22	16	0.32
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	3	0.32
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	9	0.32
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	33	0.32
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	39	0.32
(2,252)	1:22:C:THR:HG23	1:23:C:ASP:HB3	31	0.32
(2,246)	1:32:C:ALA:HB1	1:27:C:CYS:HB3	31	0.32
(2,207)	1:40:C:PHE:HE2	1:54:C:ARG:HB2	41	0.32
(2,168)	1:44:C:THR:HG21	1:46:C:ARG:HA	34	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,150)	1:38:C:CYS:HB2	1:17:C:VAL:HB	22	0.32
(2,92)	1:24:C:VAL:HG23	1:21:C:GLY:HA2	21	0.32
(2,62)	1:17:C:VAL:HG13	1:18:C:CYS:HB2	12	0.32
(2,769)	1:53:C:CYS:H	1:57:C:SER:HB2	47	0.31
(2,757)	1:54:C:ARG:H	1:54:C:ARG:HG2	24	0.31
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG3	8	0.31
(2,676)	1:57:C:SER:HA	1:52:C:ARG:HB3	10	0.31
(2,585)	1:54:C:ARG:HG3	1:39:C:HIS:HE1	27	0.31
(2,585)	1:54:C:ARG:HG3	1:39:C:HIS:HE1	28	0.31
(2,575)	1:36:C:TRP:HE1	1:46:C:ARG:HB2	6	0.31
(2,556)	1:65:C:VAL:H	1:65:C:VAL:HG21	41	0.31
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	2	0.31
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	43	0.31
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	47	0.31
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	10	0.31
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG22	6	0.31
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	6	0.31
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG21	27	0.31
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	27	0.31
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	37	0.31
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	28	0.31
(2,234)	1:36:C:TRP:HZ3	1:51:C:LEU:HD21	14	0.31
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	12	0.31
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	40	0.31
(2,126)	1:13:C:ALA:HA	1:33:C:ALA:HB1	32	0.31
(2,125)	1:32:C:ALA:HB1	1:33:C:ALA:HA	38	0.31
(2,92)	1:24:C:VAL:HG21	1:21:C:GLY:HA2	32	0.31
(2,92)	1:24:C:VAL:HG23	1:21:C:GLY:HA2	35	0.31
(2,91)	1:24:C:VAL:HG23	1:14:C:ARG:HA	24	0.31
(2,62)	1:17:C:VAL:HG13	1:18:C:CYS:HB2	11	0.31
(2,62)	1:17:C:VAL:HG11	1:18:C:CYS:HB2	26	0.31
(2,62)	1:17:C:VAL:HG13	1:18:C:CYS:HB2	41	0.31
(2,38)	1:54:C:ARG:HG2	1:40:C:PHE:HE1	40	0.31
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD22	25	0.3
(2,716)	1:6:C:GLN:H	1:7:C:GLN:HB2	49	0.3
(2,715)	1:6:C:GLN:H	1:6:C:GLN:HG3	36	0.3
(2,704)	1:34:C:PHE:HE1	1:25:C:LEU:HB3	45	0.3
(2,678)	1:57:C:SER:HB3	1:52:C:ARG:HB2	43	0.3
(2,676)	1:57:C:SER:HA	1:52:C:ARG:HB2	5	0.3
(2,585)	1:54:C:ARG:HG2	1:39:C:HIS:HE1	8	0.3
(2,585)	1:54:C:ARG:HG2	1:39:C:HIS:HE1	9	0.3
(2,556)	1:65:C:VAL:H	1:65:C:VAL:HG23	9	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,556)	1:65:C:VAL:H	1:65:C:VAL:HG22	44	0.3
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	8	0.3
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	12	0.3
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	25	0.3
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	33	0.3
(2,453)	1:29:C:HIS:H	1:29:C:HIS:HD2	19	0.3
(2,420)	1:21:C:GLY:H	1:24:C:VAL:HG21	33	0.3
(2,412)	1:20:C:ASP:H	1:20:C:ASP:HB2	28	0.3
(2,387)	1:12:C:GLY:H	1:10:C:ALA:HB1	6	0.3
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG23	42	0.3
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	44	0.3
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	50	0.3
(2,168)	1:44:C:THR:HG21	1:46:C:ARG:HA	1	0.3
(2,92)	1:24:C:VAL:HG23	1:21:C:GLY:HA2	23	0.3
(2,85)	1:24:C:VAL:HG11	1:14:C:ARG:HA	14	0.3
(2,769)	1:53:C:CYS:H	1:57:C:SER:HB2	32	0.29
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD21	50	0.29
(2,716)	1:6:C:GLN:H	1:7:C:GLN:HB3	46	0.29
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	38	0.29
(2,556)	1:65:C:VAL:H	1:65:C:VAL:HG23	12	0.29
(2,556)	1:65:C:VAL:H	1:65:C:VAL:HG22	16	0.29
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	1	0.29
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	15	0.29
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	20	0.29
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	24	0.29
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	26	0.29
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	40	0.29
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	12	0.29
(2,495)	1:39:C:HIS:H	1:38:C:CYS:HB3	21	0.29
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG22	38	0.29
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	21	0.29
(2,326)	1:36:C:TRP:HH2	1:44:C:THR:HG21	17	0.29
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	49	0.29
(2,234)	1:36:C:TRP:HZ3	1:51:C:LEU:HD21	48	0.29
(2,168)	1:44:C:THR:HG23	1:46:C:ARG:HA	46	0.29
(2,92)	1:24:C:VAL:HG21	1:21:C:GLY:HA2	49	0.29
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD21	27	0.28
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD13	49	0.28
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG2	17	0.28
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG3	23	0.28
(2,716)	1:6:C:GLN:H	1:7:C:GLN:HB2	18	0.28
(2,701)	1:34:C:PHE:HE1	1:27:C:CYS:HA	33	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,585)	1:54:C:ARG:HG2	1:39:C:HIS:HE1	39	0.28
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	5	0.28
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	6	0.28
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	18	0.28
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	22	0.28
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	27	0.28
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	35	0.28
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	14	0.28
(2,412)	1:20:C:ASP:H	1:20:C:ASP:HB2	35	0.28
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG13	4	0.28
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG23	22	0.28
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	28	0.28
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG23	31	0.28
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB2	10	0.28
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	14	0.28
(2,260)	1:39:C:HIS:HD2	1:17:C:VAL:HG23	14	0.28
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	22	0.28
(2,234)	1:36:C:TRP:HZ3	1:51:C:LEU:HD23	2	0.28
(2,168)	1:44:C:THR:HG23	1:46:C:ARG:HA	18	0.28
(2,168)	1:44:C:THR:HG21	1:46:C:ARG:HA	41	0.28
(2,145)	1:39:C:HIS:HD2	1:38:C:CYS:HB3	28	0.28
(2,126)	1:13:C:ALA:HA	1:33:C:ALA:HB2	44	0.28
(2,125)	1:32:C:ALA:HB2	1:33:C:ALA:HA	17	0.28
(2,92)	1:24:C:VAL:HG22	1:21:C:GLY:HA2	9	0.28
(2,92)	1:24:C:VAL:HG21	1:21:C:GLY:HA2	16	0.28
(2,92)	1:24:C:VAL:HG21	1:21:C:GLY:HA2	38	0.28
(2,92)	1:24:C:VAL:HG22	1:21:C:GLY:HA2	39	0.28
(2,62)	1:17:C:VAL:HG12	1:18:C:CYS:HB2	2	0.28
(2,715)	1:6:C:GLN:H	1:6:C:GLN:HG3	13	0.27
(2,702)	1:34:C:PHE:HZ	1:51:C:LEU:HD22	1	0.27
(2,556)	1:65:C:VAL:H	1:65:C:VAL:HG22	18	0.27
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	12	0.27
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	9	0.27
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	10	0.27
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	29	0.27
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	30	0.27
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	37	0.27
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	32	0.27
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	37	0.27
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG23	43	0.27
(2,252)	1:22:C:THR:HG23	1:23:C:ASP:HB3	42	0.27
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	16	0.27
(2,168)	1:44:C:THR:HG22	1:46:C:ARG:HA	7	0.27
(2,168)	1:44:C:THR:HG22	1:46:C:ARG:HA	16	0.27
(2,145)	1:39:C:HIS:HD2	1:38:C:CYS:HB3	46	0.27
(2,92)	1:24:C:VAL:HG23	1:21:C:GLY:HA2	14	0.27
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	38	0.26
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG3	39	0.26
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	12	0.26
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD22	48	0.26
(2,678)	1:57:C:SER:HB2	1:52:C:ARG:HB2	41	0.26
(2,678)	1:57:C:SER:HB3	1:52:C:ARG:HB2	44	0.26
(2,653)	1:50:C:GLY:HA2	1:28:C:THR:HG22	40	0.26
(2,634)	1:17:C:VAL:HG21	1:38:C:CYS:HB2	16	0.26
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	24	0.26
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	13	0.26
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	19	0.26
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	28	0.26
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	36	0.26
(2,412)	1:20:C:ASP:H	1:20:C:ASP:HB2	15	0.26
(2,261)	1:25:C:LEU:H	1:24:C:VAL:HG22	42	0.26
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	17	0.26
(2,168)	1:44:C:THR:HG21	1:46:C:ARG:HA	30	0.26
(2,92)	1:24:C:VAL:HG21	1:21:C:GLY:HA2	26	0.26
(2,85)	1:24:C:VAL:HG13	1:14:C:ARG:HA	36	0.26
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD21	12	0.25
(2,716)	1:6:C:GLN:H	1:7:C:GLN:HB2	41	0.25
(2,716)	1:6:C:GLN:H	1:7:C:GLN:HB2	50	0.25
(2,715)	1:6:C:GLN:H	1:6:C:GLN:HG2	32	0.25
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD22	34	0.25
(2,676)	1:57:C:SER:HA	1:52:C:ARG:HB2	36	0.25
(2,634)	1:17:C:VAL:HG21	1:38:C:CYS:HB2	9	0.25
(2,634)	1:17:C:VAL:HG21	1:38:C:CYS:HB2	24	0.25
(2,585)	1:54:C:ARG:HG3	1:39:C:HIS:HE1	29	0.25
(2,584)	1:34:C:PHE:HE2	1:39:C:HIS:HE1	5	0.25
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	11	0.25
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	26	0.25
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	23	0.25
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	36	0.25
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	44	0.25
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	49	0.25
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	48	0.25
(2,371)	1:23:C:ASP:H	1:22:C:THR:HG21	23	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,361)	1:15:C:CYS:H	1:24:C:VAL:HG22	30	0.25
(2,260)	1:39:C:HIS:HD2	1:17:C:VAL:HG21	19	0.25
(2,234)	1:36:C:TRP:HZ3	1:51:C:LEU:HD23	23	0.25
(2,168)	1:44:C:THR:HG22	1:46:C:ARG:HA	5	0.25
(2,168)	1:44:C:THR:HG23	1:46:C:ARG:HA	20	0.25
(2,168)	1:44:C:THR:HG23	1:46:C:ARG:HA	25	0.25
(2,145)	1:39:C:HIS:HD2	1:38:C:CYS:HB3	8	0.25
(2,92)	1:24:C:VAL:HG21	1:21:C:GLY:HA2	6	0.25
(2,92)	1:24:C:VAL:HG22	1:21:C:GLY:HA2	12	0.25
(2,85)	1:24:C:VAL:HG11	1:14:C:ARG:HA	45	0.25
(2,73)	1:14:C:ARG:HB3	1:21:C:GLY:HA3	20	0.25
(2,62)	1:17:C:VAL:HG11	1:18:C:CYS:HB2	18	0.25
(2,38)	1:54:C:ARG:HG2	1:40:C:PHE:HE1	29	0.25
(2,778)	1:36:C:TRP:HE1	1:46:C:ARG:HD3	18	0.24
(2,757)	1:54:C:ARG:H	1:54:C:ARG:HG2	14	0.24
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	7	0.24
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD22	20	0.24
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG3	37	0.24
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG3	50	0.24
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	2	0.24
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	6	0.24
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	27	0.24
(2,556)	1:65:C:VAL:H	1:65:C:VAL:HG23	1	0.24
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	19	0.24
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	41	0.24
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	7	0.24
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	38	0.24
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	46	0.24
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	2	0.24
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	7	0.24
(2,503)	1:40:C:PHE:H	1:40:C:PHE:HB3	45	0.24
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	30	0.24
(2,419)	1:21:C:GLY:H	1:14:C:ARG:HG2	24	0.24
(2,412)	1:20:C:ASP:H	1:20:C:ASP:HB2	6	0.24
(2,260)	1:39:C:HIS:HD2	1:17:C:VAL:HG22	40	0.24
(2,260)	1:39:C:HIS:HD2	1:17:C:VAL:HG22	47	0.24
(2,234)	1:36:C:TRP:HZ3	1:51:C:LEU:HD23	21	0.24
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	33	0.24
(2,145)	1:39:C:HIS:HD2	1:38:C:CYS:HB3	24	0.24
(2,91)	1:24:C:VAL:HG22	1:14:C:ARG:HA	33	0.24
(2,86)	1:24:C:VAL:HG13	1:21:C:GLY:HA2	2	0.24
(2,85)	1:24:C:VAL:HG13	1:14:C:ARG:HA	19	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	40	0.23
(2,716)	1:6:C:GLN:H	1:7:C:GLN:HB3	24	0.23
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD22	33	0.23
(2,678)	1:57:C:SER:HB3	1:52:C:ARG:HB2	2	0.23
(2,676)	1:57:C:SER:HA	1:52:C:ARG:HB2	41	0.23
(2,666)	1:57:C:SER:HA	1:52:C:ARG:HD3	43	0.23
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	31	0.23
(2,556)	1:65:C:VAL:H	1:65:C:VAL:HG22	27	0.23
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	10	0.23
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	25	0.23
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	29	0.23
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	43	0.23
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	34	0.23
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	50	0.23
(2,419)	1:21:C:GLY:H	1:14:C:ARG:HG2	46	0.23
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB3	49	0.23
(2,234)	1:36:C:TRP:HZ3	1:51:C:LEU:HD21	4	0.23
(2,215)	1:52:C:ARG:HD3	1:57:C:SER:HB3	2	0.23
(2,168)	1:44:C:THR:HG21	1:46:C:ARG:HA	29	0.23
(2,156)	1:63:C:ALA:HA	1:64:C:PRO:HD2	41	0.23
(2,125)	1:32:C:ALA:HB1	1:33:C:ALA:HA	5	0.23
(2,125)	1:32:C:ALA:HB3	1:33:C:ALA:HA	12	0.23
(2,101)	1:27:C:CYS:HA	1:26:C:ARG:HB2	23	0.23
(2,92)	1:24:C:VAL:HG22	1:21:C:GLY:HA2	29	0.23
(2,92)	1:24:C:VAL:HG21	1:21:C:GLY:HA2	47	0.23
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD21	36	0.22
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD21	42	0.22
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG3	3	0.22
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG3	4	0.22
(2,715)	1:6:C:GLN:H	1:6:C:GLN:HG2	30	0.22
(2,715)	1:6:C:GLN:H	1:6:C:GLN:HG3	47	0.22
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	39	0.22
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	8	0.22
(2,634)	1:17:C:VAL:HG22	1:38:C:CYS:HB2	15	0.22
(2,615)	1:26:C:ARG:HD2	1:24:C:VAL:HG22	23	0.22
(2,556)	1:65:C:VAL:H	1:65:C:VAL:HG22	2	0.22
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	1	0.22
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	8	0.22
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	15	0.22
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	16	0.22
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	23	0.22
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	27	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	28	0.22
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	32	0.22
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	42	0.22
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	44	0.22
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	4	0.22
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	5	0.22
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	12	0.22
(2,426)	1:22:C:THR:H	1:22:C:THR:HG21	15	0.22
(2,426)	1:22:C:THR:H	1:22:C:THR:HG22	16	0.22
(2,426)	1:22:C:THR:H	1:22:C:THR:HG23	32	0.22
(2,426)	1:22:C:THR:H	1:22:C:THR:HG22	41	0.22
(2,426)	1:22:C:THR:H	1:22:C:THR:HG22	45	0.22
(2,246)	1:32:C:ALA:HB1	1:27:C:CYS:HB3	26	0.22
(2,244)	1:33:C:ALA:HB1	1:24:C:VAL:HB	47	0.22
(2,223)	1:61:C:THR:HG21	1:61:C:THR:HA	34	0.22
(2,168)	1:44:C:THR:HG23	1:46:C:ARG:HA	50	0.22
(2,125)	1:32:C:ALA:HB1	1:33:C:ALA:HA	14	0.22
(2,101)	1:27:C:CYS:HA	1:26:C:ARG:HB2	42	0.22
(2,92)	1:24:C:VAL:HG23	1:21:C:GLY:HA2	15	0.22
(2,91)	1:24:C:VAL:HG23	1:14:C:ARG:HA	7	0.22
(2,62)	1:17:C:VAL:HG11	1:18:C:CYS:HB2	3	0.22
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD13	24	0.21
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG3	30	0.21
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	16	0.21
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	9	0.21
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	30	0.21
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	3	0.21
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	6	0.21
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	12	0.21
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	13	0.21
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	17	0.21
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	37	0.21
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	43	0.21
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	45	0.21
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	47	0.21
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	10	0.21
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	26	0.21
(2,426)	1:22:C:THR:H	1:22:C:THR:HG22	17	0.21
(2,426)	1:22:C:THR:H	1:22:C:THR:HG23	19	0.21
(2,426)	1:22:C:THR:H	1:22:C:THR:HG23	22	0.21
(2,426)	1:22:C:THR:H	1:22:C:THR:HG21	37	0.21
(2,426)	1:22:C:THR:H	1:22:C:THR:HG23	42	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,419)	1:21:C:GLY:H	1:14:C:ARG:HG2	18	0.21
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG12	43	0.21
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	17	0.21
(2,244)	1:33:C:ALA:HB1	1:24:C:VAL:HB	16	0.21
(2,223)	1:61:C:THR:HG23	1:61:C:THR:HA	6	0.21
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	28	0.21
(2,101)	1:27:C:CYS:HA	1:26:C:ARG:HB2	36	0.21
(2,92)	1:24:C:VAL:HG22	1:21:C:GLY:HA2	3	0.21
(2,92)	1:24:C:VAL:HG23	1:21:C:GLY:HA2	41	0.21
(2,92)	1:24:C:VAL:HG21	1:21:C:GLY:HA2	44	0.21
(2,92)	1:24:C:VAL:HG21	1:21:C:GLY:HA2	46	0.21
(2,86)	1:24:C:VAL:HG11	1:21:C:GLY:HA2	34	0.21
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD22	14	0.2
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD12	31	0.2
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG3	5	0.2
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG2	48	0.2
(2,715)	1:6:C:GLN:H	1:6:C:GLN:HG2	29	0.2
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD22	20	0.2
(2,661)	1:56:C:CYS:HB3	1:52:C:ARG:HB3	34	0.2
(2,576)	1:61:C:THR:H	1:59:C:ASP:HB2	25	0.2
(2,556)	1:65:C:VAL:H	1:65:C:VAL:HG23	34	0.2
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	2	0.2
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	4	0.2
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	9	0.2
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	18	0.2
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	19	0.2
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	20	0.2
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	21	0.2
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	25	0.2
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	30	0.2
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	35	0.2
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	11	0.2
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	41	0.2
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	49	0.2
(2,426)	1:22:C:THR:H	1:22:C:THR:HG22	27	0.2
(2,426)	1:22:C:THR:H	1:22:C:THR:HG22	35	0.2
(2,426)	1:22:C:THR:H	1:22:C:THR:HG23	38	0.2
(2,426)	1:22:C:THR:H	1:22:C:THR:HG22	50	0.2
(2,371)	1:23:C:ASP:H	1:22:C:THR:HG23	21	0.2
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG22	44	0.2
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG11	3	0.2
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG22	24	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG22	50	0.2
(2,265)	1:37:C:ARG:H	1:36:C:TRP:HB2	6	0.2
(2,223)	1:61:C:THR:HG22	1:61:C:THR:HA	20	0.2
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	46	0.2
(2,101)	1:27:C:CYS:HA	1:26:C:ARG:HB2	19	0.2
(2,73)	1:14:C:ARG:HB3	1:21:C:GLY:HA3	5	0.2
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	3	0.19
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	47	0.19
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD21	11	0.19
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD21	19	0.19
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD23	33	0.19
(2,716)	1:6:C:GLN:H	1:7:C:GLN:HB2	5	0.19
(2,715)	1:6:C:GLN:H	1:6:C:GLN:HG3	2	0.19
(2,715)	1:6:C:GLN:H	1:6:C:GLN:HG2	17	0.19
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	40	0.19
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD23	6	0.19
(2,702)	1:34:C:PHE:HZ	1:51:C:LEU:HD22	22	0.19
(2,634)	1:17:C:VAL:HG22	1:38:C:CYS:HB2	46	0.19
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	14	0.19
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	22	0.19
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	29	0.19
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	31	0.19
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	33	0.19
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	39	0.19
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	40	0.19
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	48	0.19
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	49	0.19
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	50	0.19
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	35	0.19
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	44	0.19
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	47	0.19
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	3	0.19
(2,426)	1:22:C:THR:H	1:22:C:THR:HG23	2	0.19
(2,426)	1:22:C:THR:H	1:22:C:THR:HG23	3	0.19
(2,426)	1:22:C:THR:H	1:22:C:THR:HG21	5	0.19
(2,426)	1:22:C:THR:H	1:22:C:THR:HG23	6	0.19
(2,426)	1:22:C:THR:H	1:22:C:THR:HG21	14	0.19
(2,426)	1:22:C:THR:H	1:22:C:THR:HG22	26	0.19
(2,426)	1:22:C:THR:H	1:22:C:THR:HG23	28	0.19
(2,426)	1:22:C:THR:H	1:22:C:THR:HG21	29	0.19
(2,426)	1:22:C:THR:H	1:22:C:THR:HG23	30	0.19
(2,426)	1:22:C:THR:H	1:22:C:THR:HG21	33	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,426)	1:22:C:THR:H	1:22:C:THR:HG22	36	0.19
(2,426)	1:22:C:THR:H	1:22:C:THR:HG21	49	0.19
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG11	45	0.19
(2,352)	1:34:C:PHE:HE1	1:34:C:PHE:H	24	0.19
(2,352)	1:34:C:PHE:HE1	1:34:C:PHE:H	33	0.19
(2,281)	1:66:C:GLU:H	1:65:C:VAL:HA	5	0.19
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	46	0.19
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	13	0.19
(2,145)	1:39:C:HIS:HD2	1:38:C:CYS:HB3	34	0.19
(2,126)	1:13:C:ALA:HA	1:33:C:ALA:HB2	43	0.19
(2,125)	1:32:C:ALA:HB1	1:33:C:ALA:HA	23	0.19
(2,125)	1:32:C:ALA:HB3	1:33:C:ALA:HA	26	0.19
(2,125)	1:32:C:ALA:HB3	1:33:C:ALA:HA	31	0.19
(2,125)	1:32:C:ALA:HB1	1:33:C:ALA:HA	47	0.19
(2,101)	1:27:C:CYS:HA	1:26:C:ARG:HB2	12	0.19
(2,92)	1:24:C:VAL:HG22	1:21:C:GLY:HA2	1	0.19
(2,92)	1:24:C:VAL:HG23	1:21:C:GLY:HA2	8	0.19
(2,92)	1:24:C:VAL:HG21	1:21:C:GLY:HA2	50	0.19
(2,91)	1:24:C:VAL:HG23	1:14:C:ARG:HA	48	0.19
(2,51)	1:24:C:VAL:HG23	1:15:C:CYS:HA	48	0.19
(2,744)	1:42:C:ALA:H	1:41:C:PRO:HD2	40	0.18
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	24	0.18
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG3	34	0.18
(2,706)	1:34:C:PHE:HE2	1:51:C:LEU:HG	3	0.18
(2,701)	1:34:C:PHE:HE1	1:27:C:CYS:HA	50	0.18
(2,676)	1:57:C:SER:HA	1:52:C:ARG:HB3	34	0.18
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	50	0.18
(2,576)	1:61:C:THR:H	1:59:C:ASP:HB2	27	0.18
(2,556)	1:65:C:VAL:H	1:65:C:VAL:HG22	17	0.18
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	5	0.18
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	36	0.18
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	16	0.18
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	19	0.18
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	22	0.18
(2,456)	1:30:C:CYS:H	1:30:C:CYS:HB3	31	0.18
(2,426)	1:22:C:THR:H	1:22:C:THR:HG21	4	0.18
(2,426)	1:22:C:THR:H	1:22:C:THR:HG22	25	0.18
(2,412)	1:20:C:ASP:H	1:20:C:ASP:HB2	4	0.18
(2,395)	1:17:C:VAL:H	1:18:C:CYS:HB2	41	0.18
(2,385)	1:12:C:GLY:H	1:11:C:PRO:HA	29	0.18
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG23	9	0.18
(2,352)	1:34:C:PHE:HE2	1:34:C:PHE:H	31	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,352)	1:34:C:PHE:HE1	1:34:C:PHE:H	46	0.18
(2,244)	1:33:C:ALA:HB1	1:24:C:VAL:HB	35	0.18
(2,223)	1:61:C:THR:HG23	1:61:C:THR:HA	37	0.18
(2,223)	1:61:C:THR:HG21	1:61:C:THR:HA	38	0.18
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	2	0.18
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	9	0.18
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	34	0.18
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	36	0.18
(2,101)	1:27:C:CYS:HA	1:26:C:ARG:HB2	41	0.18
(2,86)	1:24:C:VAL:HG11	1:21:C:GLY:HA2	20	0.18
(2,73)	1:14:C:ARG:HB3	1:21:C:GLY:HA3	3	0.18
(2,73)	1:14:C:ARG:HB3	1:21:C:GLY:HA3	22	0.18
(2,62)	1:17:C:VAL:HG12	1:18:C:CYS:HB2	5	0.18
(2,38)	1:54:C:ARG:HG2	1:40:C:PHE:HE2	3	0.18
(2,765)	1:61:C:THR:H	1:60:C:VAL:HG13	30	0.17
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG3	20	0.17
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG3	28	0.17
(2,717)	1:7:C:GLN:H	1:7:C:GLN:HG3	31	0.17
(2,715)	1:6:C:GLN:H	1:6:C:GLN:HG2	21	0.17
(2,676)	1:57:C:SER:HA	1:52:C:ARG:HB3	11	0.17
(2,624)	1:33:C:ALA:HA	1:26:C:ARG:HD3	38	0.17
(2,618)	1:26:C:ARG:HA	1:26:C:ARG:HD2	50	0.17
(2,544)	1:60:C:VAL:H	1:60:C:VAL:HB	5	0.17
(2,543)	1:60:C:VAL:H	1:59:C:ASP:HA	18	0.17
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	38	0.17
(2,533)	1:53:C:CYS:H	1:53:C:CYS:HB2	41	0.17
(2,524)	1:50:C:GLY:H	1:49:C:THR:HA	28	0.17
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	3	0.17
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	15	0.17
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	18	0.17
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	38	0.17
(2,468)	1:32:C:ALA:H	1:27:C:CYS:HB2	10	0.17
(2,456)	1:30:C:CYS:H	1:30:C:CYS:HB3	50	0.17
(2,426)	1:22:C:THR:H	1:22:C:THR:HG23	7	0.17
(2,426)	1:22:C:THR:H	1:22:C:THR:HG23	10	0.17
(2,426)	1:22:C:THR:H	1:22:C:THR:HG23	11	0.17
(2,426)	1:22:C:THR:H	1:22:C:THR:HG21	13	0.17
(2,426)	1:22:C:THR:H	1:22:C:THR:HG21	24	0.17
(2,426)	1:22:C:THR:H	1:22:C:THR:HG23	47	0.17
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	2	0.17
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	7	0.17
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	12	0.17
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	18	0.17
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	29	0.17
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	34	0.17
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	48	0.17
(2,395)	1:17:C:VAL:H	1:18:C:CYS:HB2	3	0.17
(2,352)	1:34:C:PHE:HE1	1:34:C:PHE:H	27	0.17
(2,327)	1:36:C:TRP:HZ2	1:51:C:LEU:HD11	24	0.17
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	20	0.17
(2,164)	1:45:C:SER:HB3	1:44:C:THR:HG22	17	0.17
(2,145)	1:39:C:HIS:HD2	1:38:C:CYS:HB3	36	0.17
(2,125)	1:32:C:ALA:HB1	1:33:C:ALA:HA	34	0.17
(2,125)	1:32:C:ALA:HB3	1:33:C:ALA:HA	49	0.17
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	47	0.17
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	50	0.17
(2,101)	1:27:C:CYS:HA	1:26:C:ARG:HB2	16	0.17
(2,101)	1:27:C:CYS:HA	1:26:C:ARG:HB2	20	0.17
(2,92)	1:24:C:VAL:HG22	1:21:C:GLY:HA2	40	0.17
(2,86)	1:24:C:VAL:HG12	1:21:C:GLY:HA2	18	0.17
(2,85)	1:24:C:VAL:HG13	1:14:C:ARG:HA	38	0.17
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	20	0.16
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD23	8	0.16
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD22	46	0.16
(2,692)	1:52:C:ARG:HG2	1:50:C:GLY:HA2	11	0.16
(2,663)	1:57:C:SER:HB3	1:52:C:ARG:HB2	17	0.16
(2,624)	1:33:C:ALA:HA	1:26:C:ARG:HD2	16	0.16
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	39	0.16
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	21	0.16
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	24	0.16
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	37	0.16
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	45	0.16
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	50	0.16
(2,458)	1:30:C:CYS:H	1:28:C:THR:HG21	43	0.16
(2,457)	1:30:C:CYS:H	1:27:C:CYS:HB2	31	0.16
(2,448)	1:28:C:THR:H	1:51:C:LEU:HD21	48	0.16
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	26	0.16
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	50	0.16
(2,426)	1:22:C:THR:H	1:22:C:THR:HG21	43	0.16
(2,426)	1:22:C:THR:H	1:22:C:THR:HG22	48	0.16
(2,419)	1:21:C:GLY:H	1:14:C:ARG:HG2	7	0.16
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	8	0.16
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	22	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	23	0.16
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	26	0.16
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	30	0.16
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	31	0.16
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	42	0.16
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	46	0.16
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	49	0.16
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	50	0.16
(2,395)	1:17:C:VAL:H	1:18:C:CYS:HB2	20	0.16
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG22	37	0.16
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG21	36	0.16
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG21	35	0.16
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	8	0.16
(2,168)	1:44:C:THR:HG21	1:46:C:ARG:HA	28	0.16
(2,145)	1:39:C:HIS:HD2	1:38:C:CYS:HB3	31	0.16
(2,125)	1:32:C:ALA:HB1	1:33:C:ALA:HA	37	0.16
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	2	0.16
(2,62)	1:17:C:VAL:HG12	1:18:C:CYS:HB2	37	0.16
(2,38)	1:54:C:ARG:HG2	1:40:C:PHE:HE2	31	0.16
(2,778)	1:36:C:TRP:HE1	1:46:C:ARG:HD3	38	0.15
(2,772)	1:57:C:SER:H	1:57:C:SER:HB3	39	0.15
(2,769)	1:53:C:CYS:H	1:57:C:SER:HB2	1	0.15
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	4	0.15
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	49	0.15
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD22	2	0.15
(2,727)	1:14:C:ARG:H	1:14:C:ARG:HB3	28	0.15
(2,718)	1:7:C:GLN:H	1:7:C:GLN:HB2	13	0.15
(2,716)	1:6:C:GLN:H	1:7:C:GLN:HB2	20	0.15
(2,715)	1:6:C:GLN:H	1:6:C:GLN:HG2	18	0.15
(2,706)	1:34:C:PHE:HZ	1:51:C:LEU:HG	27	0.15
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD23	38	0.15
(2,701)	1:34:C:PHE:HE1	1:27:C:CYS:HA	24	0.15
(2,676)	1:57:C:SER:HA	1:52:C:ARG:HB3	44	0.15
(2,624)	1:33:C:ALA:HA	1:26:C:ARG:HD3	25	0.15
(2,524)	1:50:C:GLY:H	1:49:C:THR:HA	20	0.15
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	2	0.15
(2,456)	1:30:C:CYS:H	1:30:C:CYS:HB3	3	0.15
(2,456)	1:30:C:CYS:H	1:30:C:CYS:HB3	26	0.15
(2,426)	1:22:C:THR:H	1:22:C:THR:HG21	1	0.15
(2,426)	1:22:C:THR:H	1:22:C:THR:HG22	8	0.15
(2,426)	1:22:C:THR:H	1:22:C:THR:HG23	34	0.15
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	3	0.15
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	5	0.15
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	9	0.15
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	13	0.15
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	14	0.15
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	20	0.15
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	21	0.15
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	25	0.15
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	27	0.15
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	41	0.15
(2,352)	1:34:C:PHE:HE1	1:34:C:PHE:H	50	0.15
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG22	47	0.15
(2,327)	1:36:C:TRP:HZ2	1:51:C:LEU:HD12	18	0.15
(2,252)	1:22:C:THR:HG22	1:23:C:ASP:HB3	36	0.15
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	49	0.15
(2,190)	1:52:C:ARG:HA	1:52:C:ARG:HG3	5	0.15
(2,125)	1:32:C:ALA:HB3	1:33:C:ALA:HA	6	0.15
(2,125)	1:32:C:ALA:HB1	1:33:C:ALA:HA	45	0.15
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	15	0.15
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	16	0.15
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	20	0.15
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	21	0.15
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	25	0.15
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	38	0.15
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	40	0.15
(2,101)	1:27:C:CYS:HA	1:26:C:ARG:HB2	6	0.15
(2,92)	1:24:C:VAL:HG22	1:21:C:GLY:HA2	43	0.15
(2,68)	1:14:C:ARG:HG2	1:20:C:ASP:HA	13	0.15
(2,62)	1:17:C:VAL:HG13	1:18:C:CYS:HB2	50	0.15
(2,765)	1:61:C:THR:H	1:60:C:VAL:HG23	18	0.14
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	46	0.14
(2,715)	1:6:C:GLN:H	1:6:C:GLN:HG3	25	0.14
(2,701)	1:34:C:PHE:HE1	1:27:C:CYS:HA	27	0.14
(2,678)	1:57:C:SER:HB2	1:52:C:ARG:HB3	1	0.14
(2,678)	1:57:C:SER:HB2	1:52:C:ARG:HB3	24	0.14
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	39	0.14
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	13	0.14
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	31	0.14
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	40	0.14
(2,486)	1:37:C:ARG:H	1:35:C:HIS:HB2	32	0.14
(2,468)	1:32:C:ALA:H	1:27:C:CYS:HB2	11	0.14
(2,456)	1:30:C:CYS:H	1:30:C:CYS:HB3	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,448)	1:28:C:THR:H	1:51:C:LEU:HD23	21	0.14
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	17	0.14
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	34	0.14
(2,426)	1:22:C:THR:H	1:22:C:THR:HG22	9	0.14
(2,426)	1:22:C:THR:H	1:22:C:THR:HG21	12	0.14
(2,426)	1:22:C:THR:H	1:22:C:THR:HG22	31	0.14
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	24	0.14
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	33	0.14
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	40	0.14
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	44	0.14
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	47	0.14
(2,395)	1:17:C:VAL:H	1:18:C:CYS:HB2	42	0.14
(2,362)	1:35:C:HIS:HE1	1:24:C:VAL:HG23	19	0.14
(2,339)	1:35:C:HIS:HE2	1:24:C:VAL:HG22	16	0.14
(2,246)	1:32:C:ALA:HB1	1:27:C:CYS:HB3	12	0.14
(2,168)	1:44:C:THR:HG21	1:46:C:ARG:HA	43	0.14
(2,145)	1:39:C:HIS:HD2	1:38:C:CYS:HB3	1	0.14
(2,126)	1:13:C:ALA:HA	1:33:C:ALA:HB2	29	0.14
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	12	0.14
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	19	0.14
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	37	0.14
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	44	0.14
(2,91)	1:24:C:VAL:HG23	1:14:C:ARG:HA	11	0.14
(2,62)	1:17:C:VAL:HG12	1:18:C:CYS:HB2	15	0.14
(2,62)	1:17:C:VAL:HG11	1:18:C:CYS:HB2	47	0.14
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	1	0.14
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	9	0.14
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	14	0.14
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	16	0.14
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	17	0.14
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	25	0.14
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	27	0.14
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	28	0.14
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	32	0.14
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	36	0.14
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	37	0.14
(2,51)	1:24:C:VAL:HG22	1:15:C:CYS:HA	30	0.14
(2,41)	1:9:C:LEU:HD13	1:9:C:LEU:HA	40	0.14
(2,40)	1:9:C:LEU:HD23	1:9:C:LEU:HA	18	0.14
(2,40)	1:9:C:LEU:HD22	1:9:C:LEU:HA	44	0.14
(2,769)	1:53:C:CYS:H	1:57:C:SER:HB2	26	0.13
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD21	40	0.13
(2,727)	1:14:C:ARG:H	1:14:C:ARG:HB3	17	0.13
(2,716)	1:6:C:GLN:H	1:7:C:GLN:HB2	33	0.13
(2,715)	1:6:C:GLN:H	1:6:C:GLN:HG2	35	0.13
(2,692)	1:52:C:ARG:HG2	1:50:C:GLY:HA3	20	0.13
(2,676)	1:57:C:SER:HA	1:52:C:ARG:HB3	26	0.13
(2,676)	1:57:C:SER:HA	1:52:C:ARG:HB3	28	0.13
(2,663)	1:57:C:SER:HB3	1:52:C:ARG:HB3	11	0.13
(2,663)	1:57:C:SER:HB3	1:52:C:ARG:HB2	26	0.13
(2,634)	1:17:C:VAL:HG21	1:38:C:CYS:HB2	17	0.13
(2,624)	1:33:C:ALA:HA	1:26:C:ARG:HD2	23	0.13
(2,624)	1:33:C:ALA:HA	1:26:C:ARG:HD3	36	0.13
(2,615)	1:26:C:ARG:HD2	1:24:C:VAL:HG23	6	0.13
(2,593)	1:6:C:GLN:HB2	1:6:C:GLN:HA	40	0.13
(2,584)	1:34:C:PHE:HE1	1:39:C:HIS:HE1	39	0.13
(2,543)	1:60:C:VAL:H	1:59:C:ASP:HA	38	0.13
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	42	0.13
(2,524)	1:50:C:GLY:H	1:49:C:THR:HA	22	0.13
(2,501)	1:40:C:PHE:H	1:40:C:PHE:HE1	43	0.13
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	20	0.13
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	42	0.13
(2,456)	1:30:C:CYS:H	1:30:C:CYS:HB3	34	0.13
(2,448)	1:28:C:THR:H	1:51:C:LEU:HD23	30	0.13
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	6	0.13
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	21	0.13
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	23	0.13
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	25	0.13
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	37	0.13
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	47	0.13
(2,419)	1:21:C:GLY:H	1:14:C:ARG:HG2	45	0.13
(2,412)	1:20:C:ASP:H	1:20:C:ASP:HB2	41	0.13
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	6	0.13
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	16	0.13
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	32	0.13
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG11	40	0.13
(2,357)	1:34:C:PHE:H	1:24:C:VAL:HG23	33	0.13
(2,352)	1:34:C:PHE:HE1	1:34:C:PHE:H	9	0.13
(2,252)	1:22:C:THR:HG23	1:23:C:ASP:HB3	38	0.13
(2,164)	1:45:C:SER:HB3	1:44:C:THR:HG22	33	0.13
(2,125)	1:32:C:ALA:HB2	1:33:C:ALA:HA	25	0.13
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	4	0.13
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	35	0.13
(2,101)	1:27:C:CYS:HA	1:26:C:ARG:HB2	37	0.13
(2,85)	1:24:C:VAL:HG12	1:14:C:ARG:HA	21	0.13
(2,73)	1:14:C:ARG:HB3	1:21:C:GLY:HA3	26	0.13
(2,62)	1:17:C:VAL:HG11	1:18:C:CYS:HB2	17	0.13
(2,62)	1:17:C:VAL:HG11	1:18:C:CYS:HB2	45	0.13
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	4	0.13
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	6	0.13
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	8	0.13
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	15	0.13
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	19	0.13
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	24	0.13
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	31	0.13
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	33	0.13
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	35	0.13
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	38	0.13
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	39	0.13
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	40	0.13
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	43	0.13
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	45	0.13
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	46	0.13
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	47	0.13
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	50	0.13
(2,40)	1:9:C:LEU:HD23	1:9:C:LEU:HA	48	0.13
(2,778)	1:36:C:TRP:HE1	1:46:C:ARG:HD2	9	0.12
(2,743)	1:42:C:ALA:H	1:41:C:PRO:HB2	21	0.12
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD23	29	0.12
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD22	30	0.12
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD23	37	0.12
(2,706)	1:34:C:PHE:HZ	1:51:C:LEU:HG	5	0.12
(2,706)	1:34:C:PHE:HZ	1:51:C:LEU:HG	44	0.12
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	35	0.12
(2,692)	1:52:C:ARG:HG2	1:50:C:GLY:HA3	5	0.12
(2,678)	1:57:C:SER:HB3	1:52:C:ARG:HB2	36	0.12
(2,678)	1:57:C:SER:HB3	1:52:C:ARG:HB3	46	0.12
(2,634)	1:17:C:VAL:HG21	1:38:C:CYS:HB2	32	0.12
(2,614)	1:14:C:ARG:HG2	1:21:C:GLY:HA2	16	0.12
(2,614)	1:14:C:ARG:HG2	1:21:C:GLY:HA2	18	0.12
(2,593)	1:6:C:GLN:HB2	1:6:C:GLN:HA	6	0.12
(2,593)	1:6:C:GLN:HB2	1:6:C:GLN:HA	7	0.12
(2,593)	1:7:C:GLN:HB2	1:7:C:GLN:HA	11	0.12
(2,593)	1:6:C:GLN:HB2	1:6:C:GLN:HA	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,593)	1:7:C:GLN:HB2	1:7:C:GLN:HA	19	0.12
(2,593)	1:6:C:GLN:HB2	1:6:C:GLN:HA	26	0.12
(2,593)	1:6:C:GLN:HB2	1:6:C:GLN:HA	33	0.12
(2,458)	1:30:C:CYS:H	1:28:C:THR:HG23	7	0.12
(2,448)	1:28:C:THR:H	1:51:C:LEU:HD21	26	0.12
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	9	0.12
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	12	0.12
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	15	0.12
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	19	0.12
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	32	0.12
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	43	0.12
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	46	0.12
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	10	0.12
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	38	0.12
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	39	0.12
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	43	0.12
(2,395)	1:17:C:VAL:H	1:18:C:CYS:HB2	5	0.12
(2,385)	1:12:C:GLY:H	1:11:C:PRO:HA	8	0.12
(2,371)	1:23:C:ASP:H	1:22:C:THR:HG21	20	0.12
(2,352)	1:34:C:PHE:HE1	1:34:C:PHE:H	38	0.12
(2,281)	1:66:C:GLU:H	1:65:C:VAL:HA	16	0.12
(2,252)	1:22:C:THR:HG23	1:23:C:ASP:HB3	11	0.12
(2,252)	1:22:C:THR:HG22	1:23:C:ASP:HB3	12	0.12
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	43	0.12
(2,234)	1:36:C:TRP:HZ3	1:51:C:LEU:HD23	17	0.12
(2,190)	1:52:C:ARG:HA	1:52:C:ARG:HG3	36	0.12
(2,149)	1:38:C:CYS:HB3	1:17:C:VAL:HB	13	0.12
(2,145)	1:39:C:HIS:HD2	1:38:C:CYS:HB3	50	0.12
(2,125)	1:32:C:ALA:HB2	1:33:C:ALA:HA	13	0.12
(2,125)	1:32:C:ALA:HB2	1:33:C:ALA:HA	18	0.12
(2,125)	1:32:C:ALA:HB3	1:33:C:ALA:HA	42	0.12
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	9	0.12
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	13	0.12
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	23	0.12
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	26	0.12
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	49	0.12
(2,107)	1:52:C:ARG:HA	1:27:C:CYS:HA	10	0.12
(2,101)	1:27:C:CYS:HA	1:26:C:ARG:HB2	49	0.12
(2,92)	1:24:C:VAL:HG21	1:21:C:GLY:HA2	28	0.12
(2,85)	1:24:C:VAL:HG11	1:14:C:ARG:HA	13	0.12
(2,63)	1:17:C:VAL:HG13	1:18:C:CYS:HB3	44	0.12
(2,62)	1:17:C:VAL:HG12	1:18:C:CYS:HB2	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,62)	1:17:C:VAL:HG11	1:18:C:CYS:HB2	23	0.12
(2,62)	1:17:C:VAL:HG13	1:18:C:CYS:HB2	27	0.12
(2,62)	1:17:C:VAL:HG13	1:18:C:CYS:HB2	33	0.12
(2,62)	1:17:C:VAL:HG13	1:18:C:CYS:HB2	38	0.12
(2,62)	1:17:C:VAL:HG12	1:18:C:CYS:HB2	49	0.12
(2,772)	1:57:C:SER:H	1:57:C:SER:HB3	29	0.11
(2,765)	1:61:C:THR:H	1:60:C:VAL:HG11	12	0.11
(2,765)	1:61:C:THR:H	1:60:C:VAL:HG13	48	0.11
(2,739)	1:37:C:ARG:H	1:35:C:HIS:HB3	5	0.11
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD12	7	0.11
(2,733)	1:25:C:LEU:H	1:25:C:LEU:HD21	16	0.11
(2,706)	1:34:C:PHE:HZ	1:51:C:LEU:HG	36	0.11
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	33	0.11
(2,702)	1:34:C:PHE:HZ	1:51:C:LEU:HD22	9	0.11
(2,702)	1:34:C:PHE:HE2	1:51:C:LEU:HD21	44	0.11
(2,692)	1:52:C:ARG:HG2	1:50:C:GLY:HA3	26	0.11
(2,663)	1:57:C:SER:HB3	1:52:C:ARG:HB2	4	0.11
(2,614)	1:14:C:ARG:HG2	1:21:C:GLY:HA2	35	0.11
(2,614)	1:14:C:ARG:HG2	1:21:C:GLY:HA2	46	0.11
(2,593)	1:6:C:GLN:HB2	1:6:C:GLN:HA	9	0.11
(2,593)	1:7:C:GLN:HB2	1:7:C:GLN:HA	49	0.11
(2,575)	1:36:C:TRP:HE1	1:46:C:ARG:HB2	31	0.11
(2,575)	1:36:C:TRP:HE1	1:46:C:ARG:HB2	44	0.11
(2,553)	1:65:C:VAL:H	1:64:C:PRO:HA	7	0.11
(2,544)	1:60:C:VAL:H	1:60:C:VAL:HB	37	0.11
(2,544)	1:60:C:VAL:H	1:60:C:VAL:HB	48	0.11
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	26	0.11
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	27	0.11
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	4	0.11
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	24	0.11
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	38	0.11
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	44	0.11
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	48	0.11
(2,420)	1:21:C:GLY:H	1:24:C:VAL:HG22	11	0.11
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	15	0.11
(2,379)	1:8:C:ASN:H	1:7:C:GLN:HA	32	0.11
(2,367)	1:35:C:HIS:HD2	1:24:C:VAL:HG23	43	0.11
(2,361)	1:15:C:CYS:H	1:24:C:VAL:HG23	5	0.11
(2,360)	1:22:C:THR:H	1:24:C:VAL:HG12	47	0.11
(2,330)	1:39:C:HIS:HE1	1:32:C:ALA:HB1	15	0.11
(2,246)	1:32:C:ALA:HB1	1:27:C:CYS:HB3	48	0.11
(2,177)	1:36:C:TRP:HD1	1:47:C:PRO:HD3	49	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,125)	1:32:C:ALA:HB3	1:33:C:ALA:HA	33	0.11
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	41	0.11
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	45	0.11
(2,86)	1:24:C:VAL:HG12	1:21:C:GLY:HA2	32	0.11
(2,85)	1:24:C:VAL:HG12	1:14:C:ARG:HA	32	0.11
(2,84)	1:24:C:VAL:HG13	1:24:C:VAL:HA	41	0.11
(2,68)	1:14:C:ARG:HG2	1:20:C:ASP:HA	11	0.11
(2,68)	1:14:C:ARG:HG2	1:20:C:ASP:HA	23	0.11
(2,62)	1:17:C:VAL:HG13	1:18:C:CYS:HB2	9	0.11
(2,60)	1:18:C:CYS:HB2	1:18:C:CYS:HA	44	0.11
(2,40)	1:9:C:LEU:HD23	1:9:C:LEU:HA	50	0.11
(2,778)	1:36:C:TRP:HE1	1:46:C:ARG:HD3	16	0.1
(2,726)	1:13:C:ALA:H	1:12:C:GLY:HA2	23	0.1
(2,706)	1:34:C:PHE:HZ	1:51:C:LEU:HG	9	0.1
(2,704)	1:34:C:PHE:HZ	1:25:C:LEU:HB3	13	0.1
(2,634)	1:17:C:VAL:HG23	1:38:C:CYS:HB2	35	0.1
(2,623)	1:27:C:CYS:HA	1:26:C:ARG:HB3	36	0.1
(2,610)	1:24:C:VAL:HG11	1:26:C:ARG:HD3	6	0.1
(2,544)	1:60:C:VAL:H	1:60:C:VAL:HB	29	0.1
(2,543)	1:60:C:VAL:H	1:59:C:ASP:HA	44	0.1
(2,537)	1:54:C:ARG:H	1:39:C:HIS:HB2	18	0.1
(2,496)	1:39:C:HIS:H	1:39:C:HIS:HB3	12	0.1
(2,468)	1:32:C:ALA:H	1:27:C:CYS:HB2	28	0.1
(2,458)	1:30:C:CYS:H	1:28:C:THR:HG22	32	0.1
(2,448)	1:28:C:THR:H	1:51:C:LEU:HD22	7	0.1
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	11	0.1
(2,437)	1:25:C:LEU:H	1:25:C:LEU:HB3	39	0.1
(2,412)	1:20:C:ASP:H	1:20:C:ASP:HB2	39	0.1
(2,402)	1:19:C:GLY:H	1:19:C:GLY:HA3	17	0.1
(2,388)	1:13:C:ALA:H	1:13:C:ALA:HB3	11	0.1
(2,385)	1:12:C:GLY:H	1:11:C:PRO:HA	18	0.1
(2,385)	1:12:C:GLY:H	1:11:C:PRO:HA	41	0.1
(2,359)	1:22:C:THR:H	1:24:C:VAL:HG23	13	0.1
(2,252)	1:22:C:THR:HG21	1:23:C:ASP:HB3	7	0.1
(2,252)	1:22:C:THR:HG22	1:23:C:ASP:HB3	18	0.1
(2,244)	1:33:C:ALA:HB2	1:24:C:VAL:HB	14	0.1
(2,190)	1:52:C:ARG:HA	1:52:C:ARG:HG3	41	0.1
(2,155)	1:54:C:ARG:HB2	1:39:C:HIS:HB2	45	0.1
(2,149)	1:38:C:CYS:HB3	1:17:C:VAL:HB	21	0.1
(2,125)	1:32:C:ALA:HB1	1:33:C:ALA:HA	2	0.1
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	17	0.1
(2,124)	1:24:C:VAL:HB	1:33:C:ALA:HA	39	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,44)	1:21:C:GLY:HA2	1:14:C:ARG:HA	41	0.1
(2,40)	1:9:C:LEU:HD23	1:9:C:LEU:HA	28	0.1

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

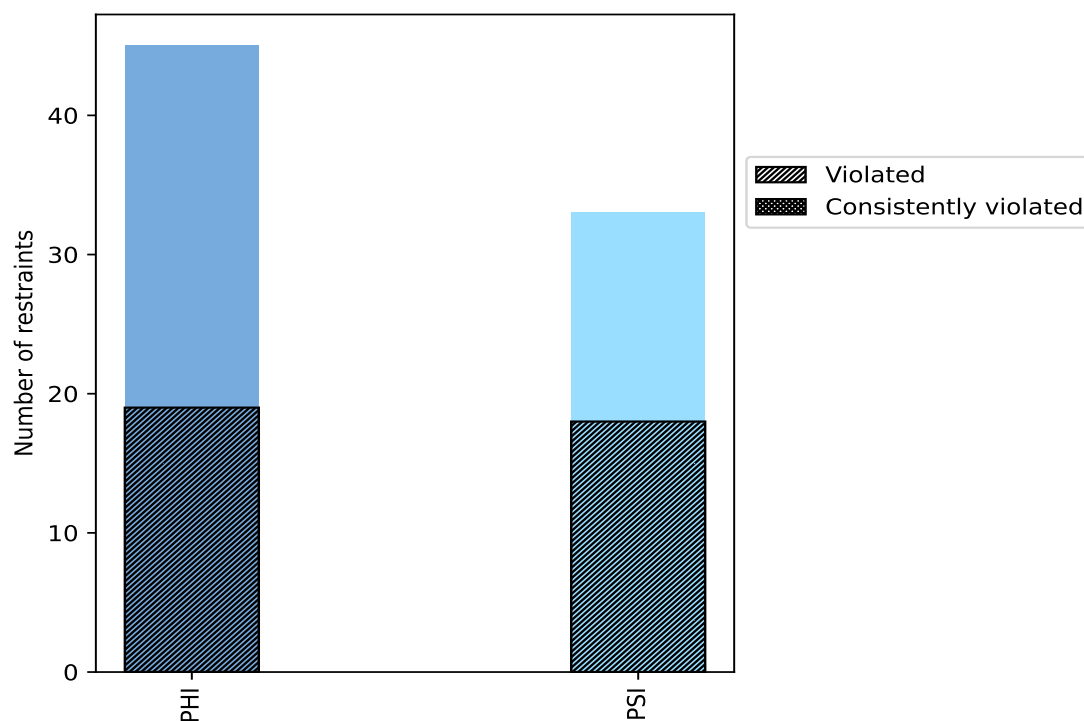
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	45	57.7	19	42.2	24.4	0	0.0	0.0
PSI	33	42.3	18	54.5	23.1	0	0.0	0.0
Total	78	100.0	37	47.4	47.4	0	0.0	0.0

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

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



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

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

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

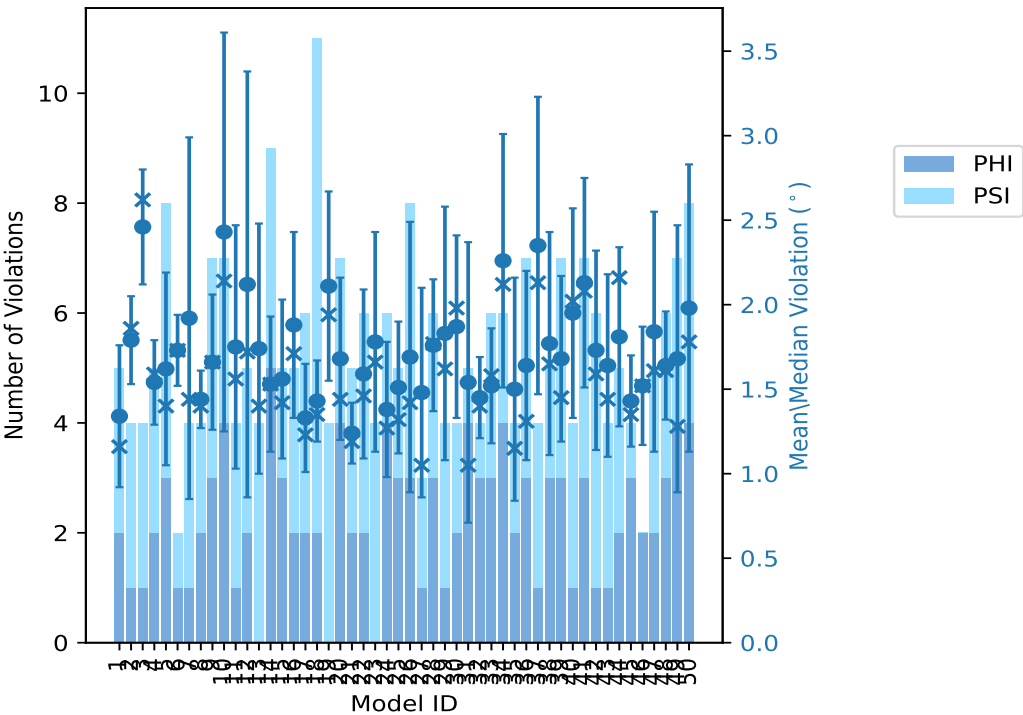
Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	2	3	5	1.34	2.16	0.42	1.16
2	1	3	4	1.79	2.04	0.26	1.86
3	1	3	4	2.46	2.72	0.34	2.62
4	2	3	5	1.54	1.87	0.25	1.59
5	3	5	8	1.62	3.08	0.57	1.4
6	1	1	2	1.73	1.94	0.21	1.73
7	1	3	4	1.92	3.74	1.07	1.44
8	2	2	4	1.44	1.7	0.17	1.4
9	3	4	7	1.66	2.21	0.4	1.66
10	4	3	7	2.43	5.08	1.18	2.14
11	1	3	4	1.75	2.83	0.72	1.56
12	2	3	5	2.12	4.51	1.26	1.72
13	0	4	4	1.74	3.01	0.74	1.4
14	5	4	9	1.53	2.02	0.4	1.53
15	3	2	5	1.56	2.43	0.47	1.42
16	2	3	5	1.88	2.96	0.55	1.71
17	2	4	6	1.33	1.99	0.32	1.23
18	2	9	11	1.43	1.8	0.24	1.35
19	0	4	4	2.11	3.0	0.56	1.94
20	4	3	7	1.68	2.74	0.48	1.44
21	2	3	5	1.24	1.57	0.18	1.19
22	2	4	6	1.59	2.43	0.5	1.46
23	0	4	4	1.78	2.73	0.65	1.66
24	4	2	6	1.38	2.26	0.4	1.27
25	3	2	5	1.51	2.24	0.39	1.32
26	3	5	8	1.69	3.5	0.8	1.42
27	1	2	3	1.48	2.36	0.62	1.05
28	3	3	6	1.76	2.32	0.39	1.77
29	1	3	4	1.83	3.03	0.75	1.62
30	2	2	4	1.87	2.46	0.54	1.98
31	4	1	5	1.54	3.18	0.83	1.05
32	3	1	4	1.45	1.79	0.24	1.4
33	3	3	6	1.52	2.11	0.34	1.58
34	4	2	6	2.26	3.43	0.75	2.12
35	2	2	4	1.5	2.64	0.66	1.15
36	3	4	7	1.64	2.77	0.56	1.31
37	1	3	4	2.35	3.75	0.88	2.13
38	3	2	5	1.77	3.01	0.66	1.65

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Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
39	3	4	7	1.68	2.52	0.49	1.45
40	1	3	4	1.95	2.72	0.62	2.02
41	3	4	7	2.13	3.08	0.62	2.08
42	1	5	6	1.73	2.6	0.59	1.59
43	1	3	4	1.64	2.51	0.54	1.44
44	2	3	5	1.81	2.27	0.53	2.16
45	3	1	4	1.43	1.85	0.27	1.35
46	2	0	2	1.52	1.87	0.35	1.52
47	2	3	5	1.84	3.16	0.71	1.61
48	3	3	6	1.64	2.27	0.32	1.61
49	4	3	7	1.68	3.22	0.79	1.28
50	4	4	8	1.98	3.6	0.85	1.78

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 [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
8	6	14	1	2.0
1	2	3	2	4.0
2	1	3	3	6.0
2	0	2	4	8.0
0	2	2	5	10.0
1	2	3	6	12.0
0	0	0	7	14.0
1	0	1	8	16.0
0	0	0	9	18.0
0	0	0	10	20.0
1	0	1	11	22.0
0	0	0	12	24.0
0	0	0	13	26.0
1	0	1	14	28.0
1	0	1	15	30.0
0	0	0	16	32.0
0	1	1	17	34.0
0	1	1	18	36.0
0	0	0	19	38.0
0	0	0	20	40.0
0	0	0	21	42.0
0	1	1	22	44.0
0	0	0	23	46.0
0	0	0	24	48.0
0	0	0	25	50.0
0	0	0	26	52.0
0	0	0	27	54.0
0	0	0	28	56.0
0	0	0	29	58.0
0	1	1	30	60.0
0	1	1	31	62.0
0	0	0	32	64.0
0	0	0	33	66.0
0	0	0	34	68.0
0	0	0	35	70.0
1	0	1	36	72.0
0	0	0	37	74.0

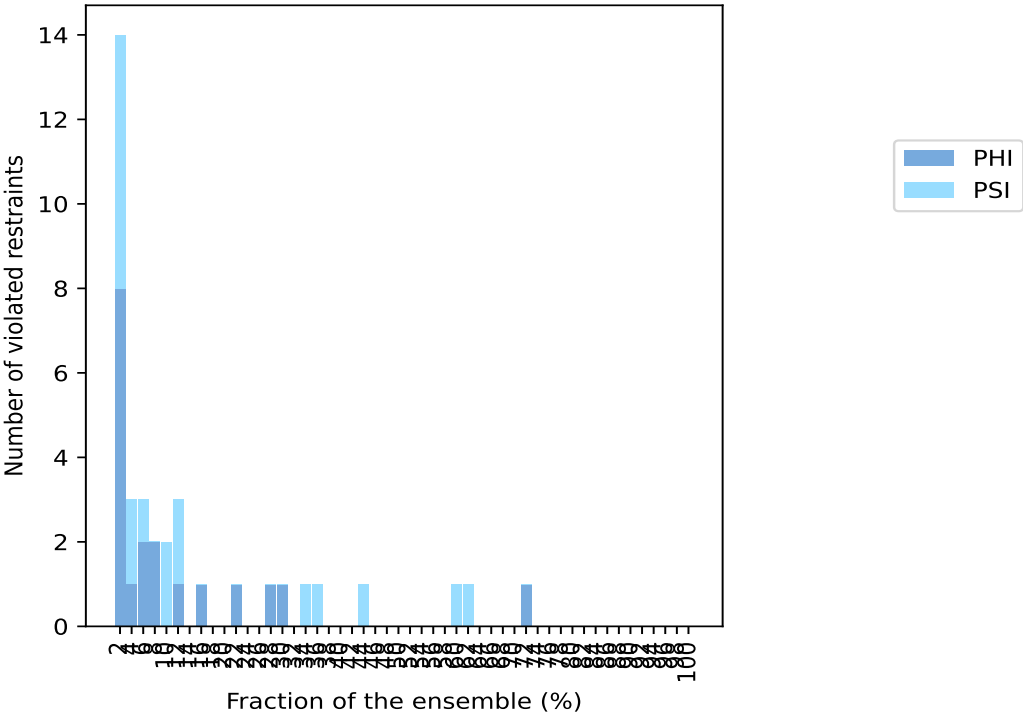
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	38	76.0
0	0	0	39	78.0
0	0	0	40	80.0
0	0	0	41	82.0
0	0	0	42	84.0
0	0	0	43	86.0
0	0	0	44	88.0
0	0	0	45	90.0
0	0	0	46	92.0
0	0	0	47	94.0
0	0	0	48	96.0
0	0	0	49	98.0
0	0	0	50	100.0

¹ Number of models with violations

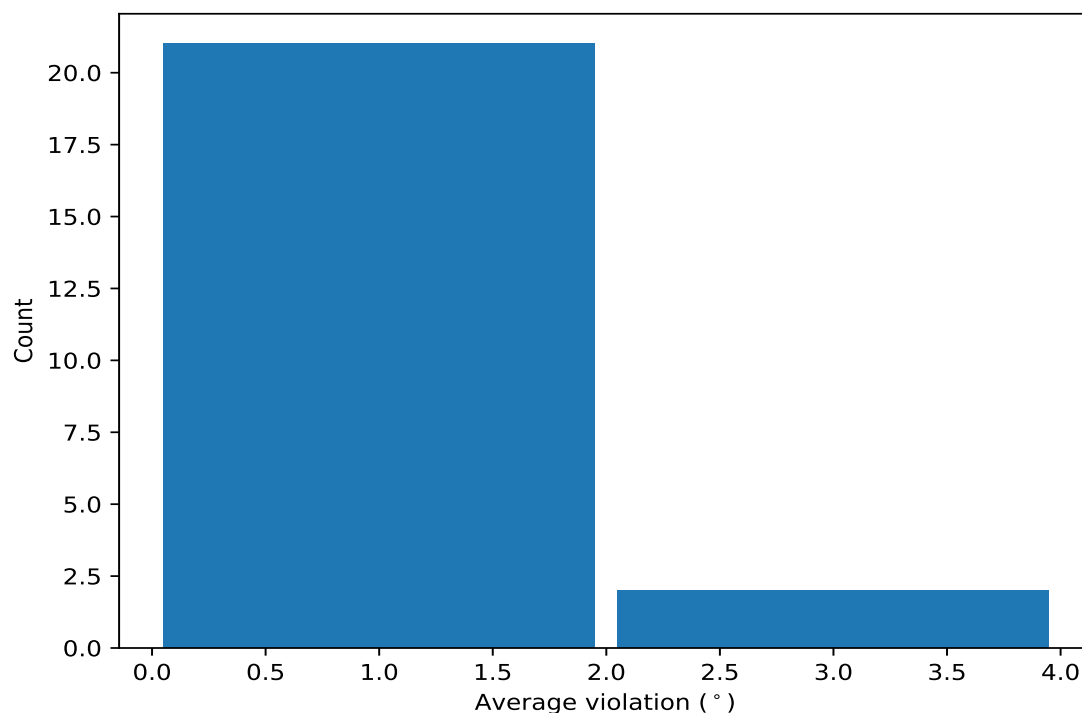
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	36	1.67	0.49	1.59
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	31	1.82	0.77	1.68
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	30	1.85	0.67	1.69
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	22	2.44	0.69	2.58
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	18	2.07	0.75	2.05
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	17	1.61	0.39	1.49
(1,35)	1:46:C:ARG:C	1:47:C:PRO:N	1:47:C:PRO:CA	1:47:C:PRO:C	15	1.65	0.48	1.46
(1,15)	1:10:C:ALA:C	1:11:C:PRO:N	1:11:C:PRO:CA	1:11:C:PRO:C	14	1.62	0.57	1.48
(1,41)	1:55:C:SER:C	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	11	1.6	0.49	1.42
(1,10)	1:58:C:GLY:C	1:59:C:ASP:N	1:59:C:ASP:CA	1:59:C:ASP:C	8	1.73	1.29	1.16
(1,74)	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	1:57:C:SER:N	6	1.65	0.49	1.63
(1,2)	1:23:C:ASP:C	1:24:C:VAL:N	1:24:C:VAL:CA	1:24:C:VAL:C	6	1.44	0.33	1.46
(1,59)	1:33:C:ALA:N	1:33:C:ALA:CA	1:33:C:ALA:C	1:34:C:PHE:N	6	1.12	0.06	1.14

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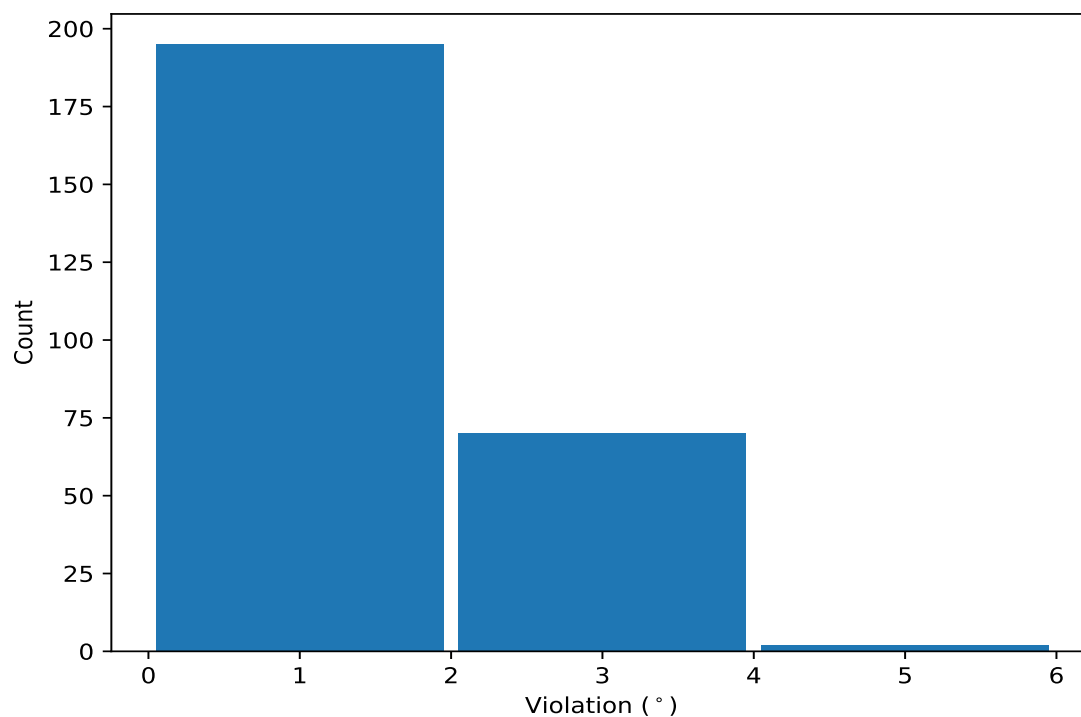
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,52)	1:22:C:THR:N	1:22:C:THR:CA	1:22:C:THR:C	1:23:C:ASP:N	5	1.47	0.12	1.44
(1,46)	1:10:C:ALA:N	1:10:C:ALA:CA	1:10:C:ALA:C	1:11:C:PRO:N	5	1.43	0.49	1.18
(1,21)	1:21:C:GLY:C	1:22:C:THR:N	1:22:C:THR:CA	1:22:C:THR:C	4	1.5	0.29	1.6
(1,11)	1:59:C:ASP:C	1:60:C:VAL:N	1:60:C:VAL:CA	1:60:C:VAL:C	4	1.18	0.09	1.19
(1,76)	1:61:C:THR:N	1:61:C:THR:CA	1:61:C:THR:C	1:62:C:PRO:N	3	1.82	0.56	1.81
(1,38)	1:52:C:ARG:C	1:53:C:CYS:N	1:53:C:CYS:CA	1:53:C:CYS:C	3	1.35	0.32	1.22
(1,9)	1:48:C:GLY:C	1:49:C:THR:N	1:49:C:THR:CA	1:49:C:THR:C	3	1.16	0.08	1.17
(1,40)	1:54:C:ARG:C	1:55:C:SER:N	1:55:C:SER:CA	1:55:C:SER:C	2	1.58	0.3	1.58
(1,77)	1:62:C:PRO:N	1:62:C:PRO:CA	1:62:C:PRO:C	1:63:C:ALA:N	2	1.42	0.17	1.42
(1,65)	1:42:C:ALA:N	1:42:C:ALA:CA	1:42:C:ALA:C	1:43:C:GLY:N	2	1.14	0.1	1.14

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,10)	1:58:C:GLY:C	1:59:C:ASP:N	1:59:C:ASP:CA	1:59:C:ASP:C	10	5.08
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	12	4.51
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	37	3.75
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	7	3.74
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	50	3.6
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	26	3.5
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	34	3.43
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	49	3.22
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	31	3.18
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	47	3.16
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	41	3.08
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	5	3.08
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	50	3.04
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	29	3.03
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	38	3.01
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	13	3.01
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	19	3.0
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	16	2.96
(1,15)	1:10:C:ALA:C	1:11:C:PRO:N	1:11:C:PRO:CA	1:11:C:PRO:C	34	2.94
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	11	2.83
(1,41)	1:55:C:SER:C	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	36	2.77
(1,15)	1:10:C:ALA:C	1:11:C:PRO:N	1:11:C:PRO:CA	1:11:C:PRO:C	20	2.74
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	23	2.73
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	40	2.72
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	3	2.72
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	3	2.71
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	35	2.64
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	10	2.63
(1,35)	1:46:C:ARG:C	1:47:C:PRO:N	1:47:C:PRO:CA	1:47:C:PRO:C	41	2.62
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	42	2.6
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	41	2.57
(1,35)	1:46:C:ARG:C	1:47:C:PRO:N	1:47:C:PRO:CA	1:47:C:PRO:C	49	2.55
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	3	2.54
(1,76)	1:61:C:THR:N	1:61:C:THR:CA	1:61:C:THR:C	1:62:C:PRO:N	39	2.52
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	43	2.51
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	30	2.46
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	22	2.43
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	15	2.43
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	42	2.39
(1,46)	1:10:C:ALA:N	1:10:C:ALA:CA	1:10:C:ALA:C	1:11:C:PRO:N	27	2.36
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	37	2.35
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	28	2.32
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	26	2.31
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	40	2.29
(1,74)	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	1:57:C:SER:N	10	2.27
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	44	2.27
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	48	2.27
(1,74)	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	1:57:C:SER:N	44	2.26
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	24	2.26
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	25	2.24
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	9	2.21
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	30	2.19

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	19	2.18
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	44	2.16
(1,35)	1:46:C:ARG:C	1:47:C:PRO:N	1:47:C:PRO:CA	1:47:C:PRO:C	1	2.16
(1,41)	1:55:C:SER:C	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	10	2.14
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	12	2.13
(1,35)	1:46:C:ARG:C	1:47:C:PRO:N	1:47:C:PRO:CA	1:47:C:PRO:C	34	2.12
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	34	2.11
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	33	2.11
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	9	2.1
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	36	2.1
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	39	2.09
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	10	2.09
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	41	2.08
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	50	2.06
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	2	2.04
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	22	2.03
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	2	2.02
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	23	2.02
(1,15)	1:10:C:ALA:C	1:11:C:PRO:N	1:11:C:PRO:CA	1:11:C:PRO:C	14	2.02
(1,41)	1:55:C:SER:C	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	14	2.0
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	17	1.99
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	28	1.99
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	39	1.99
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	11	1.97
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	6	1.94
(1,2)	1:23:C:ASP:C	1:24:C:VAL:N	1:24:C:VAL:CA	1:24:C:VAL:C	47	1.94
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	9	1.91
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	37	1.91
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	14	1.9
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	3	1.89
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	41	1.88
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	20	1.88
(1,40)	1:54:C:ARG:C	1:55:C:SER:N	1:55:C:SER:CA	1:55:C:SER:C	14	1.88
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	4	1.87
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	50	1.87
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	46	1.87
(1,17)	1:13:C:ALA:C	1:14:C:ARG:N	1:14:C:ARG:CA	1:14:C:ARG:C	28	1.86
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	45	1.85
(1,76)	1:61:C:THR:N	1:61:C:THR:CA	1:61:C:THR:C	1:62:C:PRO:N	29	1.81
(1,38)	1:52:C:ARG:C	1:53:C:CYS:N	1:53:C:CYS:CA	1:53:C:CYS:C	34	1.8
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	18	1.8
(1,15)	1:10:C:ALA:C	1:11:C:PRO:N	1:11:C:PRO:CA	1:11:C:PRO:C	32	1.79
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	30	1.78
(1,21)	1:21:C:GLY:C	1:22:C:THR:N	1:22:C:THR:CA	1:22:C:THR:C	10	1.76
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	20	1.76
(1,35)	1:46:C:ARG:C	1:47:C:PRO:N	1:47:C:PRO:CA	1:47:C:PRO:C	40	1.75
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	4	1.73
(1,10)	1:58:C:GLY:C	1:59:C:ASP:N	1:59:C:ASP:CA	1:59:C:ASP:C	38	1.73
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	42	1.72
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	12	1.72
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	16	1.71

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	36	1.71
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	19	1.71
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	16	1.71
(1,2)	1:23:C:ASP:C	1:24:C:VAL:N	1:24:C:VAL:CA	1:24:C:VAL:C	26	1.71
(1,52)	1:22:C:THR:N	1:22:C:THR:CA	1:22:C:THR:C	1:23:C:ASP:N	8	1.7
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	2	1.7
(1,21)	1:21:C:GLY:C	1:22:C:THR:N	1:22:C:THR:CA	1:22:C:THR:C	18	1.7
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	18	1.69
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	48	1.68
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	43	1.68
(1,41)	1:55:C:SER:C	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	50	1.68
(1,35)	1:46:C:ARG:C	1:47:C:PRO:N	1:47:C:PRO:CA	1:47:C:PRO:C	28	1.68
(1,74)	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	1:57:C:SER:N	28	1.67
(1,35)	1:46:C:ARG:C	1:47:C:PRO:N	1:47:C:PRO:CA	1:47:C:PRO:C	9	1.66
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	38	1.65
(1,15)	1:10:C:ALA:C	1:11:C:PRO:N	1:11:C:PRO:CA	1:11:C:PRO:C	15	1.63
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	33	1.63
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	48	1.62
(1,15)	1:10:C:ALA:C	1:11:C:PRO:N	1:11:C:PRO:CA	1:11:C:PRO:C	5	1.62
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	47	1.61
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	5	1.6
(1,2)	1:23:C:ASP:C	1:24:C:VAL:N	1:24:C:VAL:CA	1:24:C:VAL:C	48	1.6
(1,77)	1:62:C:PRO:N	1:62:C:PRO:CA	1:62:C:PRO:C	1:63:C:ALA:N	4	1.59
(1,74)	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	1:57:C:SER:N	18	1.59
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	33	1.58
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	16	1.58
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	33	1.57
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	21	1.57
(1,10)	1:58:C:GLY:C	1:59:C:ASP:N	1:59:C:ASP:CA	1:59:C:ASP:C	22	1.57
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	25	1.57
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	19	1.56
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	32	1.56
(1,15)	1:10:C:ALA:C	1:11:C:PRO:N	1:11:C:PRO:CA	1:11:C:PRO:C	26	1.55
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	14	1.53
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	6	1.52
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	18	1.5
(1,21)	1:21:C:GLY:C	1:22:C:THR:N	1:22:C:THR:CA	1:22:C:THR:C	45	1.5
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	5	1.49
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	8	1.49
(1,41)	1:55:C:SER:C	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	41	1.47
(1,52)	1:22:C:THR:N	1:22:C:THR:CA	1:22:C:THR:C	1:23:C:ASP:N	42	1.46
(1,35)	1:46:C:ARG:C	1:47:C:PRO:N	1:47:C:PRO:CA	1:47:C:PRO:C	7	1.46
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	9	1.46
(1,53)	1:25:C:LEU:N	1:25:C:LEU:CA	1:25:C:LEU:C	1:26:C:ARG:N	39	1.45
(1,75)	1:57:C:SER:N	1:57:C:SER:CA	1:57:C:SER:C	1:58:C:GLY:N	50	1.44
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	13	1.44
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	29	1.44
(1,52)	1:22:C:THR:N	1:22:C:THR:CA	1:22:C:THR:C	1:23:C:ASP:N	48	1.44
(1,46)	1:10:C:ALA:N	1:10:C:ALA:CA	1:10:C:ALA:C	1:11:C:PRO:N	20	1.44
(1,35)	1:46:C:ARG:C	1:47:C:PRO:N	1:47:C:PRO:CA	1:47:C:PRO:C	16	1.43
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	15	1.42

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	39	1.42
(1,41)	1:55:C:SER:C	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	49	1.42
(1,12)	1:64:C:PRO:C	1:65:C:VAL:N	1:65:C:VAL:CA	1:65:C:VAL:C	20	1.42
(1,52)	1:22:C:THR:N	1:22:C:THR:CA	1:22:C:THR:C	1:23:C:ASP:N	7	1.41
(1,15)	1:10:C:ALA:C	1:11:C:PRO:N	1:11:C:PRO:CA	1:11:C:PRO:C	2	1.41
(1,15)	1:10:C:ALA:C	1:11:C:PRO:N	1:11:C:PRO:CA	1:11:C:PRO:C	31	1.41
(1,43)	1:60:C:VAL:C	1:61:C:THR:N	1:61:C:THR:CA	1:61:C:THR:C	38	1.4
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	17	1.39
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	37	1.39
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	47	1.37
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	18	1.35
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	13	1.35
(1,68)	1:47:C:PRO:N	1:47:C:PRO:CA	1:47:C:PRO:C	1:48:C:GLY:N	18	1.34
(1,52)	1:22:C:THR:N	1:22:C:THR:CA	1:22:C:THR:C	1:23:C:ASP:N	18	1.34
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	22	1.34
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	25	1.32
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	24	1.32
(1,41)	1:55:C:SER:C	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	5	1.32
(1,42)	1:56:C:CYS:C	1:57:C:SER:N	1:57:C:SER:CA	1:57:C:SER:C	36	1.31
(1,2)	1:23:C:ASP:C	1:24:C:VAL:N	1:24:C:VAL:CA	1:24:C:VAL:C	20	1.31
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	23	1.3
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	5	1.3
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	8	1.3
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	44	1.3
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	1	1.3
(1,35)	1:46:C:ARG:C	1:47:C:PRO:N	1:47:C:PRO:CA	1:47:C:PRO:C	8	1.29
(1,15)	1:10:C:ALA:C	1:11:C:PRO:N	1:11:C:PRO:CA	1:11:C:PRO:C	4	1.29
(1,35)	1:46:C:ARG:C	1:47:C:PRO:N	1:47:C:PRO:CA	1:47:C:PRO:C	26	1.28
(1,11)	1:59:C:ASP:C	1:60:C:VAL:N	1:60:C:VAL:CA	1:60:C:VAL:C	49	1.28
(1,61)	1:35:C:HIS:N	1:35:C:HIS:CA	1:35:C:HIS:C	1:36:C:TRP:N	14	1.27
(1,40)	1:54:C:ARG:C	1:55:C:SER:N	1:55:C:SER:CA	1:55:C:SER:C	24	1.27
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	36	1.27
(1,77)	1:62:C:PRO:N	1:62:C:PRO:CA	1:62:C:PRO:C	1:63:C:ALA:N	5	1.26
(1,41)	1:55:C:SER:C	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	25	1.26
(1,11)	1:59:C:ASP:C	1:60:C:VAL:N	1:60:C:VAL:CA	1:60:C:VAL:C	24	1.26
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	5	1.26
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	36	1.25
(1,41)	1:55:C:SER:C	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	21	1.25
(1,9)	1:48:C:GLY:C	1:49:C:THR:N	1:49:C:THR:CA	1:49:C:THR:C	39	1.25
(1,65)	1:42:C:ALA:N	1:42:C:ALA:CA	1:42:C:ALA:C	1:43:C:GLY:N	17	1.24
(1,15)	1:10:C:ALA:C	1:11:C:PRO:N	1:11:C:PRO:CA	1:11:C:PRO:C	48	1.24
(1,13)	1:65:C:VAL:C	1:66:C:GLU:N	1:66:C:GLU:CA	1:66:C:GLU:C	32	1.23
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	20	1.22
(1,38)	1:52:C:ARG:C	1:53:C:CYS:N	1:53:C:CYS:CA	1:53:C:CYS:C	41	1.22
(1,78)	1:63:C:ALA:N	1:63:C:ALA:CA	1:63:C:ALA:C	1:64:C:PRO:N	32	1.21
(1,35)	1:46:C:ARG:C	1:47:C:PRO:N	1:47:C:PRO:CA	1:47:C:PRO:C	4	1.21
(1,32)	1:41:C:PRO:C	1:42:C:ALA:N	1:42:C:ALA:CA	1:42:C:ALA:C	17	1.21
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	43	1.2
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	45	1.2
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	21	1.19
(1,35)	1:46:C:ARG:C	1:47:C:PRO:N	1:47:C:PRO:CA	1:47:C:PRO:C	12	1.19

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	35	1.18
(1,46)	1:10:C:ALA:N	1:10:C:ALA:CA	1:10:C:ALA:C	1:11:C:PRO:N	49	1.18
(1,10)	1:58:C:GLY:C	1:59:C:ASP:N	1:59:C:ASP:CA	1:59:C:ASP:C	25	1.18
(1,59)	1:33:C:ALA:N	1:33:C:ALA:CA	1:33:C:ALA:C	1:34:C:PHE:N	18	1.17
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	15	1.17
(1,41)	1:55:C:SER:C	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	15	1.17
(1,35)	1:46:C:ARG:C	1:47:C:PRO:N	1:47:C:PRO:CA	1:47:C:PRO:C	46	1.17
(1,9)	1:48:C:GLY:C	1:49:C:THR:N	1:49:C:THR:CA	1:49:C:THR:C	45	1.17
(1,59)	1:33:C:ALA:N	1:33:C:ALA:CA	1:33:C:ALA:C	1:34:C:PHE:N	1	1.16
(1,59)	1:33:C:ALA:N	1:33:C:ALA:CA	1:33:C:ALA:C	1:34:C:PHE:N	43	1.16
(1,35)	1:46:C:ARG:C	1:47:C:PRO:N	1:47:C:PRO:CA	1:47:C:PRO:C	33	1.16
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	13	1.15
(1,10)	1:58:C:GLY:C	1:59:C:ASP:N	1:59:C:ASP:CA	1:59:C:ASP:C	9	1.15
(1,76)	1:61:C:THR:N	1:61:C:THR:CA	1:61:C:THR:C	1:62:C:PRO:N	9	1.14
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	22	1.14
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	11	1.14
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	42	1.14
(1,59)	1:33:C:ALA:N	1:33:C:ALA:CA	1:33:C:ALA:C	1:34:C:PHE:N	21	1.13
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	34	1.13
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	47	1.13
(1,11)	1:59:C:ASP:C	1:60:C:VAL:N	1:60:C:VAL:CA	1:60:C:VAL:C	50	1.13
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	35	1.13
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	17	1.12
(1,69)	1:51:C:LEU:N	1:51:C:LEU:CA	1:51:C:LEU:C	1:52:C:ARG:N	18	1.11
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	24	1.11
(1,46)	1:10:C:ALA:N	1:10:C:ALA:CA	1:10:C:ALA:C	1:11:C:PRO:N	18	1.1
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	14	1.08
(1,41)	1:55:C:SER:C	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	33	1.08
(1,74)	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	1:57:C:SER:N	26	1.07
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	23	1.07
(1,15)	1:10:C:ALA:C	1:11:C:PRO:N	1:11:C:PRO:CA	1:11:C:PRO:C	49	1.07
(1,10)	1:58:C:GLY:C	1:59:C:ASP:N	1:59:C:ASP:CA	1:59:C:ASP:C	24	1.07
(1,2)	1:23:C:ASP:C	1:24:C:VAL:N	1:24:C:VAL:CA	1:24:C:VAL:C	39	1.07
(1,74)	1:56:C:CYS:N	1:56:C:CYS:CA	1:56:C:CYS:C	1:57:C:SER:N	11	1.06
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	42	1.06
(1,59)	1:33:C:ALA:N	1:33:C:ALA:CA	1:33:C:ALA:C	1:34:C:PHE:N	14	1.06
(1,49)	1:15:C:CYS:N	1:15:C:CYS:CA	1:15:C:CYS:C	1:16:C:GLY:N	36	1.06
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	1	1.05
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	7	1.05
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	26	1.05
(1,57)	1:31:C:ALA:N	1:31:C:ALA:CA	1:31:C:ALA:C	1:32:C:ALA:N	40	1.05
(1,46)	1:10:C:ALA:N	1:10:C:ALA:CA	1:10:C:ALA:C	1:11:C:PRO:N	28	1.05
(1,31)	1:37:C:ARG:C	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	31	1.05
(1,11)	1:59:C:ASP:C	1:60:C:VAL:N	1:60:C:VAL:CA	1:60:C:VAL:C	14	1.05
(1,10)	1:58:C:GLY:C	1:59:C:ASP:N	1:59:C:ASP:CA	1:59:C:ASP:C	27	1.05
(1,9)	1:48:C:GLY:C	1:49:C:THR:N	1:49:C:THR:CA	1:49:C:THR:C	31	1.05
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	21	1.05
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	38	1.05
(1,65)	1:42:C:ALA:N	1:42:C:ALA:CA	1:42:C:ALA:C	1:43:C:GLY:N	1	1.04
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	27	1.04
(1,38)	1:52:C:ARG:C	1:53:C:CYS:N	1:53:C:CYS:CA	1:53:C:CYS:C	30	1.04

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,10)	1:58:C:GLY:C	1:59:C:ASP:N	1:59:C:ASP:CA	1:59:C:ASP:C	44	1.04
(1,21)	1:21:C:GLY:C	1:22:C:THR:N	1:22:C:THR:CA	1:22:C:THR:C	31	1.03
(1,8)	1:44:C:THR:C	1:45:C:SER:N	1:45:C:SER:CA	1:45:C:SER:C	29	1.03
(1,6)	1:38:C:CYS:C	1:39:C:HIS:N	1:39:C:HIS:CA	1:39:C:HIS:C	12	1.03
(1,2)	1:23:C:ASP:C	1:24:C:VAL:N	1:24:C:VAL:CA	1:24:C:VAL:C	35	1.03
(1,59)	1:33:C:ALA:N	1:33:C:ALA:CA	1:33:C:ALA:C	1:34:C:PHE:N	26	1.02
(1,55)	1:27:C:CYS:N	1:27:C:CYS:CA	1:27:C:CYS:C	1:28:C:THR:N	49	1.02
(1,47)	1:13:C:ALA:N	1:13:C:ALA:CA	1:13:C:ALA:C	1:14:C:ARG:N	22	1.02
(1,15)	1:10:C:ALA:C	1:11:C:PRO:N	1:11:C:PRO:CA	1:11:C:PRO:C	50	1.02
(1,64)	1:38:C:CYS:N	1:38:C:CYS:CA	1:38:C:CYS:C	1:39:C:HIS:N	10	1.01
(1,15)	1:10:C:ALA:C	1:11:C:PRO:N	1:11:C:PRO:CA	1:11:C:PRO:C	17	1.01