



Full wwPDB NMR Structure Validation Report ⓘ

Jun 3, 2023 – 04:51 PM EDT

PDB ID : 2KNI
BMRB ID : 16468
Title : High-resolution solution structure of the ASIC1a blocker PcTX1
Authors : King, G.F.; Mobli, M.; Saez, N.J.
Deposited on : 2009-08-25

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

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

A user guide is available at

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

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

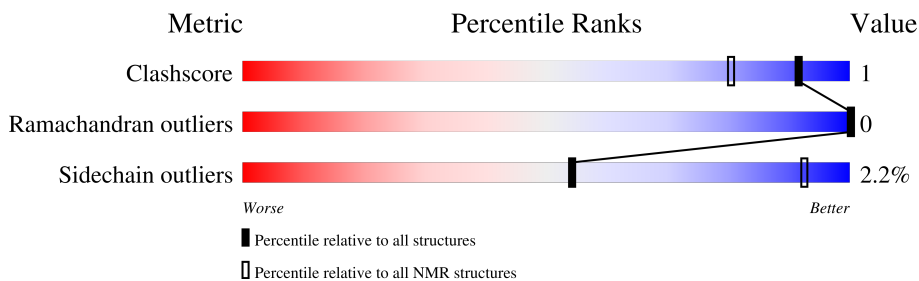
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 85%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	41	 78% 5% 17%

2 Ensemble composition and analysis i

This entry contains 25 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:37 (34)	0.25	1

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

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

The models can be grouped into 6 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 9, 14, 16, 17, 22, 23
2	11, 13, 15, 20, 25
3	5, 6, 10, 19, 24
4	2, 7, 18, 21
5	4, 12
6	3, 8

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 648 atoms, of which 318 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Psalmotoxin-1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	41	648	203	318	63	58	6	0

There is a discrepancy between the modelled and reference sequences:

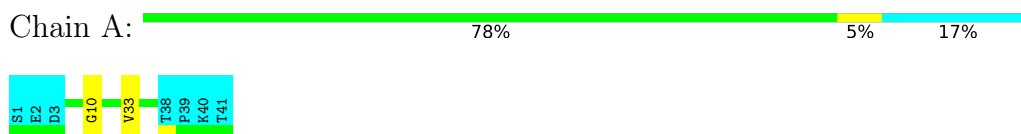
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P60514

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Psalmotoxin-1

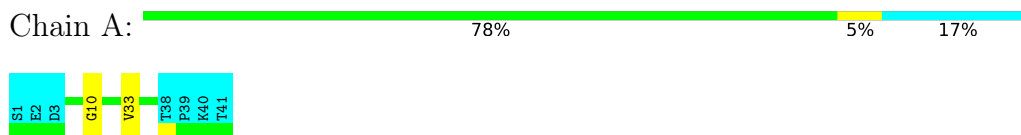


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

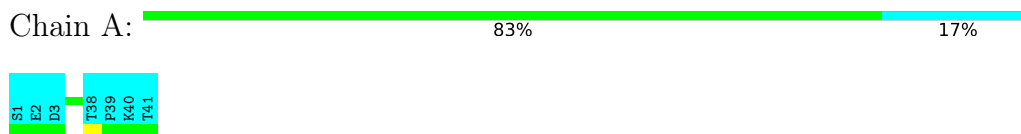
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Psalmotoxin-1



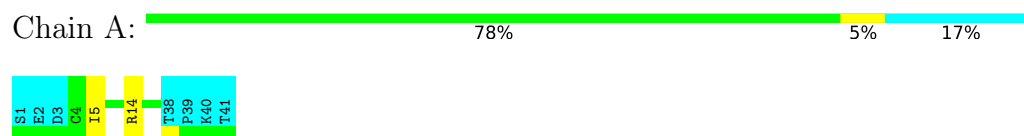
4.2.2 Score per residue for model 2

- Molecule 1: Psalmotoxin-1



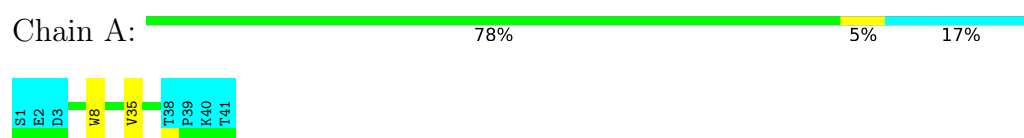
4.2.3 Score per residue for model 3

- Molecule 1: Psalmotoxin-1



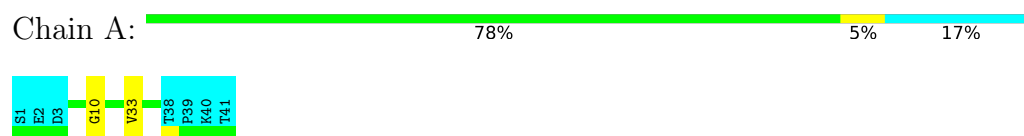
4.2.4 Score per residue for model 4

- Molecule 1: Psalmotoxin-1



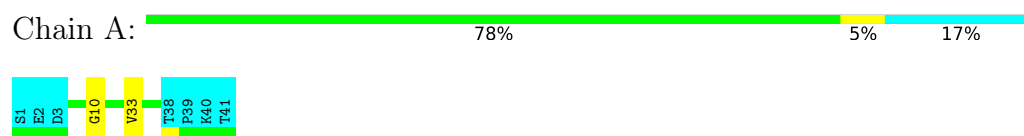
4.2.5 Score per residue for model 5

- Molecule 1: Psalmotoxin-1



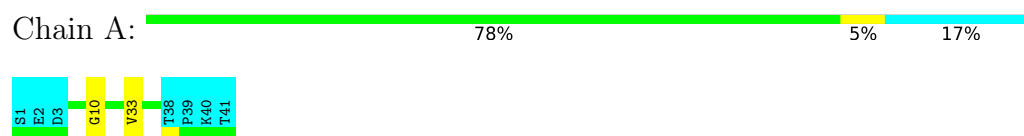
4.2.6 Score per residue for model 6

- Molecule 1: Psalmotoxin-1



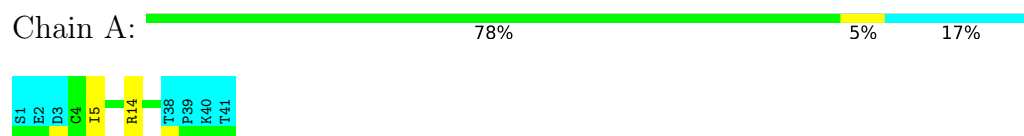
4.2.7 Score per residue for model 7

- Molecule 1: Psalmotoxin-1



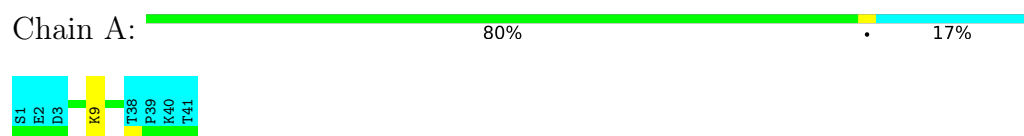
4.2.8 Score per residue for model 8

- Molecule 1: Psalmotoxin-1



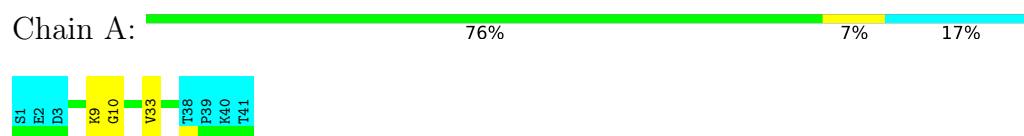
4.2.9 Score per residue for model 9

- Molecule 1: Psalmotoxin-1



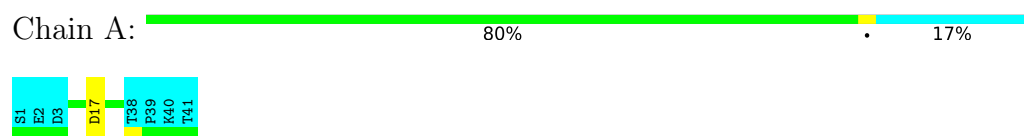
4.2.10 Score per residue for model 10

- Molecule 1: Psalmotoxin-1



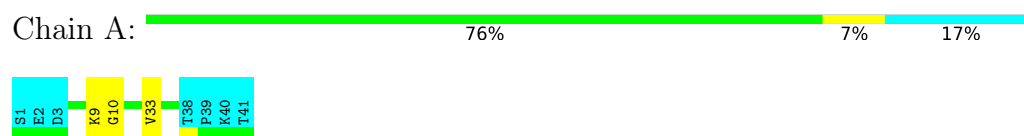
4.2.11 Score per residue for model 11

- Molecule 1: Psalmotoxin-1




4.2.12 Score per residue for model 12

- Molecule 1: Psalmotoxin-1



4.2.13 Score per residue for model 13


- Molecule 1: Psalmotoxin-1

Chain A:  76% 7% 17%



4.2.14 Score per residue for model 14


- Molecule 1: Psalmotoxin-1

Chain A:  76% 7% 17%



4.2.15 Score per residue for model 15


- Molecule 1: Psalmotoxin-1

Chain A:  76% 7% 17%



4.2.16 Score per residue for model 16


- Molecule 1: Psalmotoxin-1

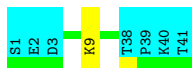
Chain A:  78% 5% 17%



4.2.17 Score per residue for model 17

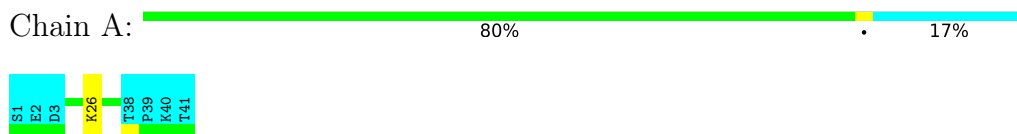
- Molecule 1: Psalmotoxin-1

Chain A:  80% 0% 17%



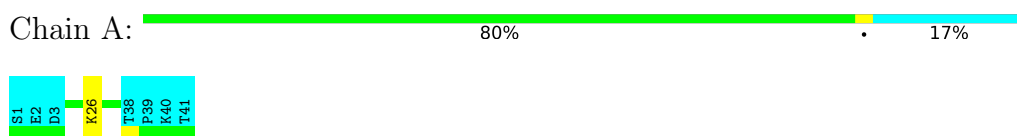
4.2.18 Score per residue for model 18

- Molecule 1: Psalmotoxin-1



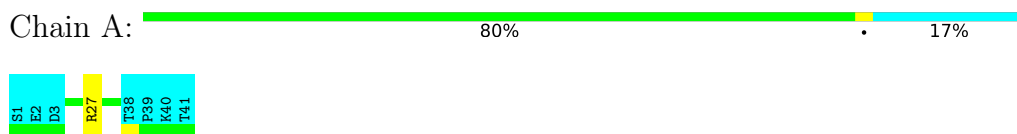
4.2.19 Score per residue for model 19

- Molecule 1: Psalmotoxin-1



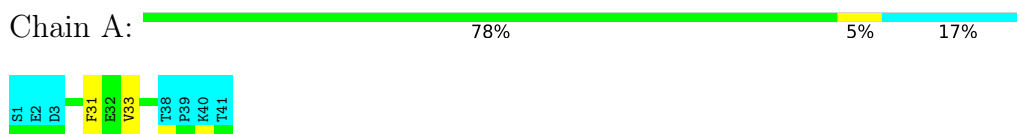
4.2.20 Score per residue for model 20

- Molecule 1: Psalmotoxin-1



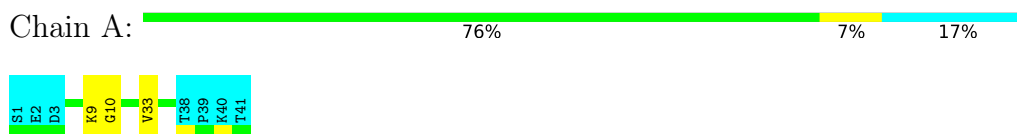
4.2.21 Score per residue for model 21

- Molecule 1: Psalmotoxin-1



4.2.22 Score per residue for model 22

- Molecule 1: Psalmotoxin-1



4.2.23 Score per residue for model 23

- Molecule 1: Psalmotoxin-1

Chain A:  73% 10% 17%



4.2.24 Score per residue for model 24


- Molecule 1: Psalmotoxin-1

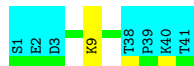
Chain A:  68% 15% 17%



4.2.25 Score per residue for model 25

- Molecule 1: Psalmotoxin-1

Chain A:  80% 0% 17%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 300 calculated structures, 25 were deposited, based on the following criterion: *Best Mol-Probity score*.

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

Software name	Classification	Version
CYANA	refinement	2.1
CYANA	structure solution	2.1

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	476
Number of shifts mapped to atoms	476
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	277	269	269	1±1
All	All	6925	6725	6725	20

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:GLY:HA2	1:A:33:VAL:HG12	0.49	1.84	14	13
1:A:5:ILE:HD11	1:A:14:ARG:CB	0.47	2.39	3	3
1:A:5:ILE:HD11	1:A:14:ARG:HB2	0.44	1.88	24	2
1:A:8:TRP:CD1	1:A:35:VAL:HG12	0.42	2.50	4	1
1:A:31:PHE:O	1:A:33:VAL:HG13	0.41	2.15	21	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	34/41 (83%)	28±1 (82±2%)	6±1 (18±2%)	0±0 (0±0%)	100	100
All	All	850/1025 (83%)	696 (82%)	154 (18%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	31/38 (82%)	30±1 (98±2%)	1±1 (2±2%)	54	92
All	All	775/950 (82%)	758 (98%)	17 (2%)	54	92

All 6 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	9	LYS	8
1	A	17	ASP	2
1	A	28	ARG	2
1	A	27	ARG	2
1	A	26	LYS	2
1	A	13	ASN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 86% 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 i

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	476
Number of shifts mapped to atoms	476
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 i

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	41	0.92 \pm 0.10	Should be applied
$^{13}\text{C}_\beta$	37	0.51 \pm 0.32	None needed (imprecise)
$^{13}\text{C}'$	36	-0.21 \pm 0.24	None needed (< 0.5 ppm)
^{15}N	36	0.60 \pm 0.46	None needed (imprecise)

7.1.3 Completeness of resonance assignments i

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 85%, i.e. 402 atoms were assigned a chemical shift out of a possible 473. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	164/169 (97%)	68/69 (99%)	65/68 (96%)	31/32 (97%)
Sidechain	221/263 (84%)	149/167 (89%)	69/79 (87%)	3/17 (18%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	17/41 (41%)	14/21 (67%)	0/17 (0%)	3/3 (100%)
Overall	402/473 (85%)	231/257 (90%)	134/164 (82%)	37/52 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 476 atoms were assigned a chemical shift out of a possible 554. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	193/202 (96%)	80/82 (98%)	77/82 (94%)	36/38 (95%)
Sidechain	266/311 (86%)	179/197 (91%)	84/96 (88%)	3/18 (17%)
Aromatic	17/41 (41%)	14/21 (67%)	0/17 (0%)	3/3 (100%)
Overall	476/554 (86%)	273/300 (91%)	161/195 (83%)	42/59 (71%)

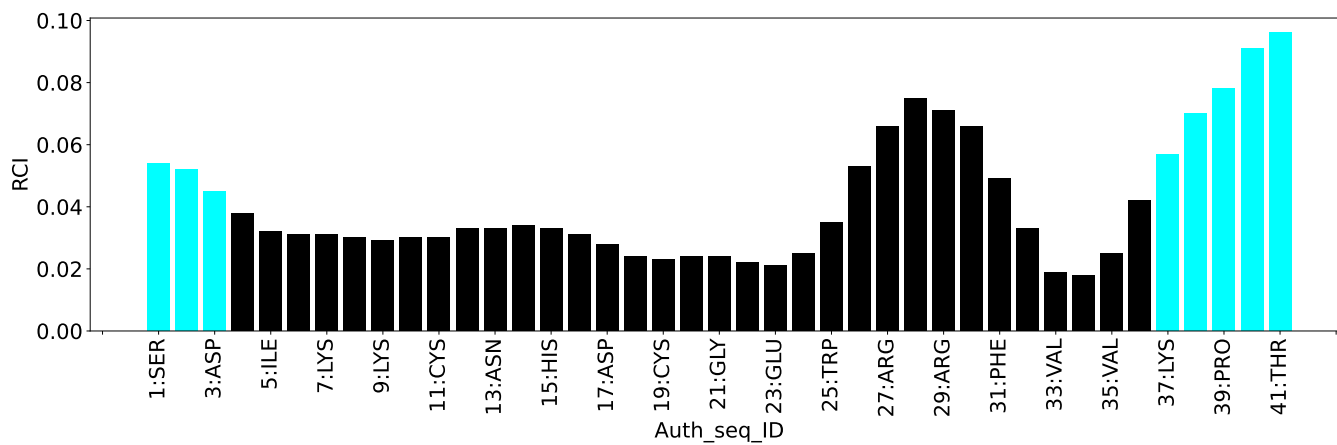
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



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	515
Intra-residue ($ i-j =0$)	136
Sequential ($ i-j =1$)	122
Medium range ($ i-j >1$ and $ i-j <5$)	63
Long range ($ i-j \geq 5$)	136
Inter-chain	0
Hydrogen bond restraints	40
Disulfide bond restraints	18
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	12.6
Number of long range restraints per residue ¹	4.6

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)	11.9	0.2
0.2-0.5 (Medium)	17.6	0.5
>0.5 (Large)	2.1	3.97

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis

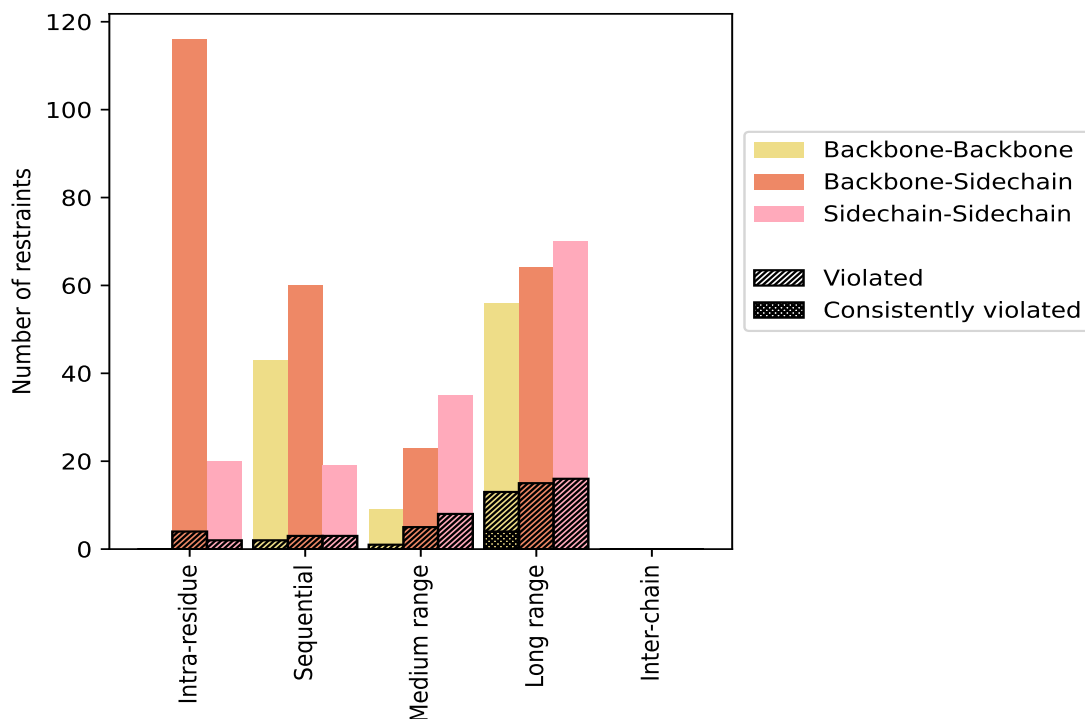
9.1 Summary of distance violations

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	136	26.4	6	4.4	1.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	116	22.5	4	3.4	0.8	0	0.0	0.0
Sidechain-Sidechain	20	3.9	2	10.0	0.4	0	0.0	0.0
Sequential ($i-j =1$)	122	23.7	8	6.6	1.6	0	0.0	0.0
Backbone-Backbone	43	8.3	2	4.7	0.4	0	0.0	0.0
Backbone-Sidechain	60	11.7	3	5.0	0.6	0	0.0	0.0
Sidechain-Sidechain	19	3.7	3	15.8	0.6	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	63	12.2	14	22.2	2.7	0	0.0	0.0
Backbone-Backbone	5	1.0	1	20.0	0.2	0	0.0	0.0
Backbone-Sidechain	23	4.5	5	21.7	1.0	0	0.0	0.0
Sidechain-Sidechain	35	6.8	8	22.9	1.6	0	0.0	0.0
Long range ($i-j \geq 5$)	136	26.4	28	20.6	5.4	0	0.0	0.0
Backbone-Backbone	20	3.9	1	5.0	0.2	0	0.0	0.0
Backbone-Sidechain	64	12.4	15	23.4	2.9	0	0.0	0.0
Sidechain-Sidechain	52	10.1	12	23.1	2.3	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	40	7.8	12	30.0	2.3	4	10.0	0.8
Disulfide bond	18	3.5	4	22.2	0.8	0	0.0	0.0
Total	515	100.0	72	14.0	14.0	4	0.8	0.8
Backbone-Backbone	108	21.0	16	14.8	3.1	4	3.7	0.8
Backbone-Sidechain	263	51.1	27	10.3	5.2	0	0.0	0.0
Sidechain-Sidechain	144	28.0	29	20.1	5.6	0	0.0	0.0

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

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



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfid 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	3	1	5	26	0	35	0.29	0.54	0.12	0.27
2	0	0	0	8	0	8	0.25	0.42	0.11	0.25
3	3	4	9	34	0	50	0.66	3.97	1.01	0.27
4	0	0	0	9	0	9	0.24	0.42	0.11	0.23
5	3	2	7	23	0	35	0.28	0.63	0.13	0.27
6	4	3	7	24	0	38	0.27	0.59	0.14	0.25
7	0	0	0	9	0	9	0.23	0.42	0.1	0.2
8	4	3	7	29	0	43	0.29	0.83	0.15	0.26
9	4	3	6	23	0	36	0.29	0.82	0.15	0.26
10	3	4	7	24	0	38	0.28	0.65	0.13	0.24
11	3	2	6	29	0	40	0.27	0.53	0.13	0.24

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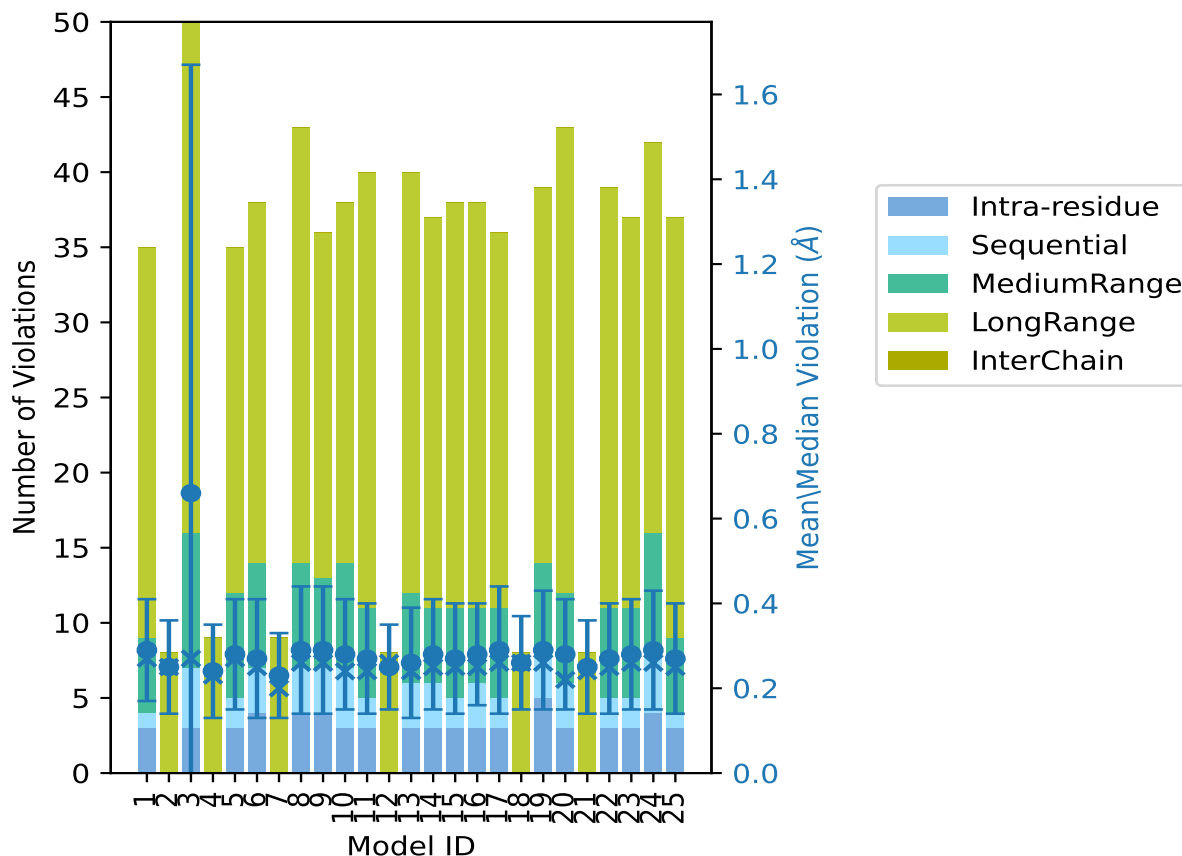
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
12	0	0	0	8	0	8	0.25	0.42	0.1	0.26
13	3	3	6	28	0	40	0.26	0.55	0.13	0.24
14	3	3	5	26	0	37	0.28	0.55	0.13	0.25
15	3	2	6	27	0	38	0.27	0.58	0.13	0.25
16	3	3	5	27	0	38	0.28	0.55	0.12	0.25
17	3	2	6	25	0	36	0.29	0.78	0.15	0.26
18	0	0	0	8	0	8	0.26	0.42	0.11	0.26
19	5	3	6	25	0	39	0.29	0.77	0.14	0.26
20	3	3	6	31	0	43	0.28	0.54	0.13	0.22
21	0	0	0	8	0	8	0.25	0.42	0.11	0.24
22	3	2	6	28	0	39	0.27	0.51	0.13	0.25
23	3	2	6	26	0	37	0.28	0.66	0.13	0.26
24	4	4	8	26	0	42	0.29	0.81	0.14	0.26
25	3	1	5	28	0	37	0.27	0.55	0.13	0.25

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 401(IR:130, SQ:114, MR:49, LR:108, 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	%
1	3	4	3	0	11	1	4.0
0	0	2	0	0	2	2	8.0
1	1	0	3	0	5	3	12.0
1	0	2	0	0	3	4	16.0
0	1	0	1	0	2	5	20.0
0	0	0	2	0	2	6	24.0

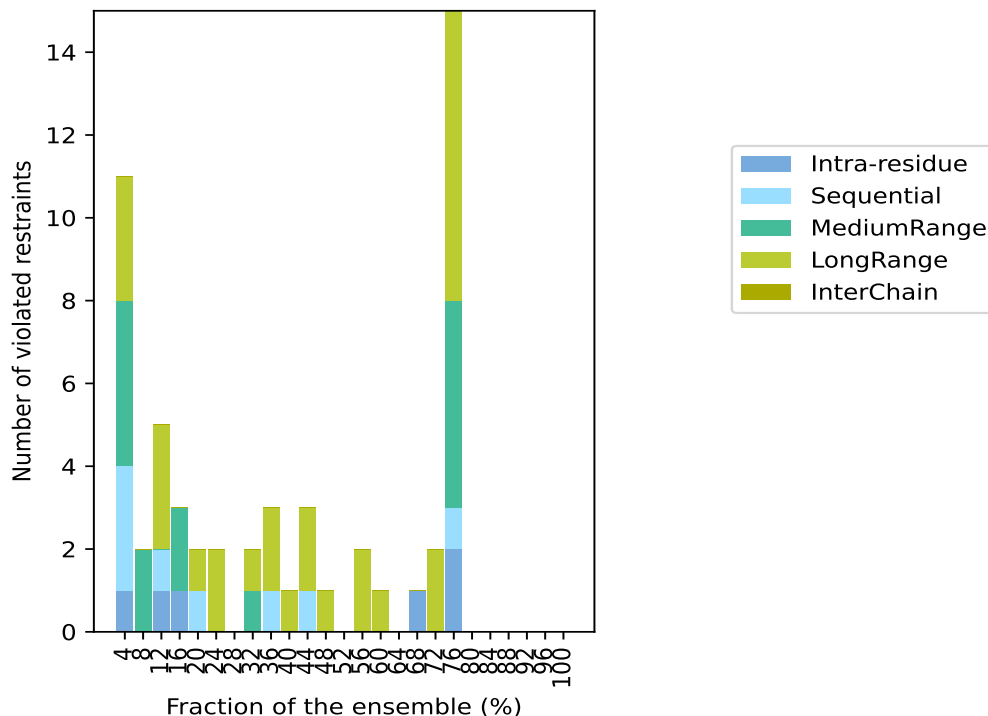
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	7	28.0
0	0	1	1	0	2	8	32.0
0	1	0	2	0	3	9	36.0
0	0	0	1	0	1	10	40.0
0	1	0	2	0	3	11	44.0
0	0	0	1	0	1	12	48.0
0	0	0	0	0	0	13	52.0
0	0	0	2	0	2	14	56.0
0	0	0	1	0	1	15	60.0
0	0	0	0	0	0	16	64.0
1	0	0	0	0	1	17	68.0
0	0	0	2	0	2	18	72.0
2	1	5	7	0	15	19	76.0
0	0	0	0	0	0	20	80.0
0	0	0	0	0	0	21	84.0
0	0	0	0	0	0	22	88.0
0	0	0	0	0	0	23	92.0
0	0	0	0	0	0	24	96.0
0	0	0	0	0	0	25	100.0

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

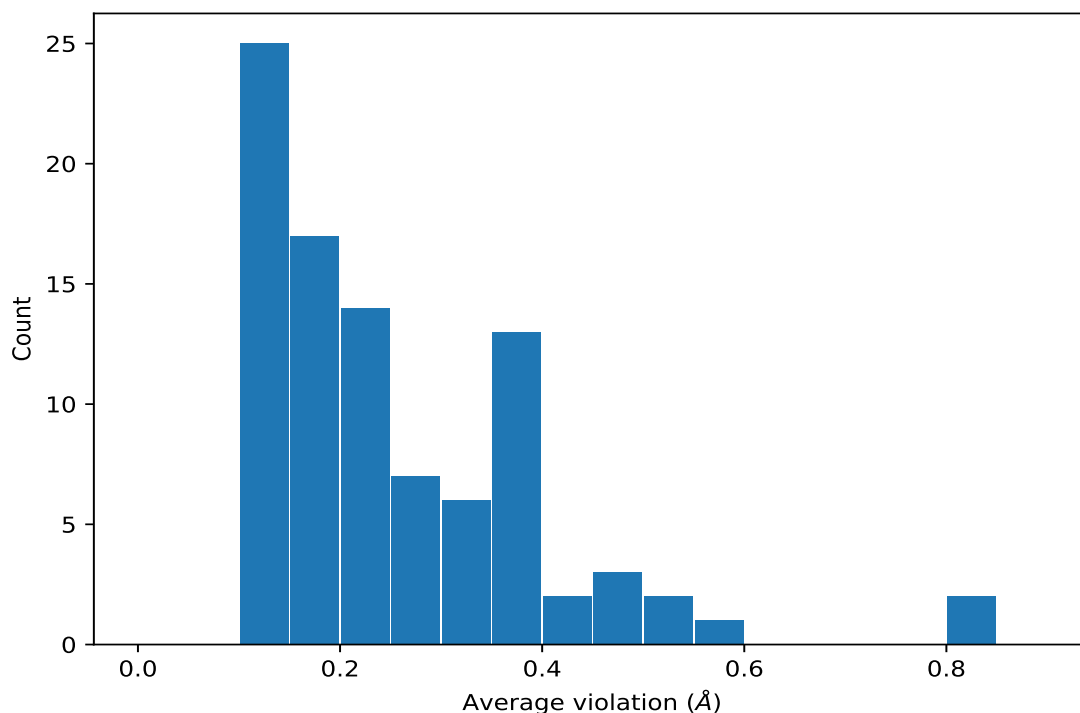
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	25	0.37	0.04	0.4
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	25	0.36	0.06	0.39
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	25	0.28	0.07	0.31
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	25	0.19	0.02	0.18
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	22	0.11	0.01	0.11
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	19	0.52	0.03	0.53
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	19	0.5	0.02	0.5
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	19	0.47	0.08	0.47
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	19	0.47	0.08	0.47
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	19	0.42	0.05	0.41
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	19	0.38	0.02	0.39
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	19	0.38	0.02	0.39
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	19	0.38	0.02	0.39
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	19	0.38	0.08	0.35
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	19	0.38	0.06	0.38
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	19	0.38	0.06	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	19	0.38	0.06	0.38
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	19	0.36	0.01	0.37
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	19	0.36	0.01	0.37
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	19	0.36	0.01	0.37
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	19	0.35	0.04	0.34
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	19	0.32	0.05	0.33
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	19	0.26	0.04	0.28
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	19	0.25	0.06	0.24
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	19	0.24	0.1	0.27
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	19	0.23	0.02	0.24
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	19	0.23	0.06	0.25
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	19	0.19	0.01	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	19	0.19	0.01	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	19	0.19	0.01	0.18
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	19	0.16	0.02	0.16
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	18	0.33	0.16	0.41
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	18	0.33	0.16	0.41
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	18	0.33	0.16	0.41
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	18	0.27	0.08	0.26
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	18	0.23	0.08	0.23
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	18	0.23	0.08	0.23
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	18	0.23	0.08	0.23
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	18	0.21	0.04	0.21
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	17	0.2	0.03	0.21
(1,259)	1:A:10:GLY:HA3	1:A:31:PHE:HD1	15	0.46	0.94	0.2
(1,278)	1:A:21:GLY:HA2	1:A:37:LYS:HG3	14	0.38	0.12	0.43
(1,374)	1:A:15:HIS:HD2	1:A:24:CYS:HB2	14	0.27	0.15	0.25
(5,9)	1:A:25:TRP:O	1:A:33:VAL:N	14	0.14	0.02	0.14
(2,4)	1:A:4:CYS:SG	1:A:19:CYS:SG	14	0.11	0.0	0.11
(2,5)	1:A:11:CYS:SG	1:A:24:CYS:SG	13	0.11	0.0	0.11
(1,320)	1:A:23:GLU:HG3	1:A:37:LYS:HA	12	0.15	0.03	0.16
(1,378)	1:A:5:ILE:HB	1:A:11:CYS:HB3	11	0.24	0.02	0.24
(1,239)	1:A:5:ILE:HD11	1:A:6:PRO:HD2	11	0.23	0.08	0.27
(1,239)	1:A:5:ILE:HD12	1:A:6:PRO:HD2	11	0.23	0.08	0.27
(1,239)	1:A:5:ILE:HD13	1:A:6:PRO:HD2	11	0.23	0.08	0.27
(1,234)	1:A:5:ILE:HG21	1:A:11:CYS:HB3	11	0.15	0.02	0.15
(1,234)	1:A:5:ILE:HG22	1:A:11:CYS:HB3	11	0.15	0.02	0.15
(1,234)	1:A:5:ILE:HG23	1:A:11:CYS:HB3	11	0.15	0.02	0.15
(1,240)	1:A:5:ILE:HD11	1:A:11:CYS:HB2	10	0.14	0.01	0.14
(1,240)	1:A:5:ILE:HD12	1:A:11:CYS:HB2	10	0.14	0.01	0.14
(1,240)	1:A:5:ILE:HD13	1:A:11:CYS:HB2	10	0.14	0.01	0.14
(1,362)	1:A:23:GLU:HB3	1:A:37:LYS:HD3	9	0.34	0.08	0.36

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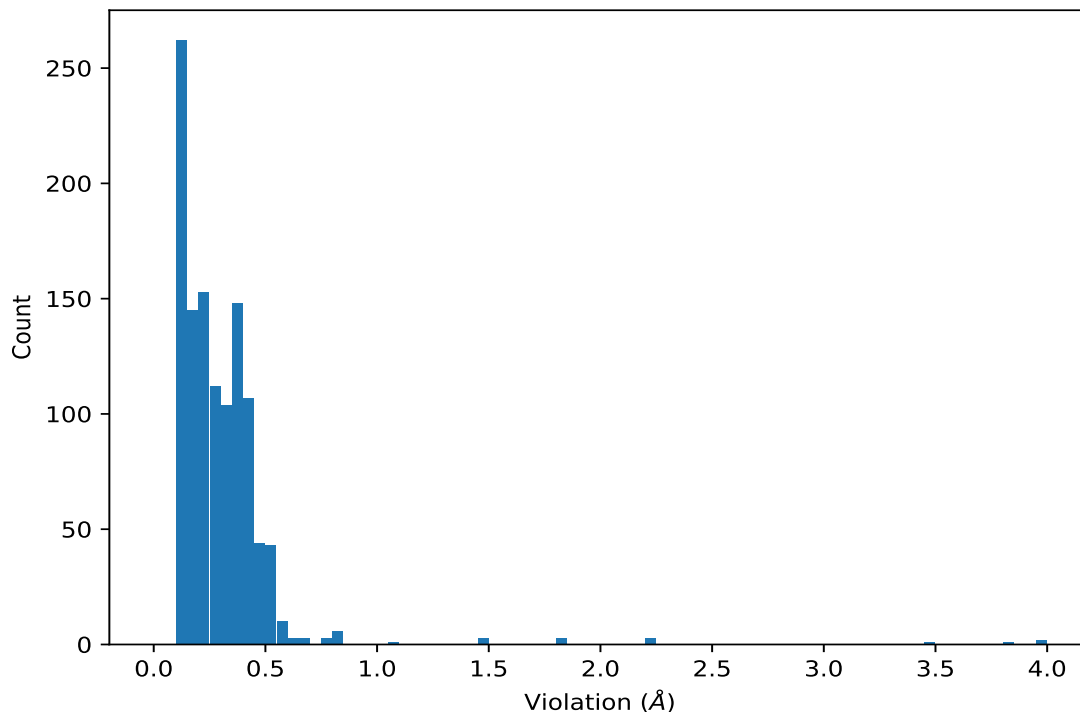
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,25)	1:A:3:ASP:HA	1:A:4:CYS:H	9	0.28	0.08	0.28
(1,339)	1:A:22:LEU:HB2	1:A:34:CYS:HB3	9	0.13	0.02	0.12
(1,273)	1:A:14:ARG:HA	1:A:17:ASP:HB2	8	0.58	0.06	0.6
(1,225)	1:A:4:CYS:HB3	1:A:19:CYS:HA	8	0.25	0.05	0.26
(5,10)	1:A:37:LYS:N	1:A:21:GLY:O	6	0.2	0.0	0.2
(1,226)	1:A:4:CYS:HB2	1:A:19:CYS:HB2	6	0.17	0.03	0.18
(1,423)	1:A:21:GLY:HA2	1:A:37:LYS:HE2	6	0.16	0.03	0.16
(1,423)	1:A:21:GLY:HA2	1:A:37:LYS:HE3	6	0.16	0.03	0.16
(1,423)	1:A:21:GLY:HA3	1:A:37:LYS:HE2	6	0.16	0.03	0.16
(1,423)	1:A:21:GLY:HA3	1:A:37:LYS:HE3	6	0.16	0.03	0.16
(1,157)	1:A:40:LYS:H	1:A:41:THR:H	5	0.19	0.05	0.23
(1,64)	1:A:11:CYS:H	1:A:33:VAL:HB	5	0.14	0.03	0.14
(1,441)	1:A:29:ARG:H	1:A:29:ARG:HG2	4	0.81	0.02	0.82
(1,441)	1:A:29:ARG:H	1:A:29:ARG:HG3	4	0.81	0.02	0.82
(1,76)	1:A:14:ARG:HA	1:A:17:ASP:H	4	0.12	0.02	0.12
(1,79)	1:A:18:CYS:H	1:A:22:LEU:HB2	4	0.12	0.02	0.12
(1,210)	1:A:25:TRP:HA	1:A:25:TRP:HE3	3	0.42	0.12	0.46
(1,260)	1:A:10:GLY:HA2	1:A:33:VAL:HB	3	0.22	0.0	0.22
(1,322)	1:A:24:CYS:HA	1:A:35:VAL:HG21	3	0.19	0.03	0.18
(1,322)	1:A:24:CYS:HA	1:A:35:VAL:HG22	3	0.19	0.03	0.18
(1,322)	1:A:24:CYS:HA	1:A:35:VAL:HG23	3	0.19	0.03	0.18
(5,2)	1:A:5:ILE:N	1:A:17:ASP:O	3	0.13	0.01	0.13
(1,229)	1:A:5:ILE:HG21	1:A:6:PRO:HD3	3	0.12	0.01	0.11
(1,229)	1:A:5:ILE:HG22	1:A:6:PRO:HD3	3	0.12	0.01	0.11
(1,229)	1:A:5:ILE:HG23	1:A:6:PRO:HD3	3	0.12	0.01	0.11
(1,328)	1:A:12:VAL:HG11	1:A:31:PHE:HA	3	0.11	0.0	0.11
(1,328)	1:A:12:VAL:HG12	1:A:31:PHE:HA	3	0.11	0.0	0.11
(1,328)	1:A:12:VAL:HG13	1:A:31:PHE:HA	3	0.11	0.0	0.11
(1,329)	1:A:31:PHE:HA	1:A:33:VAL:HG11	2	0.16	0.02	0.16
(1,329)	1:A:31:PHE:HA	1:A:33:VAL:HG12	2	0.16	0.02	0.16
(1,329)	1:A:31:PHE:HA	1:A:33:VAL:HG13	2	0.16	0.02	0.16
(1,245)	1:A:5:ILE:HD11	1:A:9:LYS:HB3	2	0.13	0.02	0.13
(1,245)	1:A:5:ILE:HD12	1:A:9:LYS:HB3	2	0.13	0.02	0.13
(1,245)	1:A:5:ILE:HD13	1:A:9:LYS:HB3	2	0.13	0.02	0.13

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)
(1,259)	1:A:10:GLY:HA3	1:A:31:PHE:HD1	3	3.97
(1,331)	1:A:31:PHE:HD1	1:A:33:VAL:HA	3	3.96
(1,264)	1:A:10:GLY:HA2	1:A:31:PHE:HD1	3	3.81
(1,63)	1:A:11:CYS:H	1:A:31:PHE:HD1	3	3.49
(1,332)	1:A:31:PHE:HD1	1:A:33:VAL:HG11	3	2.21
(1,332)	1:A:31:PHE:HD1	1:A:33:VAL:HG12	3	2.21
(1,332)	1:A:31:PHE:HD1	1:A:33:VAL:HG13	3	2.21
(1,269)	1:A:12:VAL:HG11	1:A:31:PHE:HD1	3	1.84
(1,269)	1:A:12:VAL:HG12	1:A:31:PHE:HD1	3	1.84
(1,269)	1:A:12:VAL:HG13	1:A:31:PHE:HD1	3	1.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,333)	1:A:31:PHE:HE1	1:A:33:VAL:HG11	3	1.46
(1,333)	1:A:31:PHE:HE1	1:A:33:VAL:HG12	3	1.46
(1,333)	1:A:31:PHE:HE1	1:A:33:VAL:HG13	3	1.46
(1,213)	1:A:31:PHE:HB2	1:A:31:PHE:HD1	3	1.08
(1,441)	1:A:29:ARG:H	1:A:29:ARG:HG2	8	0.83
(1,441)	1:A:29:ARG:H	1:A:29:ARG:HG3	8	0.83
(1,441)	1:A:29:ARG:H	1:A:29:ARG:HG2	9	0.82
(1,441)	1:A:29:ARG:H	1:A:29:ARG:HG3	9	0.82
(1,441)	1:A:29:ARG:H	1:A:29:ARG:HG2	24	0.81
(1,441)	1:A:29:ARG:H	1:A:29:ARG:HG3	24	0.81
(1,374)	1:A:15:HIS:HD2	1:A:24:CYS:HB2	17	0.78
(1,441)	1:A:29:ARG:H	1:A:29:ARG:HG2	19	0.77
(1,441)	1:A:29:ARG:H	1:A:29:ARG:HG3	19	0.77
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	23	0.66
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	23	0.66
(1,273)	1:A:14:ARG:HA	1:A:17:ASP:HB2	10	0.65
(1,273)	1:A:14:ARG:HA	1:A:17:ASP:HB2	5	0.63
(1,273)	1:A:14:ARG:HA	1:A:17:ASP:HB2	19	0.63
(1,273)	1:A:14:ARG:HA	1:A:17:ASP:HB2	9	0.62
(1,273)	1:A:14:ARG:HA	1:A:17:ASP:HB2	6	0.59
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	15	0.58
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	15	0.58
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	8	0.57
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	8	0.57
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	10	0.55
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	13	0.55
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	14	0.55
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	16	0.55
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	25	0.55
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	25	0.54
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	25	0.54
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	20	0.54
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	1	0.54
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	9	0.54
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	23	0.54
(1,210)	1:A:25:TRP:HA	1:A:25:TRP:HE3	6	0.54
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	20	0.53
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	20	0.53
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	5	0.53
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	10	0.53
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	1	0.53
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	20	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	20	0.53
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	20	0.53
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	11	0.53
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	15	0.53
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	17	0.53
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	11	0.52
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	14	0.52
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	5	0.52
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	13	0.51
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	16	0.51
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	22	0.51
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	25	0.51
(1,278)	1:A:21:GLY:HA2	1:A:37:LYS:HG3	20	0.51
(1,273)	1:A:14:ARG:HA	1:A:17:ASP:HB2	8	0.51
(1,273)	1:A:14:ARG:HA	1:A:17:ASP:HB2	24	0.51
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	6	0.51
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	20	0.51
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	22	0.51
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	19	0.5
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	15	0.5
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	17	0.5
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	23	0.5
(1,273)	1:A:14:ARG:HA	1:A:17:ASP:HB2	3	0.5
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	1	0.5
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	1	0.5
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	1	0.5
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	22	0.5
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	22	0.5
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	22	0.5
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	10	0.5
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	6	0.49
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	19	0.49
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	11	0.49
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	11	0.49
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	11	0.49
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	17	0.49
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	3	0.49
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	9	0.48
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	3	0.48
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	5	0.48
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	8	0.48
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	9	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	10	0.48
(1,278)	1:A:21:GLY:HA2	1:A:37:LYS:HG3	13	0.48
(1,278)	1:A:21:GLY:HA2	1:A:37:LYS:HG3	15	0.48
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	14	0.48
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	5	0.48
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	8	0.48
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	1	0.47
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	1	0.47
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	11	0.47
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	11	0.47
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	14	0.47
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	14	0.47
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	16	0.47
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	16	0.47
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	17	0.47
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	17	0.47
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	22	0.47
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	22	0.47
(1,370)	1:A:5:ILE:HG12	1:A:18:CYS:HA	24	0.47
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	17	0.47
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	17	0.47
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	17	0.47
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	19	0.47
(1,224)	1:A:4:CYS:HA	1:A:5:ILE:HG12	24	0.47
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	13	0.46
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	13	0.46
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	24	0.46
(1,210)	1:A:25:TRP:HA	1:A:25:TRP:HE3	24	0.46
(1,278)	1:A:21:GLY:HA2	1:A:37:LYS:HG3	1	0.45
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	14	0.45
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	14	0.45
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	14	0.45
(1,362)	1:A:23:GLU:HB3	1:A:37:LYS:HD3	8	0.44
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	11	0.44
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	11	0.44
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	11	0.44
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	20	0.44
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	20	0.44
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	20	0.44
(1,278)	1:A:21:GLY:HA2	1:A:37:LYS:HG3	11	0.44
(1,278)	1:A:21:GLY:HA2	1:A:37:LYS:HG3	14	0.44
(1,278)	1:A:21:GLY:HA2	1:A:37:LYS:HG3	25	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	16	0.44
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	16	0.44
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	16	0.44
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	6	0.44
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	16	0.44
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	20	0.44
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	22	0.43
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	22	0.43
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	22	0.43
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	2	0.42
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	4	0.42
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	7	0.42
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	12	0.42
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	18	0.42
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	21	0.42
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	16	0.42
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	25	0.42
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	25	0.42
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	25	0.42
(1,278)	1:A:21:GLY:HA2	1:A:37:LYS:HG3	17	0.42
(1,278)	1:A:21:GLY:HA2	1:A:37:LYS:HG3	22	0.42
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	15	0.42
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	15	0.42
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	15	0.42
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	1	0.41
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	13	0.41
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	14	0.41
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	15	0.41
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	23	0.41
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	24	0.41
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	3	0.41
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	20	0.41
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	14	0.41
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	14	0.41
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	14	0.41
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	16	0.41
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	16	0.41
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	16	0.41
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	23	0.41
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	23	0.41
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	23	0.41
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	13	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	13	0.41
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	13	0.41
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	23	0.41
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	23	0.41
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	23	0.41
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	13	0.41
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	22	0.41
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	23	0.41
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	19	0.41
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	19	0.41
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	19	0.41
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	8	0.4
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	24	0.4
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	3	0.4
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	11	0.4
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	5	0.4
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	6	0.4
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	9	0.4
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	17	0.4
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	19	0.4
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	22	0.4
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	4	0.4
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	6	0.4
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	8	0.4
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	20	0.4
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	24	0.4
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	3	0.4
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	3	0.4
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	1	0.4
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	6	0.4
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	11	0.4
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	22	0.4
(1,278)	1:A:21:GLY:HA2	1:A:37:LYS:HG3	16	0.4
(1,278)	1:A:21:GLY:HA2	1:A:37:LYS:HG3	23	0.4
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	25	0.4
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	25	0.4
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	25	0.4
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	8	0.4
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	15	0.4
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	25	0.4
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	5	0.4
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	5	0.4
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	9	0.4
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	9	0.4
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	9	0.4
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	10	0.4
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	10	0.4
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	10	0.4
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	11	0.4
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	11	0.4
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	11	0.4
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	13	0.4
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	13	0.4
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	13	0.4
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	3	0.39
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	8	0.39
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	20	0.39
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	1	0.39
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	13	0.39
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	14	0.39
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	16	0.39
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	22	0.39
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	23	0.39
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	25	0.39
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	10	0.39
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	11	0.39
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	20	0.39
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	6	0.39
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	6	0.39
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	9	0.39
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	9	0.39
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	24	0.39
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	24	0.39
(1,362)	1:A:23:GLU:HB3	1:A:37:LYS:HD3	3	0.39
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	15	0.39
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	15	0.39
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	15	0.39
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	17	0.39
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	17	0.39
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	17	0.39
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	13	0.39
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	13	0.39
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	13	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	1	0.39
(1,259)	1:A:10:GLY:HA3	1:A:31:PHE:HD1	8	0.39
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	1	0.39
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	1	0.39
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	1	0.39
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	14	0.39
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	14	0.39
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	14	0.39
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	16	0.39
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	16	0.39
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	16	0.39
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	23	0.39
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	23	0.39
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	23	0.39
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	6	0.38
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	11	0.38
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	25	0.38
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	10	0.38
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	10	0.38
(1,362)	1:A:23:GLU:HB3	1:A:37:LYS:HD3	10	0.38
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	11	0.38
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	11	0.38
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	11	0.38
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	1	0.38
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	1	0.38
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	1	0.38
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	6	0.38
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	6	0.38
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	6	0.38
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	8	0.38
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	8	0.38
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	8	0.38
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	24	0.38
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	24	0.38
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	24	0.38
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	3	0.38
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	11	0.38
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	19	0.38
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	20	0.38
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	11	0.38
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	6	0.38
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	6	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	6	0.38
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	22	0.38
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	22	0.38
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	22	0.38
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	25	0.38
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	25	0.38
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	25	0.38
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	15	0.37
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	18	0.37
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	9	0.37
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	10	0.37
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	5	0.37
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	5	0.37
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE2	19	0.37
(1,452)	1:A:37:LYS:HG3	1:A:37:LYS:HE3	19	0.37
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	1	0.37
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	1	0.37
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	1	0.37
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	13	0.37
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	13	0.37
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	13	0.37
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	14	0.37
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	14	0.37
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	14	0.37
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	16	0.37
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	16	0.37
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	16	0.37
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	22	0.37
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	22	0.37
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	22	0.37
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	23	0.37
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	23	0.37
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	23	0.37
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	25	0.37
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	25	0.37
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	25	0.37
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	3	0.37
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	3	0.37
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	3	0.37
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	5	0.37
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	5	0.37
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	9	0.37
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	9	0.37
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	9	0.37
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	10	0.37
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	10	0.37
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	10	0.37
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	19	0.37
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	19	0.37
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	19	0.37
(1,25)	1:A:3:ASP:HA	1:A:4:CYS:H	16	0.37
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	3	0.37
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	3	0.37
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	3	0.37
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	8	0.37
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	8	0.37
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	8	0.37
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	24	0.37
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	24	0.37
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	24	0.37
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	17	0.36
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	3	0.36
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	19	0.36
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	19	0.36
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	19	0.36
(1,362)	1:A:23:GLU:HB3	1:A:37:LYS:HD3	5	0.36
(1,362)	1:A:23:GLU:HB3	1:A:37:LYS:HD3	24	0.36
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	5	0.36
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	5	0.36
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	5	0.36
(1,25)	1:A:3:ASP:HA	1:A:4:CYS:H	11	0.36
(1,25)	1:A:3:ASP:HA	1:A:4:CYS:H	14	0.36
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	1	0.36
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	15	0.36
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	22	0.36
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	20	0.36
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	2	0.35
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	20	0.35
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	25	0.35
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	15	0.35
(1,362)	1:A:23:GLU:HB3	1:A:37:LYS:HD3	9	0.35
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	6	0.35
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	6	0.35
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	9	0.35
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	9	0.35
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	9	0.35
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	10	0.35
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	10	0.35
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	10	0.35
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	19	0.35
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	19	0.35
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	19	0.35
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	20	0.35
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	20	0.35
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	20	0.35
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	24	0.35
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	24	0.35
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	24	0.35
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	25	0.35
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	15	0.35
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	15	0.35
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	15	0.35
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	17	0.35
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	17	0.35
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	17	0.35
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	22	0.35
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	24	0.34
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	20	0.34
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	1	0.34
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	2	0.34
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	21	0.34
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	22	0.34
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	1	0.34
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	13	0.34
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	13	0.34
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	17	0.34
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	9	0.34
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	9	0.34
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	9	0.34
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	10	0.34
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	10	0.34
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	10	0.34
(1,362)	1:A:23:GLU:HB3	1:A:37:LYS:HD3	6	0.34
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	3	0.34
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	3	0.34
(1,340)	1:A:22:LEU:HD11	1:A:34:CYS:HB2	8	0.34
(1,340)	1:A:22:LEU:HD12	1:A:34:CYS:HB2	8	0.34
(1,340)	1:A:22:LEU:HD13	1:A:34:CYS:HB2	8	0.34
(1,266)	1:A:11:CYS:HB2	1:A:14:ARG:HB3	9	0.34
(1,25)	1:A:3:ASP:HA	1:A:4:CYS:H	15	0.34
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	14	0.34
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	17	0.34
(1,138)	1:A:22:LEU:HD11	1:A:34:CYS:H	20	0.34
(1,138)	1:A:22:LEU:HD12	1:A:34:CYS:H	20	0.34
(1,138)	1:A:22:LEU:HD13	1:A:34:CYS:H	20	0.34
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	12	0.33
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	7	0.33
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	21	0.33
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	13	0.33
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	18	0.33
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	14	0.33
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	19	0.33
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	8	0.33
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	25	0.33
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	5	0.33
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	5	0.33
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	5	0.33
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	16	0.33
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	23	0.33
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	3	0.33
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	8	0.33
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	18	0.32
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	24	0.32
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	7	0.32
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	12	0.32
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	5	0.32
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	11	0.32
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	15	0.32
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	23	0.32
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	16	0.32
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	23	0.32
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	24	0.32
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	6	0.32
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	6	0.32
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,362)	1:A:23:GLU:HB3	1:A:37:LYS:HD3	19	0.32
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	13	0.32
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	6	0.31
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	4	0.31
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	15	0.31
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	23	0.31
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	25	0.31
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	3	0.31
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	11	0.31
(1,239)	1:A:5:ILE:HD11	1:A:6:PRO:HD2	24	0.31
(1,239)	1:A:5:ILE:HD12	1:A:6:PRO:HD2	24	0.31
(1,239)	1:A:5:ILE:HD13	1:A:6:PRO:HD2	24	0.31
(1,225)	1:A:4:CYS:HB3	1:A:19:CYS:HA	24	0.31
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	16	0.3
(1,374)	1:A:15:HIS:HD2	1:A:24:CYS:HB2	1	0.3
(1,374)	1:A:15:HIS:HD2	1:A:24:CYS:HB2	22	0.3
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	20	0.3
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	22	0.3
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	19	0.3
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	15	0.3
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	10	0.29
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	2	0.29
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	21	0.29
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	17	0.29
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	8	0.29
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	8	0.29
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	8	0.29
(1,374)	1:A:15:HIS:HD2	1:A:24:CYS:HB2	13	0.29
(1,239)	1:A:5:ILE:HD11	1:A:6:PRO:HD2	19	0.29
(1,239)	1:A:5:ILE:HD12	1:A:6:PRO:HD2	19	0.29
(1,239)	1:A:5:ILE:HD13	1:A:6:PRO:HD2	19	0.29
(1,225)	1:A:4:CYS:HB3	1:A:19:CYS:HA	19	0.29
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	16	0.29
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	17	0.29
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	5	0.28
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	17	0.28
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	3	0.28
(1,25)	1:A:3:ASP:HA	1:A:4:CYS:H	17	0.28
(1,239)	1:A:5:ILE:HD11	1:A:6:PRO:HD2	5	0.28
(1,239)	1:A:5:ILE:HD12	1:A:6:PRO:HD2	5	0.28
(1,239)	1:A:5:ILE:HD13	1:A:6:PRO:HD2	5	0.28
(1,239)	1:A:5:ILE:HD11	1:A:6:PRO:HD2	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,239)	1:A:5:ILE:HD12	1:A:6:PRO:HD2	8	0.28
(1,239)	1:A:5:ILE:HD13	1:A:6:PRO:HD2	8	0.28
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	5	0.28
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	9	0.28
(1,225)	1:A:4:CYS:HB3	1:A:19:CYS:HA	8	0.28
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	1	0.28
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	6	0.28
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	11	0.28
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	13	0.28
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	14	0.28
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	15	0.28
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	23	0.28
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	25	0.28
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	9	0.27
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	23	0.27
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	4	0.27
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	7	0.27
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	5	0.27
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	8	0.27
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	9	0.27
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	19	0.27
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	12	0.27
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	3	0.27
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	16	0.27
(1,374)	1:A:15:HIS:HD2	1:A:24:CYS:HB2	11	0.27
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	1	0.27
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	23	0.27
(1,239)	1:A:5:ILE:HD11	1:A:6:PRO:HD2	3	0.27
(1,239)	1:A:5:ILE:HD12	1:A:6:PRO:HD2	3	0.27
(1,239)	1:A:5:ILE:HD13	1:A:6:PRO:HD2	3	0.27
(1,239)	1:A:5:ILE:HD11	1:A:6:PRO:HD2	6	0.27
(1,239)	1:A:5:ILE:HD12	1:A:6:PRO:HD2	6	0.27
(1,239)	1:A:5:ILE:HD13	1:A:6:PRO:HD2	6	0.27
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	10	0.27
(1,225)	1:A:4:CYS:HB3	1:A:19:CYS:HA	3	0.27
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	5	0.27
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	19	0.27
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	24	0.27
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	17	0.27
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	19	0.26
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	25	0.26
(5,17)	1:A:23:GLU:H	1:A:35:VAL:O	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	3	0.26
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	20	0.26
(5,14)	1:A:11:CYS:H	1:A:32:GLU:O	8	0.26
(5,12)	1:A:5:ILE:H	1:A:17:ASP:O	22	0.26
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	23	0.26
(1,378)	1:A:5:ILE:HB	1:A:11:CYS:HB3	16	0.26
(1,374)	1:A:15:HIS:HD2	1:A:24:CYS:HB2	15	0.26
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	14	0.26
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	16	0.26
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	25	0.26
(1,259)	1:A:10:GLY:HA3	1:A:31:PHE:HD1	24	0.26
(1,239)	1:A:5:ILE:HD11	1:A:6:PRO:HD2	10	0.26
(1,239)	1:A:5:ILE:HD12	1:A:6:PRO:HD2	10	0.26
(1,239)	1:A:5:ILE:HD13	1:A:6:PRO:HD2	10	0.26
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	3	0.26
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	6	0.26
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	8	0.26
(1,225)	1:A:4:CYS:HB3	1:A:19:CYS:HA	5	0.26
(1,210)	1:A:25:TRP:HA	1:A:25:TRP:HE3	19	0.26
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	9	0.26
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	10	0.26
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	22	0.26
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	10	0.25
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	14	0.25
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	19	0.25
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	11	0.25
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	22	0.25
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	24	0.25
(1,378)	1:A:5:ILE:HB	1:A:11:CYS:HB3	14	0.25
(1,378)	1:A:5:ILE:HB	1:A:11:CYS:HB3	15	0.25
(1,378)	1:A:5:ILE:HB	1:A:11:CYS:HB3	17	0.25
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	14	0.25
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	14	0.25
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	14	0.25
(1,374)	1:A:15:HIS:HD2	1:A:24:CYS:HB2	23	0.25
(1,374)	1:A:15:HIS:HD2	1:A:24:CYS:HB2	25	0.25
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	13	0.25
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	15	0.25
(1,259)	1:A:10:GLY:HA3	1:A:31:PHE:HD1	14	0.25
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	9	0.25
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	23	0.25
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	16	0.24
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	8	0.24
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	13	0.24
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	22	0.24
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	12	0.24
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	3	0.24
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	5	0.24
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	6	0.24
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	8	0.24
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	9	0.24
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	10	0.24
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	19	0.24
(1,378)	1:A:5:ILE:HB	1:A:11:CYS:HB3	13	0.24
(1,378)	1:A:5:ILE:HB	1:A:11:CYS:HB3	20	0.24
(1,378)	1:A:5:ILE:HB	1:A:11:CYS:HB3	25	0.24
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	3	0.24
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	3	0.24
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	3	0.24
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	24	0.24
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	24	0.24
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	24	0.24
(1,259)	1:A:10:GLY:HA3	1:A:31:PHE:HD1	16	0.24
(1,157)	1:A:40:LYS:H	1:A:41:THR:H	10	0.24
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	1	0.24
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	16	0.24
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	24	0.24
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	23	0.23
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	8	0.23
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	4	0.23
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	8	0.23
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	1	0.23
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	14	0.23
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	16	0.23
(1,380)	1:A:14:ARG:HG2	1:A:17:ASP:HB2	14	0.23
(1,378)	1:A:5:ILE:HB	1:A:11:CYS:HB3	1	0.23
(1,378)	1:A:5:ILE:HB	1:A:11:CYS:HB3	22	0.23
(1,378)	1:A:5:ILE:HB	1:A:11:CYS:HB3	23	0.23
(1,322)	1:A:24:CYS:HA	1:A:35:VAL:HG21	8	0.23
(1,322)	1:A:24:CYS:HA	1:A:35:VAL:HG22	8	0.23
(1,322)	1:A:24:CYS:HA	1:A:35:VAL:HG23	8	0.23
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	15	0.23
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	15	0.23
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD11	17	0.23
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD12	17	0.23
(1,291)	1:A:18:CYS:HB2	1:A:22:LEU:HD13	17	0.23
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	17	0.23
(1,259)	1:A:10:GLY:HA3	1:A:31:PHE:HD1	1	0.23
(1,25)	1:A:3:ASP:HA	1:A:4:CYS:H	22	0.23
(1,25)	1:A:3:ASP:HA	1:A:4:CYS:H	23	0.23
(1,228)	1:A:5:ILE:HB	1:A:18:CYS:HB3	24	0.23
(1,157)	1:A:40:LYS:H	1:A:41:THR:H	3	0.23
(1,157)	1:A:40:LYS:H	1:A:41:THR:H	9	0.23
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	13	0.23
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	25	0.23
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	16	0.22
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	24	0.22
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	17	0.22
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	13	0.22
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	20	0.22
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	16	0.22
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	16	0.22
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	16	0.22
(1,374)	1:A:15:HIS:HD2	1:A:24:CYS:HB2	16	0.22
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	15	0.22
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	17	0.22
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	20	0.22
(1,260)	1:A:10:GLY:HA2	1:A:33:VAL:HB	8	0.22
(1,260)	1:A:10:GLY:HA2	1:A:33:VAL:HB	20	0.22
(1,259)	1:A:10:GLY:HA3	1:A:31:PHE:HD1	17	0.22
(1,225)	1:A:4:CYS:HB3	1:A:19:CYS:HA	6	0.22
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	11	0.22
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	14	0.21
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	1	0.21
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	11	0.21
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	25	0.21
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	2	0.21
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	3	0.21
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	24	0.21
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	25	0.21
(1,423)	1:A:21:GLY:HA2	1:A:37:LYS:HE2	10	0.21
(1,423)	1:A:21:GLY:HA2	1:A:37:LYS:HE3	10	0.21
(1,423)	1:A:21:GLY:HA3	1:A:37:LYS:HE2	10	0.21
(1,423)	1:A:21:GLY:HA3	1:A:37:LYS:HE3	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	13	0.21
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	13	0.21
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	13	0.21
(1,374)	1:A:15:HIS:HD2	1:A:24:CYS:HB2	20	0.21
(1,320)	1:A:23:GLU:HG3	1:A:37:LYS:HA	3	0.21
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	1	0.21
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	11	0.21
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	13	0.21
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	16	0.21
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	22	0.21
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	23	0.21
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	19	0.21
(1,260)	1:A:10:GLY:HA2	1:A:33:VAL:HB	3	0.21
(1,239)	1:A:5:ILE:HD11	1:A:6:PRO:HD2	9	0.21
(1,239)	1:A:5:ILE:HD12	1:A:6:PRO:HD2	9	0.21
(1,239)	1:A:5:ILE:HD13	1:A:6:PRO:HD2	9	0.21
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	5	0.21
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	5	0.21
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	5	0.21
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	10	0.21
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	10	0.21
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	10	0.21
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	19	0.21
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	19	0.21
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	19	0.21
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	14	0.21
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	11	0.2
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	14	0.2
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	9	0.2
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	19	0.2
(5,10)	1:A:37:LYS:N	1:A:21:GLY:O	2	0.2
(5,10)	1:A:37:LYS:N	1:A:21:GLY:O	7	0.2
(5,10)	1:A:37:LYS:N	1:A:21:GLY:O	12	0.2
(5,10)	1:A:37:LYS:N	1:A:21:GLY:O	18	0.2
(1,423)	1:A:21:GLY:HA2	1:A:37:LYS:HE2	9	0.2
(1,423)	1:A:21:GLY:HA2	1:A:37:LYS:HE3	9	0.2
(1,423)	1:A:21:GLY:HA3	1:A:37:LYS:HE2	9	0.2
(1,423)	1:A:21:GLY:HA3	1:A:37:LYS:HE3	9	0.2
(1,378)	1:A:5:ILE:HB	1:A:11:CYS:HB3	11	0.2
(1,320)	1:A:23:GLU:HG3	1:A:37:LYS:HA	8	0.2
(1,320)	1:A:23:GLU:HG3	1:A:37:LYS:HA	20	0.2
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	14	0.2
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	25	0.2
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	9	0.2
(1,259)	1:A:10:GLY:HA3	1:A:31:PHE:HD1	19	0.2
(1,259)	1:A:10:GLY:HA3	1:A:31:PHE:HD1	20	0.2
(1,259)	1:A:10:GLY:HA3	1:A:31:PHE:HD1	23	0.2
(1,234)	1:A:5:ILE:HG21	1:A:11:CYS:HB3	20	0.2
(1,234)	1:A:5:ILE:HG22	1:A:11:CYS:HB3	20	0.2
(1,234)	1:A:5:ILE:HG23	1:A:11:CYS:HB3	20	0.2
(1,226)	1:A:4:CYS:HB2	1:A:19:CYS:HB2	19	0.2
(1,226)	1:A:4:CYS:HB2	1:A:19:CYS:HB2	24	0.2
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	3	0.2
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	3	0.2
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	3	0.2
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	8	0.2
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	8	0.2
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	8	0.2
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	9	0.2
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	9	0.2
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	9	0.2
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	24	0.2
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	24	0.2
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	24	0.2
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	3	0.2
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	20	0.2
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	10	0.2
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	1	0.19
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	5	0.19
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	7	0.19
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	20	0.19
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	21	0.19
(5,10)	1:A:37:LYS:N	1:A:21:GLY:O	4	0.19
(5,10)	1:A:37:LYS:N	1:A:21:GLY:O	21	0.19
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	15	0.19
(1,90)	1:A:19:CYS:H	1:A:22:LEU:HG	17	0.19
(1,64)	1:A:11:CYS:H	1:A:33:VAL:HB	24	0.19
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	23	0.19
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	5	0.19
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	5	0.19
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	10	0.19
(1,278)	1:A:21:GLY:HA2	1:A:37:LYS:HG3	19	0.19
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	6	0.19
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	6	0.19
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	13	0.19
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	13	0.19
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	13	0.19
(5,9)	1:A:25:TRP:O	1:A:33:VAL:N	8	0.18
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	5	0.18
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	10	0.18
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	1	0.18
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	5	0.18
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	6	0.18
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	11	0.18
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	13	0.18
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	18	0.18
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	25	0.18
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	25	0.18
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	25	0.18
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	25	0.18
(1,374)	1:A:15:HIS:HD2	1:A:24:CYS:HB2	3	0.18
(1,339)	1:A:22:LEU:HB2	1:A:34:CYS:HB3	23	0.18
(1,329)	1:A:31:PHE:HA	1:A:33:VAL:HG11	17	0.18
(1,329)	1:A:31:PHE:HA	1:A:33:VAL:HG12	17	0.18
(1,329)	1:A:31:PHE:HA	1:A:33:VAL:HG13	17	0.18
(1,322)	1:A:24:CYS:HA	1:A:35:VAL:HG21	3	0.18
(1,322)	1:A:24:CYS:HA	1:A:35:VAL:HG22	3	0.18
(1,322)	1:A:24:CYS:HA	1:A:35:VAL:HG23	3	0.18
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	10	0.18
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	19	0.18
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	10	0.18
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	10	0.18
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	10	0.18
(1,259)	1:A:10:GLY:HA3	1:A:31:PHE:HD1	22	0.18
(1,226)	1:A:4:CYS:HB2	1:A:19:CYS:HB2	8	0.18
(1,225)	1:A:4:CYS:HB3	1:A:19:CYS:HA	10	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	14	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	14	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	14	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	15	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	15	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	15	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	16	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	16	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	17	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	17	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	17	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	23	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	23	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	23	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	25	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	25	0.18
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	25	0.18
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	15	0.17
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	6	0.17
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	15	0.17
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	24	0.17
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	9	0.17
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	10	0.17
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	15	0.17
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	16	0.17
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	22	0.17
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	23	0.17
(1,424)	1:A:25:TRP:HE1	1:A:27:ARG:HG2	15	0.17
(1,424)	1:A:25:TRP:HE1	1:A:27:ARG:HG3	15	0.17
(1,423)	1:A:21:GLY:HA2	1:A:37:LYS:HE2	24	0.17
(1,423)	1:A:21:GLY:HA2	1:A:37:LYS:HE3	24	0.17
(1,423)	1:A:21:GLY:HA3	1:A:37:LYS:HE2	24	0.17
(1,423)	1:A:21:GLY:HA3	1:A:37:LYS:HE3	24	0.17
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	1	0.17
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	1	0.17
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	1	0.17
(1,374)	1:A:15:HIS:HD2	1:A:24:CYS:HB2	8	0.17
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	6	0.17
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	8	0.17
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	10	0.17
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	20	0.17
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	24	0.17
(1,339)	1:A:22:LEU:HB2	1:A:34:CYS:HB3	1	0.17
(1,25)	1:A:3:ASP:HA	1:A:4:CYS:H	3	0.17
(1,240)	1:A:5:ILE:HD11	1:A:11:CYS:HB2	14	0.17
(1,240)	1:A:5:ILE:HD12	1:A:11:CYS:HB2	14	0.17
(1,240)	1:A:5:ILE:HD13	1:A:11:CYS:HB2	14	0.17
(1,226)	1:A:4:CYS:HB2	1:A:19:CYS:HB2	3	0.17
(1,226)	1:A:4:CYS:HB2	1:A:19:CYS:HB2	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	1	0.17
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	1	0.17
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	1	0.17
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	11	0.17
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	11	0.17
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	11	0.17
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	20	0.17
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	20	0.17
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	20	0.17
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD11	22	0.17
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD12	22	0.17
(1,204)	1:A:5:ILE:HA	1:A:5:ILE:HD13	22	0.17
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	5	0.17
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	6	0.17
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	15	0.16
(5,20)	1:A:37:LYS:H	1:A:21:GLY:O	20	0.16
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	5	0.16
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	9	0.16
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	10	0.16
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	14	0.16
(5,11)	1:A:5:ILE:O	1:A:19:CYS:H	17	0.16
(1,79)	1:A:18:CYS:H	1:A:22:LEU:HB2	20	0.16
(1,374)	1:A:15:HIS:HD2	1:A:24:CYS:HB2	24	0.16
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	3	0.16
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	5	0.16
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	9	0.16
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	11	0.16
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	16	0.16
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	25	0.16
(1,336)	1:A:34:CYS:HA	1:A:35:VAL:HG21	20	0.16
(1,336)	1:A:34:CYS:HA	1:A:35:VAL:HG22	20	0.16
(1,336)	1:A:34:CYS:HA	1:A:35:VAL:HG23	20	0.16
(1,320)	1:A:23:GLU:HG3	1:A:37:LYS:HA	9	0.16
(1,320)	1:A:23:GLU:HG3	1:A:37:LYS:HA	22	0.16
(1,320)	1:A:23:GLU:HG3	1:A:37:LYS:HA	24	0.16
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	6	0.16
(1,259)	1:A:10:GLY:HA3	1:A:31:PHE:HD1	15	0.16
(1,240)	1:A:5:ILE:HD11	1:A:11:CYS:HB2	16	0.16
(1,240)	1:A:5:ILE:HD12	1:A:11:CYS:HB2	16	0.16
(1,240)	1:A:5:ILE:HD13	1:A:11:CYS:HB2	16	0.16
(1,234)	1:A:5:ILE:HG21	1:A:11:CYS:HB3	15	0.16
(1,234)	1:A:5:ILE:HG22	1:A:11:CYS:HB3	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:A:5:ILE:HG23	1:A:11:CYS:HB3	15	0.16
(1,225)	1:A:4:CYS:HB3	1:A:19:CYS:HA	9	0.16
(1,157)	1:A:40:LYS:H	1:A:41:THR:H	24	0.16
(5,9)	1:A:25:TRP:O	1:A:33:VAL:N	1	0.15
(5,9)	1:A:25:TRP:O	1:A:33:VAL:N	20	0.15
(1,76)	1:A:14:ARG:HA	1:A:17:ASP:H	6	0.15
(1,64)	1:A:11:CYS:H	1:A:33:VAL:HB	8	0.15
(1,423)	1:A:21:GLY:HA2	1:A:37:LYS:HE2	6	0.15
(1,423)	1:A:21:GLY:HA2	1:A:37:LYS:HE3	6	0.15
(1,423)	1:A:21:GLY:HA3	1:A:37:LYS:HE2	6	0.15
(1,423)	1:A:21:GLY:HA3	1:A:37:LYS:HE3	6	0.15
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	11	0.15
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	11	0.15
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	11	0.15
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	22	0.15
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	22	0.15
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	22	0.15
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	23	0.15
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	23	0.15
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	23	0.15
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	1	0.15
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	14	0.15
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	19	0.15
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	22	0.15
(1,362)	1:A:23:GLU:HB3	1:A:37:LYS:HD3	22	0.15
(1,344)	1:A:35:VAL:HG11	1:A:36:PRO:HD3	20	0.15
(1,344)	1:A:35:VAL:HG12	1:A:36:PRO:HD3	20	0.15
(1,344)	1:A:35:VAL:HG13	1:A:36:PRO:HD3	20	0.15
(1,322)	1:A:24:CYS:HA	1:A:35:VAL:HG21	20	0.15
(1,322)	1:A:24:CYS:HA	1:A:35:VAL:HG22	20	0.15
(1,322)	1:A:24:CYS:HA	1:A:35:VAL:HG23	20	0.15
(1,320)	1:A:23:GLU:HG3	1:A:37:LYS:HA	17	0.15
(1,278)	1:A:21:GLY:HA2	1:A:37:LYS:HG3	5	0.15
(1,278)	1:A:21:GLY:HA2	1:A:37:LYS:HG3	9	0.15
(1,25)	1:A:3:ASP:HA	1:A:4:CYS:H	10	0.15
(1,245)	1:A:5:ILE:HD11	1:A:9:LYS:HB3	24	0.15
(1,245)	1:A:5:ILE:HD12	1:A:9:LYS:HB3	24	0.15
(1,245)	1:A:5:ILE:HD13	1:A:9:LYS:HB3	24	0.15
(1,234)	1:A:5:ILE:HG21	1:A:11:CYS:HB3	14	0.15
(1,234)	1:A:5:ILE:HG22	1:A:11:CYS:HB3	14	0.15
(1,234)	1:A:5:ILE:HG23	1:A:11:CYS:HB3	14	0.15
(1,234)	1:A:5:ILE:HG21	1:A:11:CYS:HB3	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:A:5:ILE:HG22	1:A:11:CYS:HB3	16	0.15
(1,234)	1:A:5:ILE:HG23	1:A:11:CYS:HB3	16	0.15
(1,234)	1:A:5:ILE:HG21	1:A:11:CYS:HB3	17	0.15
(1,234)	1:A:5:ILE:HG22	1:A:11:CYS:HB3	17	0.15
(1,234)	1:A:5:ILE:HG23	1:A:11:CYS:HB3	17	0.15
(1,234)	1:A:5:ILE:HG21	1:A:11:CYS:HB3	22	0.15
(1,234)	1:A:5:ILE:HG22	1:A:11:CYS:HB3	22	0.15
(1,234)	1:A:5:ILE:HG23	1:A:11:CYS:HB3	22	0.15
(1,234)	1:A:5:ILE:HG21	1:A:11:CYS:HB3	25	0.15
(1,234)	1:A:5:ILE:HG22	1:A:11:CYS:HB3	25	0.15
(1,234)	1:A:5:ILE:HG23	1:A:11:CYS:HB3	25	0.15
(1,149)	1:A:23:GLU:HG3	1:A:37:LYS:H	8	0.15
(1,109)	1:A:23:GLU:H	1:A:37:LYS:HA	19	0.15
(5,9)	1:A:25:TRP:O	1:A:33:VAL:N	3	0.14
(5,9)	1:A:25:TRP:O	1:A:33:VAL:N	11	0.14
(5,9)	1:A:25:TRP:O	1:A:33:VAL:N	16	0.14
(5,9)	1:A:25:TRP:O	1:A:33:VAL:N	22	0.14
(5,9)	1:A:25:TRP:O	1:A:33:VAL:N	23	0.14
(5,2)	1:A:5:ILE:N	1:A:17:ASP:O	7	0.14
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	6	0.14
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	25	0.14
(1,64)	1:A:11:CYS:H	1:A:33:VAL:HB	19	0.14
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	17	0.14
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	17	0.14
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	17	0.14
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	13	0.14
(1,339)	1:A:22:LEU:HB2	1:A:34:CYS:HB3	11	0.14
(1,339)	1:A:22:LEU:HB2	1:A:34:CYS:HB3	22	0.14
(1,329)	1:A:31:PHE:HA	1:A:33:VAL:HG11	13	0.14
(1,329)	1:A:31:PHE:HA	1:A:33:VAL:HG12	13	0.14
(1,329)	1:A:31:PHE:HA	1:A:33:VAL:HG13	13	0.14
(1,320)	1:A:23:GLU:HG3	1:A:37:LYS:HA	25	0.14
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	6	0.14
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	3	0.14
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	8	0.14
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	5	0.14
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	5	0.14
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	5	0.14
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	8	0.14
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	8	0.14
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	8	0.14
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	24	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	24	0.14
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	24	0.14
(1,259)	1:A:10:GLY:HA3	1:A:31:PHE:HD1	13	0.14
(1,240)	1:A:5:ILE:HD11	1:A:11:CYS:HB2	1	0.14
(1,240)	1:A:5:ILE:HD12	1:A:11:CYS:HB2	1	0.14
(1,240)	1:A:5:ILE:HD13	1:A:11:CYS:HB2	1	0.14
(1,240)	1:A:5:ILE:HD11	1:A:11:CYS:HB2	13	0.14
(1,240)	1:A:5:ILE:HD12	1:A:11:CYS:HB2	13	0.14
(1,240)	1:A:5:ILE:HD13	1:A:11:CYS:HB2	13	0.14
(1,240)	1:A:5:ILE:HD11	1:A:11:CYS:HB2	22	0.14
(1,240)	1:A:5:ILE:HD12	1:A:11:CYS:HB2	22	0.14
(1,240)	1:A:5:ILE:HD13	1:A:11:CYS:HB2	22	0.14
(1,240)	1:A:5:ILE:HD11	1:A:11:CYS:HB2	23	0.14
(1,240)	1:A:5:ILE:HD12	1:A:11:CYS:HB2	23	0.14
(1,240)	1:A:5:ILE:HD13	1:A:11:CYS:HB2	23	0.14
(1,240)	1:A:5:ILE:HD11	1:A:11:CYS:HB2	25	0.14
(1,240)	1:A:5:ILE:HD12	1:A:11:CYS:HB2	25	0.14
(1,240)	1:A:5:ILE:HD13	1:A:11:CYS:HB2	25	0.14
(1,234)	1:A:5:ILE:HG21	1:A:11:CYS:HB3	1	0.14
(1,234)	1:A:5:ILE:HG22	1:A:11:CYS:HB3	1	0.14
(1,234)	1:A:5:ILE:HG23	1:A:11:CYS:HB3	1	0.14
(1,234)	1:A:5:ILE:HG21	1:A:11:CYS:HB3	13	0.14
(1,234)	1:A:5:ILE:HG22	1:A:11:CYS:HB3	13	0.14
(1,234)	1:A:5:ILE:HG23	1:A:11:CYS:HB3	13	0.14
(1,123)	1:A:25:TRP:HD1	1:A:26:LYS:H	13	0.14
(5,9)	1:A:25:TRP:O	1:A:33:VAL:N	19	0.13
(5,9)	1:A:25:TRP:O	1:A:33:VAL:N	25	0.13
(5,2)	1:A:5:ILE:N	1:A:17:ASP:O	4	0.13
(5,16)	1:A:23:GLU:O	1:A:35:VAL:H	19	0.13
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	20	0.13
(1,76)	1:A:14:ARG:HA	1:A:17:ASP:H	10	0.13
(1,423)	1:A:21:GLY:HA2	1:A:37:LYS:HE2	19	0.13
(1,423)	1:A:21:GLY:HA2	1:A:37:LYS:HE3	19	0.13
(1,423)	1:A:21:GLY:HA3	1:A:37:LYS:HE2	19	0.13
(1,423)	1:A:21:GLY:HA3	1:A:37:LYS:HE3	19	0.13
(1,374)	1:A:15:HIS:HD2	1:A:24:CYS:HB2	14	0.13
(1,289)	1:A:18:CYS:HB2	1:A:34:CYS:HB3	24	0.13
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	19	0.13
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	19	0.13
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	19	0.13
(1,240)	1:A:5:ILE:HD11	1:A:11:CYS:HB2	11	0.13
(1,240)	1:A:5:ILE:HD12	1:A:11:CYS:HB2	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,240)	1:A:5:ILE:HD13	1:A:11:CYS:HB2	11	0.13
(1,240)	1:A:5:ILE:HD11	1:A:11:CYS:HB2	15	0.13
(1,240)	1:A:5:ILE:HD12	1:A:11:CYS:HB2	15	0.13
(1,240)	1:A:5:ILE:HD13	1:A:11:CYS:HB2	15	0.13
(1,240)	1:A:5:ILE:HD11	1:A:11:CYS:HB2	17	0.13
(1,240)	1:A:5:ILE:HD12	1:A:11:CYS:HB2	17	0.13
(1,240)	1:A:5:ILE:HD13	1:A:11:CYS:HB2	17	0.13
(1,234)	1:A:5:ILE:HG21	1:A:11:CYS:HB3	11	0.13
(1,234)	1:A:5:ILE:HG22	1:A:11:CYS:HB3	11	0.13
(1,234)	1:A:5:ILE:HG23	1:A:11:CYS:HB3	11	0.13
(1,234)	1:A:5:ILE:HG21	1:A:11:CYS:HB3	23	0.13
(1,234)	1:A:5:ILE:HG22	1:A:11:CYS:HB3	23	0.13
(1,234)	1:A:5:ILE:HG23	1:A:11:CYS:HB3	23	0.13
(1,229)	1:A:5:ILE:HG21	1:A:6:PRO:HD3	24	0.13
(1,229)	1:A:5:ILE:HG22	1:A:6:PRO:HD3	24	0.13
(1,229)	1:A:5:ILE:HG23	1:A:6:PRO:HD3	24	0.13
(5,9)	1:A:25:TRP:O	1:A:33:VAL:N	13	0.12
(5,9)	1:A:25:TRP:O	1:A:33:VAL:N	14	0.12
(5,9)	1:A:25:TRP:O	1:A:33:VAL:N	15	0.12
(5,2)	1:A:5:ILE:N	1:A:17:ASP:O	18	0.12
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	13	0.12
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	17	0.12
(5,13)	1:A:8:TRP:H	1:A:34:CYS:O	6	0.12
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	8	0.12
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	23	0.12
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	25	0.12
(2,5)	1:A:11:CYS:SG	1:A:24:CYS:SG	12	0.12
(1,79)	1:A:18:CYS:H	1:A:22:LEU:HB2	11	0.12
(1,64)	1:A:11:CYS:H	1:A:33:VAL:HB	13	0.12
(1,423)	1:A:21:GLY:HA2	1:A:37:LYS:HE2	3	0.12
(1,423)	1:A:21:GLY:HA2	1:A:37:LYS:HE3	3	0.12
(1,423)	1:A:21:GLY:HA3	1:A:37:LYS:HE2	3	0.12
(1,423)	1:A:21:GLY:HA3	1:A:37:LYS:HE3	3	0.12
(1,339)	1:A:22:LEU:HB2	1:A:34:CYS:HB3	14	0.12
(1,339)	1:A:22:LEU:HB2	1:A:34:CYS:HB3	16	0.12
(1,339)	1:A:22:LEU:HB2	1:A:34:CYS:HB3	20	0.12
(1,320)	1:A:23:GLU:HG3	1:A:37:LYS:HA	10	0.12
(1,320)	1:A:23:GLU:HG3	1:A:37:LYS:HA	11	0.12
(1,320)	1:A:23:GLU:HG3	1:A:37:LYS:HA	15	0.12
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	3	0.12
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	3	0.12
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,259)	1:A:10:GLY:HA3	1:A:31:PHE:HD1	11	0.12
(1,226)	1:A:4:CYS:HB2	1:A:19:CYS:HB2	6	0.12
(5,9)	1:A:25:TRP:O	1:A:33:VAL:N	6	0.11
(5,6)	1:A:23:GLU:O	1:A:35:VAL:N	2	0.11
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	9	0.11
(5,18)	1:A:25:TRP:H	1:A:33:VAL:O	11	0.11
(3,8)	1:A:4:CYS:CB	1:A:19:CYS:SG	20	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	1	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	3	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	4	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	5	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	6	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	7	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	9	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	10	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	11	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	12	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	13	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	14	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	15	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	16	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	17	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	21	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	22	0.11
(2,6)	1:A:18:CYS:SG	1:A:34:CYS:SG	24	0.11
(2,5)	1:A:11:CYS:SG	1:A:24:CYS:SG	2	0.11
(2,5)	1:A:11:CYS:SG	1:A:24:CYS:SG	3	0.11
(2,5)	1:A:11:CYS:SG	1:A:24:CYS:SG	4	0.11
(2,5)	1:A:11:CYS:SG	1:A:24:CYS:SG	7	0.11
(2,5)	1:A:11:CYS:SG	1:A:24:CYS:SG	8	0.11
(2,5)	1:A:11:CYS:SG	1:A:24:CYS:SG	11	0.11
(2,5)	1:A:11:CYS:SG	1:A:24:CYS:SG	15	0.11
(2,5)	1:A:11:CYS:SG	1:A:24:CYS:SG	18	0.11
(2,5)	1:A:11:CYS:SG	1:A:24:CYS:SG	20	0.11
(2,5)	1:A:11:CYS:SG	1:A:24:CYS:SG	21	0.11
(2,5)	1:A:11:CYS:SG	1:A:24:CYS:SG	22	0.11
(2,5)	1:A:11:CYS:SG	1:A:24:CYS:SG	25	0.11
(2,4)	1:A:4:CYS:SG	1:A:19:CYS:SG	1	0.11
(2,4)	1:A:4:CYS:SG	1:A:19:CYS:SG	3	0.11
(2,4)	1:A:4:CYS:SG	1:A:19:CYS:SG	5	0.11
(2,4)	1:A:4:CYS:SG	1:A:19:CYS:SG	10	0.11
(2,4)	1:A:4:CYS:SG	1:A:19:CYS:SG	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4)	1:A:4:CYS:SG	1:A:19:CYS:SG	13	0.11
(2,4)	1:A:4:CYS:SG	1:A:19:CYS:SG	14	0.11
(2,4)	1:A:4:CYS:SG	1:A:19:CYS:SG	15	0.11
(2,4)	1:A:4:CYS:SG	1:A:19:CYS:SG	16	0.11
(2,4)	1:A:4:CYS:SG	1:A:19:CYS:SG	17	0.11
(2,4)	1:A:4:CYS:SG	1:A:19:CYS:SG	20	0.11
(2,4)	1:A:4:CYS:SG	1:A:19:CYS:SG	22	0.11
(2,4)	1:A:4:CYS:SG	1:A:19:CYS:SG	23	0.11
(2,4)	1:A:4:CYS:SG	1:A:19:CYS:SG	25	0.11
(1,79)	1:A:18:CYS:H	1:A:22:LEU:HB2	22	0.11
(1,79)	1:A:18:CYS:H	1:A:22:LEU:HB2	23	0.11
(1,76)	1:A:14:ARG:HA	1:A:17:ASP:H	5	0.11
(1,76)	1:A:14:ARG:HA	1:A:17:ASP:H	24	0.11
(1,64)	1:A:11:CYS:H	1:A:33:VAL:HB	16	0.11
(1,375)	1:A:22:LEU:HD21	1:A:35:VAL:HA	20	0.11
(1,375)	1:A:22:LEU:HD22	1:A:35:VAL:HA	20	0.11
(1,375)	1:A:22:LEU:HD23	1:A:35:VAL:HA	20	0.11
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	15	0.11
(1,366)	1:A:18:CYS:HB3	1:A:22:LEU:HG	17	0.11
(1,339)	1:A:22:LEU:HB2	1:A:34:CYS:HB3	13	0.11
(1,339)	1:A:22:LEU:HB2	1:A:34:CYS:HB3	25	0.11
(1,328)	1:A:12:VAL:HG11	1:A:31:PHE:HA	3	0.11
(1,328)	1:A:12:VAL:HG12	1:A:31:PHE:HA	3	0.11
(1,328)	1:A:12:VAL:HG13	1:A:31:PHE:HA	3	0.11
(1,328)	1:A:12:VAL:HG11	1:A:31:PHE:HA	10	0.11
(1,328)	1:A:12:VAL:HG12	1:A:31:PHE:HA	10	0.11
(1,328)	1:A:12:VAL:HG13	1:A:31:PHE:HA	10	0.11
(1,328)	1:A:12:VAL:HG11	1:A:31:PHE:HA	19	0.11
(1,328)	1:A:12:VAL:HG12	1:A:31:PHE:HA	19	0.11
(1,328)	1:A:12:VAL:HG13	1:A:31:PHE:HA	19	0.11
(1,320)	1:A:23:GLU:HG3	1:A:37:LYS:HA	6	0.11
(1,31)	1:A:5:ILE:H	1:A:5:ILE:HG12	8	0.11
(1,267)	1:A:5:ILE:HD11	1:A:11:CYS:HB3	9	0.11
(1,267)	1:A:5:ILE:HD12	1:A:11:CYS:HB3	9	0.11
(1,267)	1:A:5:ILE:HD13	1:A:11:CYS:HB3	9	0.11
(1,259)	1:A:10:GLY:HA3	1:A:31:PHE:HD1	6	0.11
(1,245)	1:A:5:ILE:HD11	1:A:9:LYS:HB3	8	0.11
(1,245)	1:A:5:ILE:HD12	1:A:9:LYS:HB3	8	0.11
(1,245)	1:A:5:ILE:HD13	1:A:9:LYS:HB3	8	0.11
(1,239)	1:A:5:ILE:HD11	1:A:6:PRO:HD2	13	0.11
(1,239)	1:A:5:ILE:HD12	1:A:6:PRO:HD2	13	0.11
(1,239)	1:A:5:ILE:HD13	1:A:6:PRO:HD2	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,239)	1:A:5:ILE:HD11	1:A:6:PRO:HD2	14	0.11
(1,239)	1:A:5:ILE:HD12	1:A:6:PRO:HD2	14	0.11
(1,239)	1:A:5:ILE:HD13	1:A:6:PRO:HD2	14	0.11
(1,239)	1:A:5:ILE:HD11	1:A:6:PRO:HD2	16	0.11
(1,239)	1:A:5:ILE:HD12	1:A:6:PRO:HD2	16	0.11
(1,239)	1:A:5:ILE:HD13	1:A:6:PRO:HD2	16	0.11
(1,229)	1:A:5:ILE:HG21	1:A:6:PRO:HD3	6	0.11
(1,229)	1:A:5:ILE:HG22	1:A:6:PRO:HD3	6	0.11
(1,229)	1:A:5:ILE:HG23	1:A:6:PRO:HD3	6	0.11
(1,229)	1:A:5:ILE:HG21	1:A:6:PRO:HD3	19	0.11
(1,229)	1:A:5:ILE:HG22	1:A:6:PRO:HD3	19	0.11
(1,229)	1:A:5:ILE:HG23	1:A:6:PRO:HD3	19	0.11
(1,157)	1:A:40:LYS:H	1:A:41:THR:H	8	0.11

10 Dihedral-angle violation analysis

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value