Full wwPDB NMR Structure Validation Report (i)

Mar 28, 2026 – 08:04 PM UTC

PDB ID	:	5W9F / pdb_00005w9f
BMRB ID	:	30312
Title	:	Solution structure of the de novo mini protein gHEEE_02
Authors	:	Pulavarti, S.V.S.R.K.; Shaw, E.A.; Bahl, C.D.; Garry, B.W.; Baker, D.; Szyperski, T.
Deposited on	:	2017-06-23

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

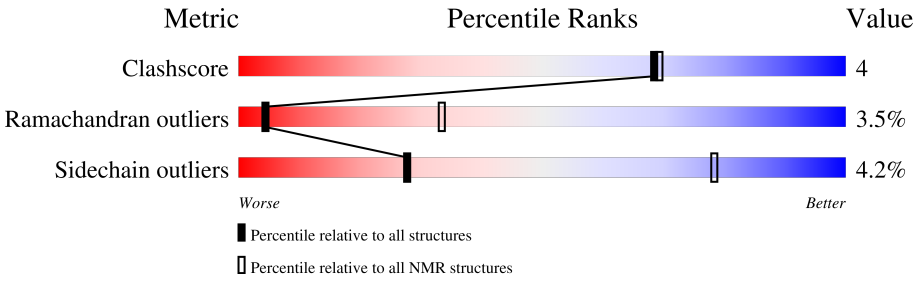
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (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 92%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	41	83% 10% 7%

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:4-A:41 (38)	0.50	11

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 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 665 atoms, of which 330 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called De novo mini protein gHEEE_02.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	41	665	199	330	62	67	7	0

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: De novo mini protein gHEEE_02

Chain A:





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: De novo mini protein gHEEE_02

Chain A:





4.2.2 Score per residue for model 2

• Molecule 1: De novo mini protein gHEEE_02

Chain A:

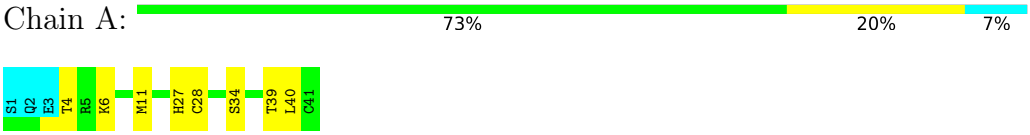




4.2.3 Score per residue for model 3

• Molecule 1: De novo mini protein gHEEE_02

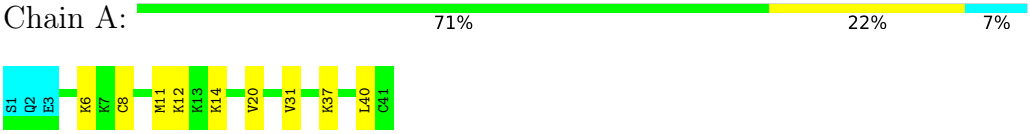
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: De novo mini protein gHEEE_02

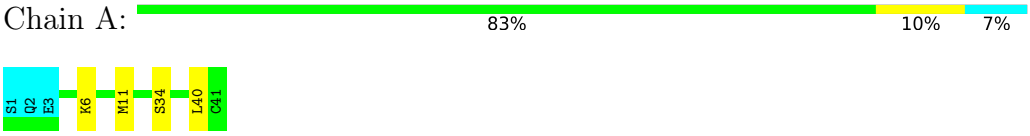
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: De novo mini protein gHEEE_02

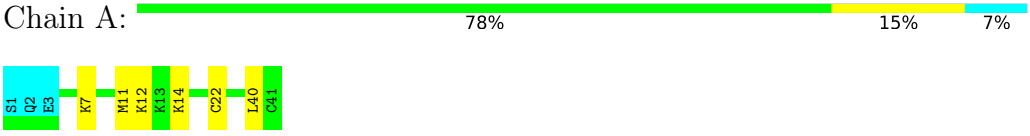
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: De novo mini protein gHEEE_02

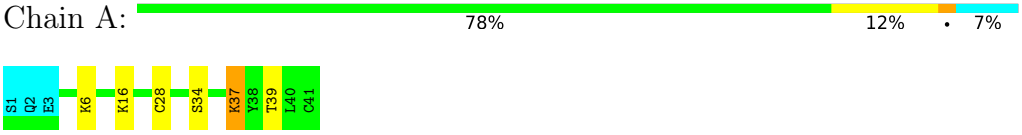
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: De novo mini protein gHEEE_02

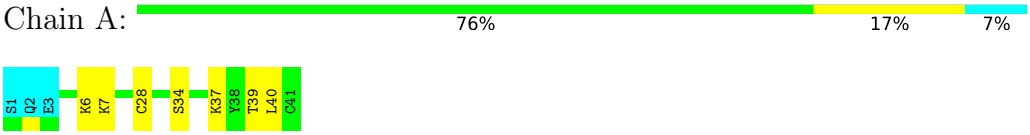
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: De novo mini protein gHEEE_02

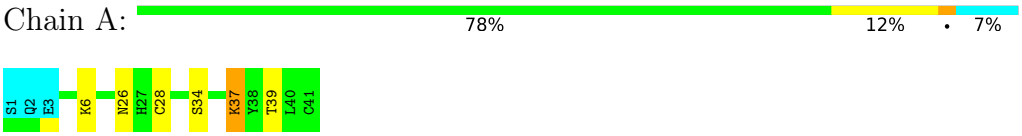
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: De novo mini protein gHEEE_02

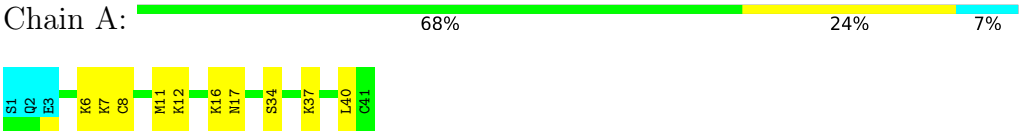
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: De novo mini protein gHEEE_02

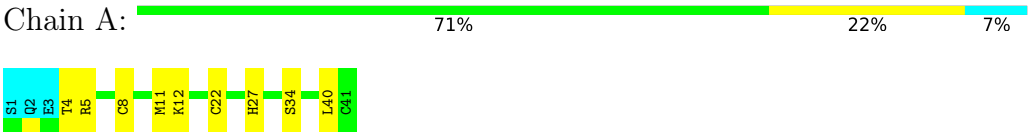
Chain A:



4.2.11 Score per residue for model 11 (medoid)

• Molecule 1: De novo mini protein gHEEE_02

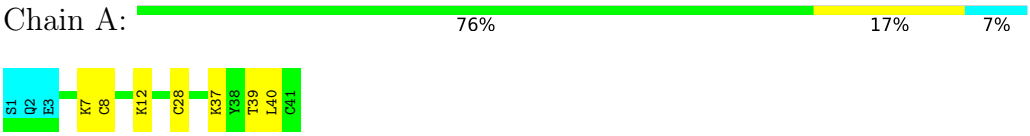
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: De novo mini protein gHEEE_02

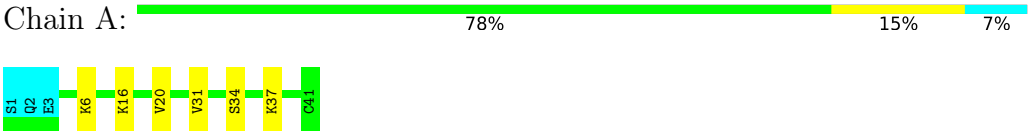
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: De novo mini protein gHEEE_02

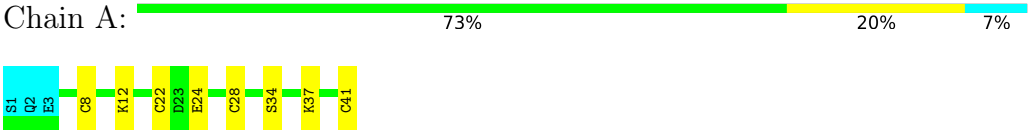
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: De novo mini protein gHEEE_02

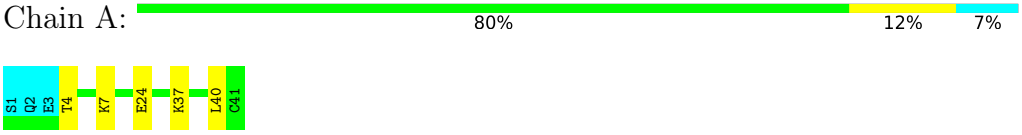
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: De novo mini protein gHEEE_02

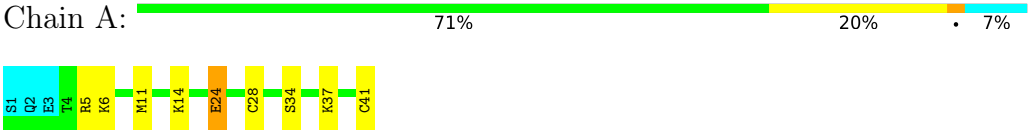
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: De novo mini protein gHEEE_02

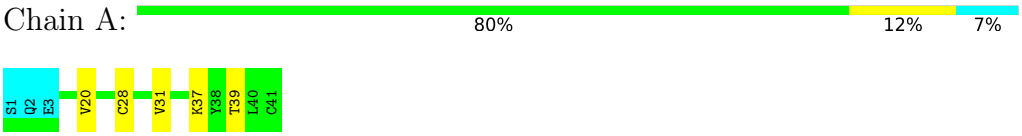
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: De novo mini protein gHEEE_02

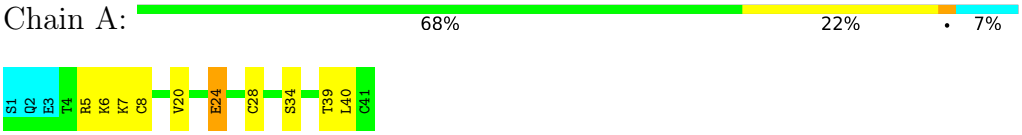
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: De novo mini protein gHEEE_02

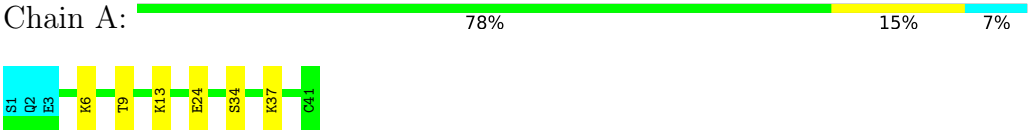
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: De novo mini protein gHEEE_02

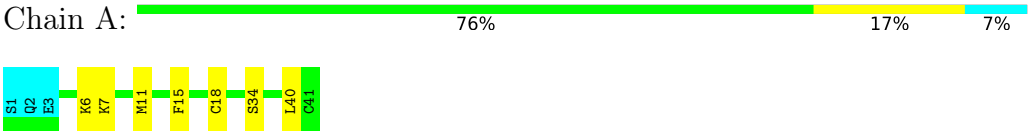
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: De novo mini protein gHEEE_02

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure calculation	3.97
CNS	refinement	1.3
CYANA	refinement	3.97

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	511
Number of shifts mapped to atoms	511
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

6 Model quality

6.1 Standard geometry

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

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	311	309	308	2±1
All	All	6220	6180	6160	46

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:CYS:SG	1:A:39:THR:HG22	0.73	2.23	7	7
1:A:12:LYS:HE3	1:A:22:CYS:SG	0.60	2.36	6	3
1:A:11:MET:SD	1:A:40:LEU:HD22	0.54	2.42	4	9
1:A:28:CYS:HA	1:A:41:CYS:HA	0.52	1.82	14	2
1:A:7:LYS:HD3	1:A:40:LEU:HB3	0.49	1.85	12	6
1:A:4:THR:HG21	1:A:24:GLU:HA	0.49	1.83	15	1
1:A:15:PHE:HB3	1:A:18:CYS:HB2	0.49	1.83	20	1
1:A:11:MET:SD	1:A:14:LYS:HD2	0.48	2.48	16	1
1:A:8:CYS:SG	1:A:20:VAL:HG12	0.47	2.48	18	1
1:A:8:CYS:SG	1:A:12:LYS:HE3	0.47	2.50	10	2
1:A:20:VAL:HG22	1:A:31:VAL:HG13	0.46	1.86	13	3
1:A:7:LYS:HE2	1:A:40:LEU:HB3	0.46	1.87	2	2
1:A:21:ARG:HD2	1:A:30:GLU:HB3	0.45	1.88	1	1
1:A:4:THR:HG21	1:A:27:HIS:HA	0.45	1.89	11	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:ARG:HE	1:A:24:GLU:HG2	0.43	1.74	16	1
1:A:5:ARG:HH21	1:A:24:GLU:HG3	0.42	1.74	18	1
1:A:26:ASN:HD22	1:A:28:CYS:HB3	0.42	1.74	9	1
1:A:9:THR:HG22	1:A:13:LYS:HE3	0.41	1.92	19	1
1:A:8:CYS:O	1:A:12:LYS:HG3	0.40	2.16	4	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	37/41 (90%)	32±2 (86±4%)	4±1 (11±3%)	1±1 (4±2%)	4	33
All	All	740/820 (90%)	633 (86%)	81 (11%)	26 (4%)	4	33

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	34	SER	14
1	A	37	LYS	11
1	A	17	ASN	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	38/41 (93%)	36±1 (96±3%)	2±1 (4±3%)	28	78
All	All	760/820 (93%)	728 (96%)	32 (4%)	28	78

All 8 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	6	LYS	13
1	A	16	LYS	5
1	A	24	GLU	4
1	A	8	CYS	3
1	A	37	LYS	3
1	A	14	LYS	2
1	A	21	ARG	1
1	A	32	ARG	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 92% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *HEEE_02nmrstar31.v1.str*

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	511
Number of shifts mapped to atoms	511
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	41	0.17 ± 0.23	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	41	0.36 ± 0.17	None needed (< 0.5 ppm)
$^{13}C'$	40	0.33 ± 0.20	None needed (< 0.5 ppm)
^{15}N	40	0.01 ± 0.53	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 92%, i.e. 480 atoms were assigned a chemical shift out of a possible 522. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	189/190 (99%)	76/76 (100%)	75/76 (99%)	38/38 (100%)
Sidechain	269/305 (88%)	180/192 (94%)	84/95 (88%)	5/18 (28%)

Continued on next page...

Continued from previous page...

	Total	^{1}H	^{13}C	^{15}N
Aromatic	22/27 (81%)	11/13 (85%)	11/12 (92%)	0/2 (0%)
Overall	480/522 (92%)	267/281 (95%)	170/183 (93%)	43/58 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 511 atoms were assigned a chemical shift out of a possible 557. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	202/205 (99%)	81/82 (99%)	81/82 (99%)	40/41 (98%)
Sidechain	287/325 (88%)	192/204 (94%)	89/102 (87%)	6/19 (32%)
Aromatic	22/27 (81%)	11/13 (85%)	11/12 (92%)	0/2 (0%)
Overall	511/557 (92%)	284/299 (95%)	181/196 (92%)	46/62 (74%)

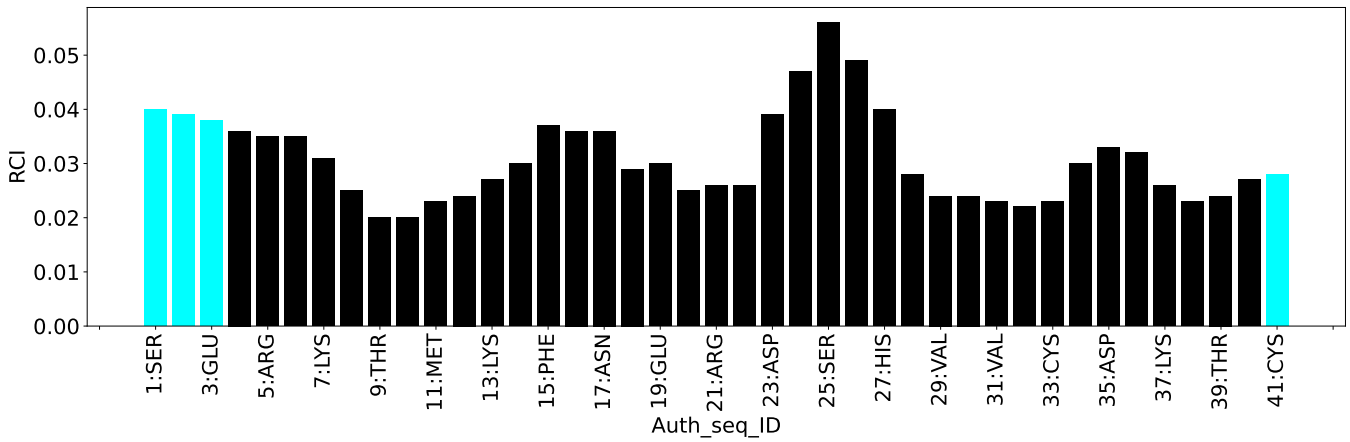
7.1.4 Statistically unusual chemical shifts (i)

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	1000
Intra-residue (|i-j|=0)	182
Sequential (|i-j|=1)	270
Medium range (|i-j|>1 and |i-j|<5)	244
Long range (|i-j|≥5)	301
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	3
Total dihedral-angle restraints	36
Number of unmapped restraints	0
Number of restraints per residue	25.3
Number of long range restraints per residue[1]	7.4

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	8.8	0.2
0.2-0.5 (Medium)	2.6	0.41
>0.5 (Large)	None	None

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	6.0	7.91
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

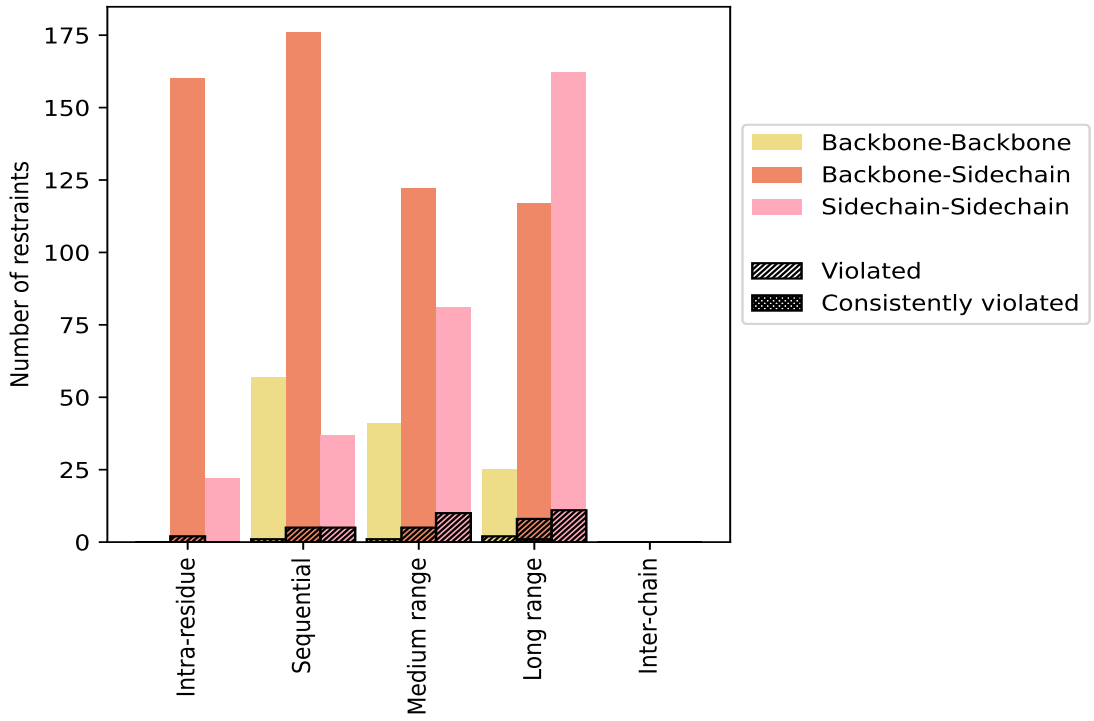
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	182	18.2	2	1.1	0.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	160	16.0	2	1.2	0.2	0	0.0	0.0
Sidechain-Sidechain	22	2.2	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	270	27.0	11	4.1	1.1	0	0.0	0.0
Backbone-Backbone	57	5.7	1	1.8	0.1	0	0.0	0.0
Backbone-Sidechain	176	17.6	5	2.8	0.5	0	0.0	0.0
Sidechain-Sidechain	37	3.7	5	13.5	0.5	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	244	24.4	16	6.6	1.6	0	0.0	0.0
Backbone-Backbone	41	4.1	1	2.4	0.1	0	0.0	0.0
Backbone-Sidechain	122	12.2	5	4.1	0.5	0	0.0	0.0
Sidechain-Sidechain	81	8.1	10	12.3	1.0	0	0.0	0.0
Long range (|i-j|≥5)	301	30.1	21	7.0	2.1	1	0.3	0.1
Backbone-Backbone	25	2.5	2	8.0	0.2	0	0.0	0.0
Backbone-Sidechain	117	11.7	8	6.8	0.8	1	0.9	0.1
Sidechain-Sidechain	159	15.9	11	6.9	1.1	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	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	3	0.3	0	0.0	0.0	0	0.0	0.0
Total	1000	100.0	50	5.0	5.0	1	0.1	0.1
Backbone-Backbone	123	12.3	4	3.3	0.4	0	0.0	0.0
Backbone-Sidechain	575	57.5	20	3.5	2.0	1	0.2	0.1
Sidechain-Sidechain	302	30.2	26	8.6	2.6	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



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	1	1	5	0	7	0.19	0.41	0.1	0.15
2	0	2	5	9	0	16	0.17	0.33	0.06	0.16
3	0	4	4	8	0	16	0.2	0.39	0.08	0.16
4	0	0	1	8	0	9	0.17	0.29	0.06	0.14
5	1	0	3	7	0	11	0.16	0.21	0.03	0.15
6	0	1	3	7	0	11	0.17	0.29	0.05	0.14
7	0	2	2	8	0	12	0.19	0.36	0.08	0.16
8	0	1	4	7	0	12	0.14	0.27	0.04	0.13
9	1	2	1	8	0	12	0.18	0.37	0.07	0.15
10	0	0	2	7	0	9	0.18	0.33	0.07	0.17

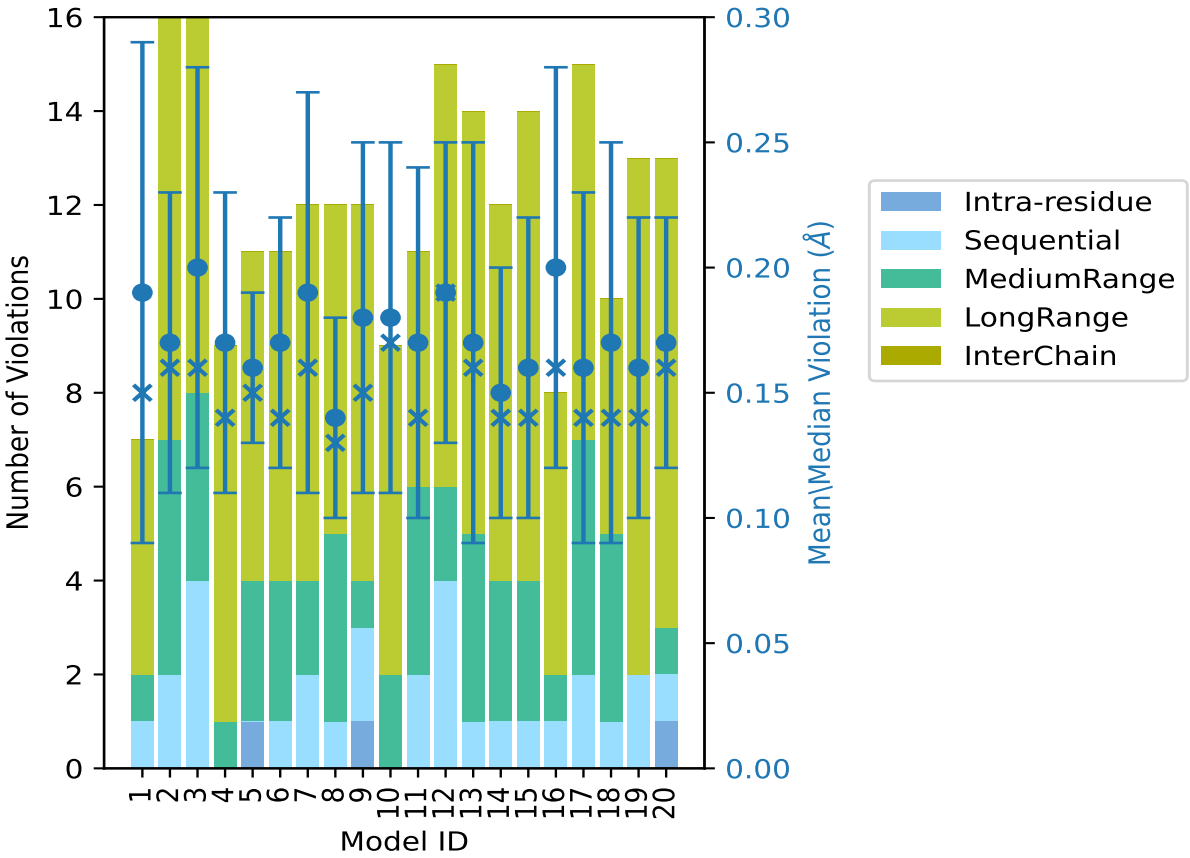
Continued on next page...

Continued from previous page...

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	0	2	4	5	0	11	0.17	0.38	0.07	0.14
12	0	4	2	9	0	15	0.19	0.35	0.06	0.19
13	0	1	4	9	0	14	0.17	0.39	0.08	0.16
14	0	1	3	8	0	12	0.15	0.27	0.05	0.14
15	0	1	3	10	0	14	0.16	0.32	0.06	0.14
16	0	1	1	6	0	8	0.2	0.33	0.08	0.16
17	0	2	5	8	0	15	0.16	0.36	0.07	0.14
18	0	1	4	5	0	10	0.17	0.36	0.08	0.14
19	0	2	0	11	0	13	0.16	0.29	0.06	0.14
20	1	1	1	10	0	13	0.17	0.28	0.05	0.16

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

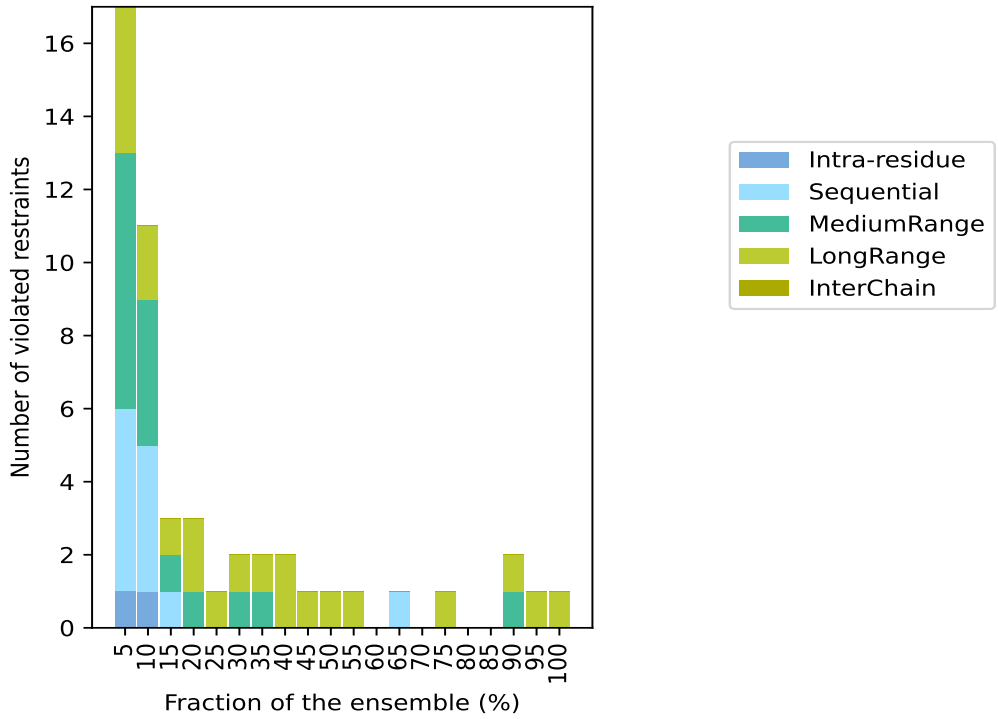
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 947(IR:180, SQ:259, MR:228, LR:280, 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	5	7	4	0	17	1	5.0
1	4	4	2	0	11	2	10.0
0	1	1	1	0	3	3	15.0
0	0	1	2	0	3	4	20.0
0	0	0	1	0	1	5	25.0
0	0	1	1	0	2	6	30.0
0	0	1	1	0	2	7	35.0
0	0	0	2	0	2	8	40.0
0	0	0	1	0	1	9	45.0
0	0	0	1	0	1	10	50.0
0	0	0	1	0	1	11	55.0
0	0	0	0	0	0	12	60.0
0	1	0	0	0	1	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	1	0	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	1	1	0	2	18	90.0
0	0	0	1	0	1	19	95.0
0	0	0	1	0	1	20	100.0

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

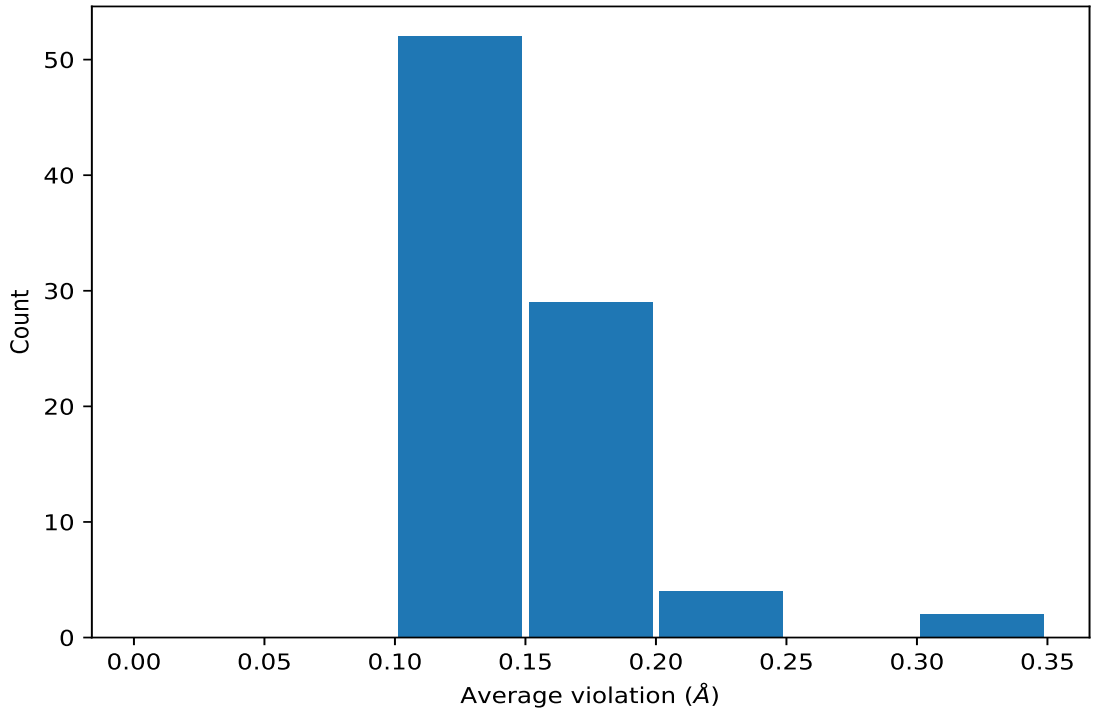
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	20	0.3	0.07	0.29
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	20	0.3	0.07	0.29
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	19	0.16	0.03	0.16
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	19	0.16	0.03	0.16
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	19	0.16	0.03	0.16
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	18	0.23	0.06	0.23
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	18	0.23	0.06	0.23
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	18	0.23	0.06	0.23
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	18	0.23	0.06	0.23
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	18	0.15	0.05	0.12
(1,690)	1:19:A:GLU:HB2	1:32:A:ARG:HG3	15	0.17	0.05	0.17
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB2	13	0.16	0.04	0.15
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB3	13	0.16	0.04	0.15
(1,300)	1:5:A:ARG:HB2	1:23:A:ASP:H	11	0.19	0.05	0.18
(1,300)	1:5:A:ARG:HB3	1:23:A:ASP:H	11	0.19	0.05	0.18
(1,644)	1:31:A:VAL:HG11	1:38:A:TYR:HB3	10	0.14	0.03	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,644)	1:31:A:VAL:HG12	1:38:A:TYR:HB3	10	0.14	0.03	0.14
(1,644)	1:31:A:VAL:HG13	1:38:A:TYR:HB3	10	0.14	0.03	0.14
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD1	9	0.16	0.04	0.15
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD2	9	0.16	0.04	0.15
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD1	9	0.16	0.04	0.15
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD2	9	0.16	0.04	0.15
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD1	9	0.16	0.04	0.15
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD2	9	0.16	0.04	0.15
(1,297)	1:21:A:ARG:H	1:30:A:GLU:HG3	8	0.15	0.03	0.15
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD21	8	0.13	0.01	0.12
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD22	8	0.13	0.01	0.12
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD23	8	0.13	0.01	0.12
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD21	8	0.13	0.01	0.12
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD22	8	0.13	0.01	0.12
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD23	8	0.13	0.01	0.12
(1,607)	1:6:A:LYS:HE2	1:9:A:THR:HB	7	0.15	0.03	0.15
(1,607)	1:6:A:LYS:HE3	1:9:A:THR:HB	7	0.15	0.03	0.15
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG21	7	0.14	0.04	0.12
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG22	7	0.14	0.04	0.12
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG23	7	0.14	0.04	0.12
(1,972)	1:32:A:ARG:HG2	1:36:A:THR:H	6	0.14	0.02	0.12
(1,972)	1:32:A:ARG:HG3	1:36:A:THR:H	6	0.14	0.02	0.12
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD11	6	0.13	0.02	0.13
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD12	6	0.13	0.02	0.13
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD13	6	0.13	0.02	0.13
(1,637)	1:31:A:VAL:HG21	1:38:A:TYR:HA	5	0.11	0.01	0.11
(1,637)	1:31:A:VAL:HG22	1:38:A:TYR:HA	5	0.11	0.01	0.11
(1,637)	1:31:A:VAL:HG23	1:38:A:TYR:HA	5	0.11	0.01	0.11
(1,308)	1:22:A:CYS:HA	1:29:A:VAL:H	4	0.14	0.04	0.12
(1,48)	1:10:A:GLU:H	1:13:A:LYS:HE2	4	0.14	0.01	0.14
(1,48)	1:10:A:GLU:H	1:13:A:LYS:HE3	4	0.14	0.01	0.14
(1,712)	1:15:A:PHE:HE1	1:29:A:VAL:HG11	4	0.13	0.01	0.13
(1,712)	1:15:A:PHE:HE1	1:29:A:VAL:HG12	4	0.13	0.01	0.13
(1,712)	1:15:A:PHE:HE1	1:29:A:VAL:HG13	4	0.13	0.01	0.13
(1,712)	1:15:A:PHE:HE2	1:29:A:VAL:HG11	4	0.13	0.01	0.13
(1,712)	1:15:A:PHE:HE2	1:29:A:VAL:HG12	4	0.13	0.01	0.13
(1,712)	1:15:A:PHE:HE2	1:29:A:VAL:HG13	4	0.13	0.01	0.13
(1,22)	1:5:A:ARG:HD2	1:6:A:LYS:H	3	0.19	0.05	0.16
(1,953)	1:28:A:CYS:HB2	1:40:A:LEU:H	3	0.15	0.02	0.14
(1,953)	1:28:A:CYS:HB3	1:40:A:LEU:H	3	0.15	0.02	0.14
(1,601)	1:8:A:CYS:HB2	1:12:A:LYS:HG2	3	0.14	0.02	0.14
(1,601)	1:8:A:CYS:HB3	1:12:A:LYS:HG2	3	0.14	0.02	0.14

Continued on next page...

Continued from previous page...

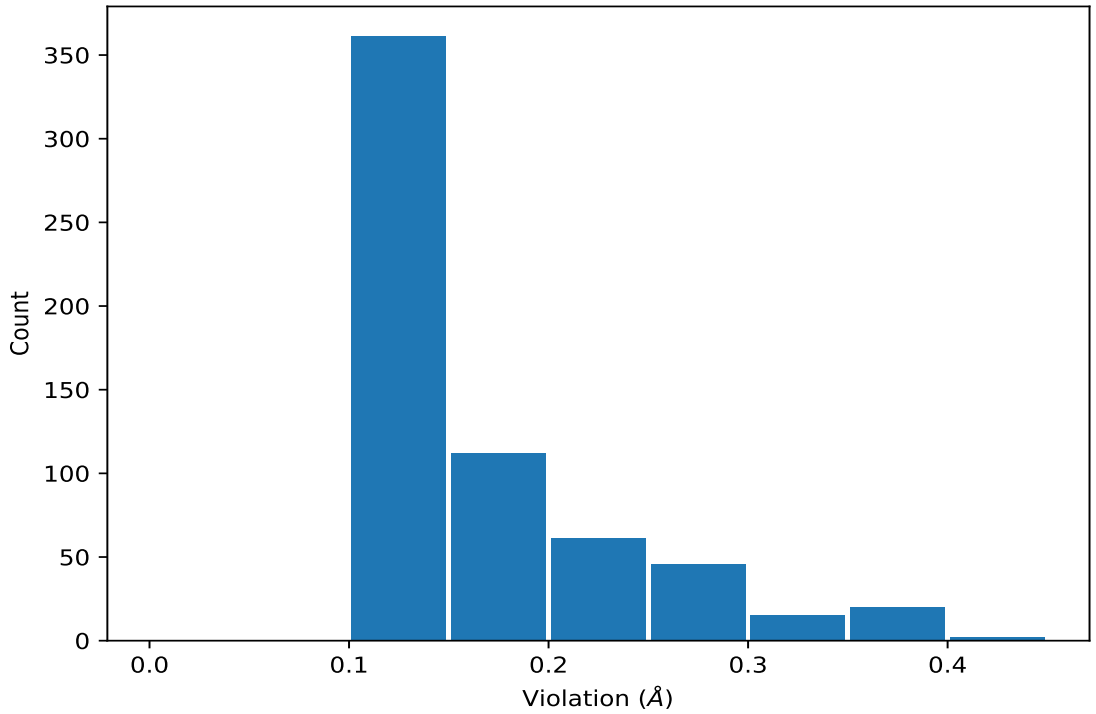
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,425)	1:14:A:LYS:HE3	1:15:A:PHE:HE1	2	0.16	0.05	0.16
(1,425)	1:14:A:LYS:HE3	1:15:A:PHE:HE2	2	0.16	0.05	0.16
(1,795)	1:38:A:TYR:HD1	1:39:A:THR:HG21	2	0.16	0.02	0.16
(1,795)	1:38:A:TYR:HD1	1:39:A:THR:HG22	2	0.16	0.02	0.16
(1,795)	1:38:A:TYR:HD1	1:39:A:THR:HG23	2	0.16	0.02	0.16
(1,795)	1:38:A:TYR:HD2	1:39:A:THR:HG21	2	0.16	0.02	0.16
(1,795)	1:38:A:TYR:HD2	1:39:A:THR:HG22	2	0.16	0.02	0.16
(1,795)	1:38:A:TYR:HD2	1:39:A:THR:HG23	2	0.16	0.02	0.16
(1,260)	1:3:A:GLU:H	1:4:A:THR:HA	2	0.14	0.02	0.14
(1,292)	1:19:A:GLU:H	1:32:A:ARG:HB2	2	0.14	0.01	0.14
(1,965)	1:30:A:GLU:HG2	1:32:A:ARG:HE	2	0.14	0.02	0.14
(1,965)	1:30:A:GLU:HG3	1:32:A:ARG:HE	2	0.14	0.02	0.14
(1,224)	1:33:A:CYS:HB2	1:35:A:ASP:H	2	0.13	0.02	0.13
(1,349)	1:37:A:LYS:H	1:37:A:LYS:HE2	2	0.13	0.01	0.13
(1,349)	1:37:A:LYS:H	1:37:A:LYS:HE3	2	0.13	0.01	0.13
(1,964)	1:30:A:GLU:HG2	1:32:A:ARG:HG2	2	0.13	0.02	0.13
(1,964)	1:30:A:GLU:HG2	1:32:A:ARG:HG3	2	0.13	0.02	0.13
(1,964)	1:30:A:GLU:HG3	1:32:A:ARG:HG2	2	0.13	0.02	0.13
(1,964)	1:30:A:GLU:HG3	1:32:A:ARG:HG3	2	0.13	0.02	0.13
(1,471)	1:31:A:VAL:HG11	1:38:A:TYR:HB2	2	0.12	0.01	0.12
(1,471)	1:31:A:VAL:HG12	1:38:A:TYR:HB2	2	0.12	0.01	0.12
(1,471)	1:31:A:VAL:HG13	1:38:A:TYR:HB2	2	0.12	0.01	0.12
(1,5)	1:3:A:GLU:H	1:4:A:THR:HG21	2	0.12	0.02	0.12
(1,5)	1:3:A:GLU:H	1:4:A:THR:HG22	2	0.12	0.02	0.12
(1,5)	1:3:A:GLU:H	1:4:A:THR:HG23	2	0.12	0.02	0.12
(1,861)	1:10:A:GLU:HG2	1:14:A:LYS:HD2	2	0.12	0.02	0.12
(1,861)	1:10:A:GLU:HG2	1:14:A:LYS:HD3	2	0.12	0.02	0.12
(1,861)	1:10:A:GLU:HG3	1:14:A:LYS:HD2	2	0.12	0.02	0.12
(1,861)	1:10:A:GLU:HG3	1:14:A:LYS:HD3	2	0.12	0.02	0.12

[1]Number of violated models, [2]Standard 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)
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	1	0.41
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	1	0.41
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	13	0.39
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	13	0.39
(1,658)	1:3:A:GLU:HB2	1:4:A:THR:HG21	3	0.39
(1,658)	1:3:A:GLU:HB2	1:4:A:THR:HG22	3	0.39
(1,658)	1:3:A:GLU:HB2	1:4:A:THR:HG23	3	0.39
(1,658)	1:3:A:GLU:HB3	1:4:A:THR:HG21	3	0.39
(1,658)	1:3:A:GLU:HB3	1:4:A:THR:HG22	3	0.39
(1,658)	1:3:A:GLU:HB3	1:4:A:THR:HG23	3	0.39
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	11	0.38
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	11	0.38
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	9	0.37
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	9	0.37
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	18	0.36
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	18	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	18	0.36
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	18	0.36
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	7	0.36
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	7	0.36
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	17	0.36
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	17	0.36
(1,427)	1:14:A:LYS:HD2	1:15:A:PHE:HD1	12	0.35
(1,427)	1:14:A:LYS:HD2	1:15:A:PHE:HD2	12	0.35
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	2	0.33
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	2	0.33
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	10	0.33
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	10	0.33
(1,217)	1:33:A:CYS:HB3	1:34:A:SER:H	16	0.33
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	3	0.32
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	3	0.32
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	3	0.32
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	3	0.32
(1,690)	1:19:A:GLU:HB2	1:32:A:ARG:HG3	15	0.32
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	3	0.31
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	3	0.31
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	7	0.31
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	7	0.3
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	7	0.3
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	7	0.3
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	7	0.3
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	13	0.29
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	13	0.29
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	13	0.29
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	13	0.29
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	4	0.29
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	4	0.29
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	6	0.29
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	6	0.29
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	16	0.29
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	16	0.29
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	19	0.29
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	19	0.29
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	20	0.28
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	20	0.28
(1,784)	1:24:A:GLU:HA	1:27:A:HIS:HE1	3	0.28
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	16	0.27
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	16	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	16	0.27
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	16	0.27
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	8	0.27
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	8	0.27
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	14	0.27
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	14	0.27
(1,300)	1:5:A:ARG:HB2	1:23:A:ASP:H	15	0.27
(1,300)	1:5:A:ARG:HB3	1:23:A:ASP:H	15	0.27
(1,300)	1:5:A:ARG:HB2	1:23:A:ASP:H	9	0.26
(1,300)	1:5:A:ARG:HB3	1:23:A:ASP:H	9	0.26
(1,22)	1:5:A:ARG:HD2	1:6:A:LYS:H	19	0.26
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	10	0.25
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	10	0.25
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	10	0.25
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	10	0.25
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	12	0.25
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	12	0.25
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	12	0.25
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	12	0.25
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	17	0.25
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	17	0.25
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	17	0.25
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	17	0.25
(1,300)	1:5:A:ARG:HB2	1:23:A:ASP:H	2	0.25
(1,300)	1:5:A:ARG:HB3	1:23:A:ASP:H	2	0.25
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	12	0.24
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	12	0.24
(1,690)	1:19:A:GLU:HB2	1:32:A:ARG:HG3	18	0.24
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG21	12	0.24
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG22	12	0.24
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG23	12	0.24
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB2	2	0.23
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB3	2	0.23
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	2	0.23
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	2	0.23
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	2	0.23
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	2	0.23
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	20	0.23
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	20	0.23
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	20	0.23
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	20	0.23
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	18	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	18	0.23
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD1	4	0.23
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD2	4	0.23
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD1	4	0.23
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD2	4	0.23
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD1	4	0.23
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD2	4	0.23
(1,300)	1:5:A:ARG:HB2	1:23:A:ASP:H	4	0.23
(1,300)	1:5:A:ARG:HB3	1:23:A:ASP:H	4	0.23
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB2	1	0.21
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB3	1	0.21
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	5	0.21
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	5	0.21
(1,690)	1:19:A:GLU:HB2	1:32:A:ARG:HG3	6	0.21
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	13	0.21
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	17	0.21
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	9	0.21
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	9	0.21
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	9	0.21
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	11	0.21
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	11	0.21
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	11	0.21
(1,425)	1:14:A:LYS:HE3	1:15:A:PHE:HE1	12	0.21
(1,425)	1:14:A:LYS:HE3	1:15:A:PHE:HE2	12	0.21
(1,308)	1:22:A:CYS:HA	1:29:A:VAL:H	2	0.21
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB2	7	0.2
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB3	7	0.2
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB2	12	0.2
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB3	12	0.2
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	1	0.2
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	1	0.2
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	1	0.2
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	1	0.2
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	6	0.2
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	6	0.2
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	6	0.2
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	6	0.2
(1,690)	1:19:A:GLU:HB2	1:32:A:ARG:HG3	9	0.2
(1,690)	1:19:A:GLU:HB2	1:32:A:ARG:HG3	20	0.2
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	10	0.2
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	14	0.2
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	14	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	14	0.2
(1,297)	1:21:A:ARG:H	1:30:A:GLU:HG3	15	0.2
(1,880)	1:12:A:LYS:HG2	1:15:A:PHE:HB2	18	0.19
(1,880)	1:12:A:LYS:HG3	1:15:A:PHE:HB2	18	0.19
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD1	10	0.19
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD2	10	0.19
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD1	10	0.19
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD2	10	0.19
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD1	10	0.19
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD2	10	0.19
(1,690)	1:19:A:GLU:HB2	1:32:A:ARG:HG3	5	0.19
(1,644)	1:31:A:VAL:HG11	1:38:A:TYR:HB3	19	0.19
(1,644)	1:31:A:VAL:HG12	1:38:A:TYR:HB3	19	0.19
(1,644)	1:31:A:VAL:HG13	1:38:A:TYR:HB3	19	0.19
(1,607)	1:6:A:LYS:HE2	1:9:A:THR:HB	12	0.19
(1,607)	1:6:A:LYS:HE3	1:9:A:THR:HB	12	0.19
(1,550)	1:7:A:LYS:HE2	1:40:A:LEU:HD11	5	0.19
(1,550)	1:7:A:LYS:HE2	1:40:A:LEU:HD12	5	0.19
(1,550)	1:7:A:LYS:HE2	1:40:A:LEU:HD13	5	0.19
(1,550)	1:7:A:LYS:HE3	1:40:A:LEU:HD11	5	0.19
(1,550)	1:7:A:LYS:HE3	1:40:A:LEU:HD12	5	0.19
(1,550)	1:7:A:LYS:HE3	1:40:A:LEU:HD13	5	0.19
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	12	0.19
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	12	0.19
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	12	0.19
(1,300)	1:5:A:ARG:HB2	1:23:A:ASP:H	3	0.19
(1,300)	1:5:A:ARG:HB3	1:23:A:ASP:H	3	0.19
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB2	14	0.18
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB3	14	0.18
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB2	19	0.18
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB3	19	0.18
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	9	0.18
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	9	0.18
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	9	0.18
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	9	0.18
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	11	0.18
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	11	0.18
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	11	0.18
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	11	0.18
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	15	0.18
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	15	0.18
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	15	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	15	0.18
(1,972)	1:32:A:ARG:HG2	1:36:A:THR:H	13	0.18
(1,972)	1:32:A:ARG:HG3	1:36:A:THR:H	13	0.18
(1,953)	1:28:A:CYS:HB2	1:40:A:LEU:H	20	0.18
(1,953)	1:28:A:CYS:HB3	1:40:A:LEU:H	20	0.18
(1,795)	1:38:A:TYR:HD1	1:39:A:THR:HG21	12	0.18
(1,795)	1:38:A:TYR:HD1	1:39:A:THR:HG22	12	0.18
(1,795)	1:38:A:TYR:HD1	1:39:A:THR:HG23	12	0.18
(1,795)	1:38:A:TYR:HD2	1:39:A:THR:HG21	12	0.18
(1,795)	1:38:A:TYR:HD2	1:39:A:THR:HG22	12	0.18
(1,795)	1:38:A:TYR:HD2	1:39:A:THR:HG23	12	0.18
(1,690)	1:19:A:GLU:HB2	1:32:A:ARG:HG3	3	0.18
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	6	0.18
(1,607)	1:6:A:LYS:HE2	1:9:A:THR:HB	3	0.18
(1,607)	1:6:A:LYS:HE3	1:9:A:THR:HB	3	0.18
(1,607)	1:6:A:LYS:HE2	1:9:A:THR:HB	14	0.18
(1,607)	1:6:A:LYS:HE3	1:9:A:THR:HB	14	0.18
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	2	0.18
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	2	0.18
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	2	0.18
(1,300)	1:5:A:ARG:HB2	1:23:A:ASP:H	20	0.18
(1,300)	1:5:A:ARG:HB3	1:23:A:ASP:H	20	0.18
(1,297)	1:21:A:ARG:H	1:30:A:GLU:HG3	8	0.18
(1,297)	1:21:A:ARG:H	1:30:A:GLU:HG3	13	0.18
(1,858)	1:10:A:GLU:HG2	1:13:A:LYS:HG2	3	0.17
(1,858)	1:10:A:GLU:HG2	1:13:A:LYS:HG3	3	0.17
(1,858)	1:10:A:GLU:HG3	1:13:A:LYS:HG2	3	0.17
(1,858)	1:10:A:GLU:HG3	1:13:A:LYS:HG3	3	0.17
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD1	2	0.17
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD2	2	0.17
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD1	2	0.17
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD2	2	0.17
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD1	2	0.17
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD2	2	0.17
(1,690)	1:19:A:GLU:HB2	1:32:A:ARG:HG3	7	0.17
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	12	0.17
(1,644)	1:31:A:VAL:HG11	1:38:A:TYR:HB3	20	0.17
(1,644)	1:31:A:VAL:HG12	1:38:A:TYR:HB3	20	0.17
(1,644)	1:31:A:VAL:HG13	1:38:A:TYR:HB3	20	0.17
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	10	0.17
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	10	0.17
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	10	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	13	0.17
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	13	0.17
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	13	0.17
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	16	0.17
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	16	0.17
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	16	0.17
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	5	0.16
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	5	0.16
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	5	0.16
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	5	0.16
(1,972)	1:32:A:ARG:HG2	1:36:A:THR:H	15	0.16
(1,972)	1:32:A:ARG:HG3	1:36:A:THR:H	15	0.16
(1,690)	1:19:A:GLU:HB2	1:32:A:ARG:HG3	14	0.16
(1,601)	1:8:A:CYS:HB2	1:12:A:LYS:HG2	2	0.16
(1,601)	1:8:A:CYS:HB3	1:12:A:LYS:HG2	2	0.16
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	3	0.16
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	3	0.16
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	3	0.16
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	15	0.16
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	15	0.16
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	15	0.16
(1,300)	1:5:A:ARG:HB2	1:23:A:ASP:H	7	0.16
(1,300)	1:5:A:ARG:HB3	1:23:A:ASP:H	7	0.16
(1,300)	1:5:A:ARG:HB2	1:23:A:ASP:H	19	0.16
(1,300)	1:5:A:ARG:HB3	1:23:A:ASP:H	19	0.16
(1,105)	1:16:A:LYS:H	1:16:A:LYS:HE2	20	0.16
(1,105)	1:16:A:LYS:H	1:16:A:LYS:HE3	20	0.16
(1,48)	1:10:A:GLU:H	1:13:A:LYS:HE2	5	0.16
(1,48)	1:10:A:GLU:H	1:13:A:LYS:HE3	5	0.16
(1,22)	1:5:A:ARG:HD2	1:6:A:LYS:H	13	0.16
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB2	17	0.15
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB3	17	0.15
(1,965)	1:30:A:GLU:HG2	1:32:A:ARG:HE	17	0.15
(1,965)	1:30:A:GLU:HG3	1:32:A:ARG:HE	17	0.15
(1,964)	1:30:A:GLU:HG2	1:32:A:ARG:HG2	5	0.15
(1,964)	1:30:A:GLU:HG2	1:32:A:ARG:HG3	5	0.15
(1,964)	1:30:A:GLU:HG3	1:32:A:ARG:HG2	5	0.15
(1,964)	1:30:A:GLU:HG3	1:32:A:ARG:HG3	5	0.15
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD1	11	0.15
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD2	11	0.15
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD1	11	0.15
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD2	11	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD1	11	0.15
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD2	11	0.15
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD1	17	0.15
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD2	17	0.15
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD1	17	0.15
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD2	17	0.15
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD1	17	0.15
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD2	17	0.15
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD11	15	0.15
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD12	15	0.15
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD13	15	0.15
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD11	17	0.15
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD12	17	0.15
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD13	17	0.15
(1,756)	1:14:A:LYS:HB2	1:15:A:PHE:HD1	9	0.15
(1,756)	1:14:A:LYS:HB2	1:15:A:PHE:HD2	9	0.15
(1,712)	1:15:A:PHE:HE1	1:29:A:VAL:HG11	13	0.15
(1,712)	1:15:A:PHE:HE1	1:29:A:VAL:HG12	13	0.15
(1,712)	1:15:A:PHE:HE1	1:29:A:VAL:HG13	13	0.15
(1,712)	1:15:A:PHE:HE2	1:29:A:VAL:HG11	13	0.15
(1,712)	1:15:A:PHE:HE2	1:29:A:VAL:HG12	13	0.15
(1,712)	1:15:A:PHE:HE2	1:29:A:VAL:HG13	13	0.15
(1,644)	1:31:A:VAL:HG11	1:38:A:TYR:HB3	9	0.15
(1,644)	1:31:A:VAL:HG12	1:38:A:TYR:HB3	9	0.15
(1,644)	1:31:A:VAL:HG13	1:38:A:TYR:HB3	9	0.15
(1,644)	1:31:A:VAL:HG11	1:38:A:TYR:HB3	12	0.15
(1,644)	1:31:A:VAL:HG12	1:38:A:TYR:HB3	12	0.15
(1,644)	1:31:A:VAL:HG13	1:38:A:TYR:HB3	12	0.15
(1,644)	1:31:A:VAL:HG11	1:38:A:TYR:HB3	14	0.15
(1,644)	1:31:A:VAL:HG12	1:38:A:TYR:HB3	14	0.15
(1,644)	1:31:A:VAL:HG13	1:38:A:TYR:HB3	14	0.15
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG21	3	0.15
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG22	3	0.15
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG23	3	0.15
(1,607)	1:6:A:LYS:HE2	1:9:A:THR:HB	7	0.15
(1,607)	1:6:A:LYS:HE3	1:9:A:THR:HB	7	0.15
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	20	0.15
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	20	0.15
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	20	0.15
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD21	1	0.15
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD22	1	0.15
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD23	1	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD21	1	0.15
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD22	1	0.15
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD23	1	0.15
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD21	2	0.15
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD22	2	0.15
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD23	2	0.15
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD21	2	0.15
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD22	2	0.15
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD23	2	0.15
(1,300)	1:5:A:ARG:HB2	1:23:A:ASP:H	5	0.15
(1,300)	1:5:A:ARG:HB3	1:23:A:ASP:H	5	0.15
(1,297)	1:21:A:ARG:H	1:30:A:GLU:HG3	3	0.15
(1,260)	1:3:A:GLU:H	1:4:A:THR:HA	7	0.15
(1,224)	1:33:A:CYS:HB2	1:35:A:ASP:H	6	0.15
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB2	6	0.14
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB3	6	0.14
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB2	8	0.14
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB3	8	0.14
(1,953)	1:28:A:CYS:HB2	1:40:A:LEU:H	4	0.14
(1,953)	1:28:A:CYS:HB3	1:40:A:LEU:H	4	0.14
(1,861)	1:10:A:GLU:HG2	1:14:A:LYS:HD2	6	0.14
(1,861)	1:10:A:GLU:HG2	1:14:A:LYS:HD3	6	0.14
(1,861)	1:10:A:GLU:HG3	1:14:A:LYS:HD2	6	0.14
(1,861)	1:10:A:GLU:HG3	1:14:A:LYS:HD3	6	0.14
(1,799)	1:26:A:ASN:HA	1:27:A:HIS:HD2	3	0.14
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD1	1	0.14
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD2	1	0.14
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD1	1	0.14
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD2	1	0.14
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD1	1	0.14
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD2	1	0.14
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD1	16	0.14
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD2	16	0.14
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD1	16	0.14
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD2	16	0.14
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD1	16	0.14
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD2	16	0.14
(1,690)	1:19:A:GLU:HB2	1:32:A:ARG:HG3	4	0.14
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	3	0.14
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG21	2	0.14
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG22	2	0.14
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG23	2	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,601)	1:8:A:CYS:HB2	1:12:A:LYS:HG2	11	0.14
(1,601)	1:8:A:CYS:HB3	1:12:A:LYS:HG2	11	0.14
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	18	0.14
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	18	0.14
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	18	0.14
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	19	0.14
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	19	0.14
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	19	0.14
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD21	8	0.14
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD22	8	0.14
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD23	8	0.14
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD21	8	0.14
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD22	8	0.14
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD23	8	0.14
(1,349)	1:37:A:LYS:H	1:37:A:LYS:HE2	9	0.14
(1,349)	1:37:A:LYS:H	1:37:A:LYS:HE3	9	0.14
(1,308)	1:22:A:CYS:HA	1:29:A:VAL:H	12	0.14
(1,297)	1:21:A:ARG:H	1:30:A:GLU:HG3	19	0.14
(1,292)	1:19:A:GLU:H	1:32:A:ARG:HB2	20	0.14
(1,48)	1:10:A:GLU:H	1:13:A:LYS:HE2	17	0.14
(1,48)	1:10:A:GLU:H	1:13:A:LYS:HE3	17	0.14
(1,22)	1:5:A:ARG:HD2	1:6:A:LYS:H	11	0.14
(1,5)	1:3:A:GLU:H	1:4:A:THR:HG21	3	0.14
(1,5)	1:3:A:GLU:H	1:4:A:THR:HG22	3	0.14
(1,5)	1:3:A:GLU:H	1:4:A:THR:HG23	3	0.14
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB2	3	0.13
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB3	3	0.13
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB2	11	0.13
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB3	11	0.13
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	8	0.13
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	8	0.13
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	8	0.13
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	8	0.13
(1,972)	1:32:A:ARG:HG2	1:36:A:THR:H	11	0.13
(1,972)	1:32:A:ARG:HG3	1:36:A:THR:H	11	0.13
(1,963)	1:30:A:GLU:HG2	1:32:A:ARG:HB2	15	0.13
(1,963)	1:30:A:GLU:HG2	1:32:A:ARG:HB3	15	0.13
(1,963)	1:30:A:GLU:HG3	1:32:A:ARG:HB2	15	0.13
(1,963)	1:30:A:GLU:HG3	1:32:A:ARG:HB3	15	0.13
(1,919)	1:19:A:GLU:HB3	1:21:A:ARG:HG2	8	0.13
(1,919)	1:19:A:GLU:HB3	1:21:A:ARG:HG3	8	0.13
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD1	5	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD2	5	0.13
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD1	5	0.13
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD2	5	0.13
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD1	5	0.13
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD2	5	0.13
(1,795)	1:38:A:TYR:HD1	1:39:A:THR:HG21	18	0.13
(1,795)	1:38:A:TYR:HD1	1:39:A:THR:HG22	18	0.13
(1,795)	1:38:A:TYR:HD1	1:39:A:THR:HG23	18	0.13
(1,795)	1:38:A:TYR:HD2	1:39:A:THR:HG21	18	0.13
(1,795)	1:38:A:TYR:HD2	1:39:A:THR:HG22	18	0.13
(1,795)	1:38:A:TYR:HD2	1:39:A:THR:HG23	18	0.13
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD11	7	0.13
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD12	7	0.13
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD13	7	0.13
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD11	8	0.13
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD12	8	0.13
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD13	8	0.13
(1,712)	1:15:A:PHE:HE1	1:29:A:VAL:HG11	3	0.13
(1,712)	1:15:A:PHE:HE1	1:29:A:VAL:HG12	3	0.13
(1,712)	1:15:A:PHE:HE1	1:29:A:VAL:HG13	3	0.13
(1,712)	1:15:A:PHE:HE2	1:29:A:VAL:HG11	3	0.13
(1,712)	1:15:A:PHE:HE2	1:29:A:VAL:HG12	3	0.13
(1,712)	1:15:A:PHE:HE2	1:29:A:VAL:HG13	3	0.13
(1,712)	1:15:A:PHE:HE1	1:29:A:VAL:HG11	6	0.13
(1,712)	1:15:A:PHE:HE1	1:29:A:VAL:HG12	6	0.13
(1,712)	1:15:A:PHE:HE1	1:29:A:VAL:HG13	6	0.13
(1,712)	1:15:A:PHE:HE2	1:29:A:VAL:HG11	6	0.13
(1,712)	1:15:A:PHE:HE2	1:29:A:VAL:HG12	6	0.13
(1,712)	1:15:A:PHE:HE2	1:29:A:VAL:HG13	6	0.13
(1,690)	1:19:A:GLU:HB2	1:32:A:ARG:HG3	11	0.13
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	14	0.13
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	15	0.13
(1,637)	1:31:A:VAL:HG21	1:38:A:TYR:HA	19	0.13
(1,637)	1:31:A:VAL:HG22	1:38:A:TYR:HA	19	0.13
(1,637)	1:31:A:VAL:HG23	1:38:A:TYR:HA	19	0.13
(1,607)	1:6:A:LYS:HE2	1:9:A:THR:HB	11	0.13
(1,607)	1:6:A:LYS:HE3	1:9:A:THR:HB	11	0.13
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	4	0.13
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	4	0.13
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	4	0.13
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	6	0.13
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	6	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	6	0.13
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	7	0.13
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	7	0.13
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	7	0.13
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	17	0.13
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	17	0.13
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	17	0.13
(1,471)	1:31:A:VAL:HG11	1:38:A:TYR:HB2	15	0.13
(1,471)	1:31:A:VAL:HG12	1:38:A:TYR:HB2	15	0.13
(1,471)	1:31:A:VAL:HG13	1:38:A:TYR:HB2	15	0.13
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD21	20	0.13
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD22	20	0.13
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD23	20	0.13
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD21	20	0.13
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD22	20	0.13
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD23	20	0.13
(1,300)	1:5:A:ARG:HB2	1:23:A:ASP:H	16	0.13
(1,300)	1:5:A:ARG:HB3	1:23:A:ASP:H	16	0.13
(1,297)	1:21:A:ARG:H	1:30:A:GLU:HG3	6	0.13
(1,297)	1:21:A:ARG:H	1:30:A:GLU:HG3	20	0.13
(1,292)	1:19:A:GLU:H	1:32:A:ARG:HB2	5	0.13
(1,251)	1:28:A:CYS:HA	1:40:A:LEU:H	16	0.13
(1,48)	1:10:A:GLU:H	1:13:A:LYS:HE2	2	0.13
(1,48)	1:10:A:GLU:H	1:13:A:LYS:HE3	2	0.13
(1,972)	1:32:A:ARG:HG2	1:36:A:THR:H	14	0.12
(1,972)	1:32:A:ARG:HG3	1:36:A:THR:H	14	0.12
(1,972)	1:32:A:ARG:HG2	1:36:A:THR:H	17	0.12
(1,972)	1:32:A:ARG:HG3	1:36:A:THR:H	17	0.12
(1,965)	1:30:A:GLU:HG2	1:32:A:ARG:HE	2	0.12
(1,965)	1:30:A:GLU:HG3	1:32:A:ARG:HE	2	0.12
(1,953)	1:28:A:CYS:HB2	1:40:A:LEU:H	17	0.12
(1,953)	1:28:A:CYS:HB3	1:40:A:LEU:H	17	0.12
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE1	15	0.12
(1,803)	1:20:A:VAL:HA	1:38:A:TYR:HE2	15	0.12
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD11	12	0.12
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD12	12	0.12
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD13	12	0.12
(1,712)	1:15:A:PHE:HE1	1:29:A:VAL:HG11	14	0.12
(1,712)	1:15:A:PHE:HE1	1:29:A:VAL:HG12	14	0.12
(1,712)	1:15:A:PHE:HE1	1:29:A:VAL:HG13	14	0.12
(1,712)	1:15:A:PHE:HE2	1:29:A:VAL:HG11	14	0.12
(1,712)	1:15:A:PHE:HE2	1:29:A:VAL:HG12	14	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,712)	1:15:A:PHE:HE2	1:29:A:VAL:HG13	14	0.12
(1,690)	1:19:A:GLU:HB2	1:32:A:ARG:HG3	10	0.12
(1,690)	1:19:A:GLU:HB2	1:32:A:ARG:HG3	13	0.12
(1,690)	1:19:A:GLU:HB2	1:32:A:ARG:HG3	19	0.12
(1,689)	1:19:A:GLU:HB2	1:32:A:ARG:HG2	2	0.12
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	5	0.12
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	9	0.12
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	16	0.12
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	20	0.12
(1,644)	1:31:A:VAL:HG11	1:38:A:TYR:HB3	6	0.12
(1,644)	1:31:A:VAL:HG12	1:38:A:TYR:HB3	6	0.12
(1,644)	1:31:A:VAL:HG13	1:38:A:TYR:HB3	6	0.12
(1,644)	1:31:A:VAL:HG11	1:38:A:TYR:HB3	7	0.12
(1,644)	1:31:A:VAL:HG12	1:38:A:TYR:HB3	7	0.12
(1,644)	1:31:A:VAL:HG13	1:38:A:TYR:HB3	7	0.12
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG21	10	0.12
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG22	10	0.12
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG23	10	0.12
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG21	13	0.12
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG22	13	0.12
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG23	13	0.12
(1,601)	1:8:A:CYS:HB2	1:12:A:LYS:HG2	14	0.12
(1,601)	1:8:A:CYS:HB3	1:12:A:LYS:HG2	14	0.12
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	8	0.12
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	8	0.12
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	8	0.12
(1,471)	1:31:A:VAL:HG11	1:38:A:TYR:HB2	19	0.12
(1,471)	1:31:A:VAL:HG12	1:38:A:TYR:HB2	19	0.12
(1,471)	1:31:A:VAL:HG13	1:38:A:TYR:HB2	19	0.12
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD21	4	0.12
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD22	4	0.12
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD23	4	0.12
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD21	4	0.12
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD22	4	0.12
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD23	4	0.12
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD21	17	0.12
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD22	17	0.12
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD23	17	0.12
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD21	17	0.12
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD22	17	0.12
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD23	17	0.12
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD21	19	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD22	19	0.12
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD23	19	0.12
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD21	19	0.12
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD22	19	0.12
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD23	19	0.12
(1,349)	1:37:A:LYS:H	1:37:A:LYS:HE2	5	0.12
(1,349)	1:37:A:LYS:H	1:37:A:LYS:HE3	5	0.12
(1,300)	1:5:A:ARG:HB2	1:23:A:ASP:H	11	0.12
(1,300)	1:5:A:ARG:HB3	1:23:A:ASP:H	11	0.12
(1,260)	1:3:A:GLU:H	1:4:A:THR:HA	2	0.12
(1,48)	1:10:A:GLU:H	1:13:A:LYS:HE2	13	0.12
(1,48)	1:10:A:GLU:H	1:13:A:LYS:HE3	13	0.12
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB2	9	0.11
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB3	9	0.11
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB2	15	0.11
(1,991)	1:40:A:LEU:H	1:41:A:CYS:HB3	15	0.11
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB2	4	0.11
(1,988)	1:38:A:TYR:HE1	1:40:A:LEU:HB3	4	0.11
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB2	4	0.11
(1,988)	1:38:A:TYR:HE2	1:40:A:LEU:HB3	4	0.11
(1,972)	1:32:A:ARG:HG2	1:36:A:THR:H	18	0.11
(1,972)	1:32:A:ARG:HG3	1:36:A:THR:H	18	0.11
(1,964)	1:30:A:GLU:HG2	1:32:A:ARG:HG2	10	0.11
(1,964)	1:30:A:GLU:HG2	1:32:A:ARG:HG3	10	0.11
(1,964)	1:30:A:GLU:HG3	1:32:A:ARG:HG2	10	0.11
(1,964)	1:30:A:GLU:HG3	1:32:A:ARG:HG3	10	0.11
(1,690)	1:19:A:GLU:HB2	1:32:A:ARG:HG3	8	0.11
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	1	0.11
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	2	0.11
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	4	0.11
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	18	0.11
(1,644)	1:31:A:VAL:HG11	1:38:A:TYR:HB3	15	0.11
(1,644)	1:31:A:VAL:HG12	1:38:A:TYR:HB3	15	0.11
(1,644)	1:31:A:VAL:HG13	1:38:A:TYR:HB3	15	0.11
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG21	9	0.11
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG22	9	0.11
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG23	9	0.11
(1,637)	1:31:A:VAL:HG21	1:38:A:TYR:HA	7	0.11
(1,637)	1:31:A:VAL:HG22	1:38:A:TYR:HA	7	0.11
(1,637)	1:31:A:VAL:HG23	1:38:A:TYR:HA	7	0.11
(1,637)	1:31:A:VAL:HG21	1:38:A:TYR:HA	9	0.11
(1,637)	1:31:A:VAL:HG22	1:38:A:TYR:HA	9	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,637)	1:31:A:VAL:HG23	1:38:A:TYR:HA	9	0.11
(1,637)	1:31:A:VAL:HG21	1:38:A:TYR:HA	12	0.11
(1,637)	1:31:A:VAL:HG22	1:38:A:TYR:HA	12	0.11
(1,637)	1:31:A:VAL:HG23	1:38:A:TYR:HA	12	0.11
(1,637)	1:31:A:VAL:HG21	1:38:A:TYR:HA	15	0.11
(1,637)	1:31:A:VAL:HG22	1:38:A:TYR:HA	15	0.11
(1,637)	1:31:A:VAL:HG23	1:38:A:TYR:HA	15	0.11
(1,607)	1:6:A:LYS:HE2	1:9:A:THR:HB	18	0.11
(1,607)	1:6:A:LYS:HE3	1:9:A:THR:HB	18	0.11
(1,549)	1:31:A:VAL:HG21	1:38:A:TYR:HB3	1	0.11
(1,549)	1:31:A:VAL:HG22	1:38:A:TYR:HB3	1	0.11
(1,549)	1:31:A:VAL:HG23	1:38:A:TYR:HB3	1	0.11
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD21	14	0.11
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD22	14	0.11
(1,382)	1:6:A:LYS:HE2	1:40:A:LEU:HD23	14	0.11
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD21	14	0.11
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD22	14	0.11
(1,382)	1:6:A:LYS:HE3	1:40:A:LEU:HD23	14	0.11
(1,308)	1:22:A:CYS:HA	1:29:A:VAL:H	17	0.11
(1,297)	1:21:A:ARG:H	1:30:A:GLU:HG3	12	0.11
(1,224)	1:33:A:CYS:HB2	1:35:A:ASP:H	8	0.11
(1,214)	1:33:A:CYS:H	1:37:A:LYS:HG2	2	0.11
(1,861)	1:10:A:GLU:HG2	1:14:A:LYS:HD2	13	0.1
(1,861)	1:10:A:GLU:HG2	1:14:A:LYS:HD3	13	0.1
(1,861)	1:10:A:GLU:HG3	1:14:A:LYS:HD2	13	0.1
(1,861)	1:10:A:GLU:HG3	1:14:A:LYS:HD3	13	0.1
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD1	13	0.1
(1,796)	1:11:A:MET:HE1	1:38:A:TYR:HD2	13	0.1
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD1	13	0.1
(1,796)	1:11:A:MET:HE2	1:38:A:TYR:HD2	13	0.1
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD1	13	0.1
(1,796)	1:11:A:MET:HE3	1:38:A:TYR:HD2	13	0.1
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD11	19	0.1
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD12	19	0.1
(1,762)	1:15:A:PHE:HZ	1:40:A:LEU:HD13	19	0.1
(1,716)	1:30:A:GLU:HG2	1:39:A:THR:HA	10	0.1
(1,679)	1:15:A:PHE:HB3	1:20:A:VAL:HB	19	0.1
(1,644)	1:31:A:VAL:HG11	1:38:A:TYR:HB3	13	0.1
(1,644)	1:31:A:VAL:HG12	1:38:A:TYR:HB3	13	0.1
(1,644)	1:31:A:VAL:HG13	1:38:A:TYR:HB3	13	0.1
(1,644)	1:31:A:VAL:HG11	1:38:A:TYR:HB3	18	0.1
(1,644)	1:31:A:VAL:HG12	1:38:A:TYR:HB3	18	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,644)	1:31:A:VAL:HG13	1:38:A:TYR:HB3	18	0.1
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG21	14	0.1
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG22	14	0.1
(1,638)	1:19:A:GLU:H	1:31:A:VAL:HG23	14	0.1
(1,607)	1:6:A:LYS:HE2	1:9:A:THR:HB	8	0.1
(1,607)	1:6:A:LYS:HE3	1:9:A:THR:HB	8	0.1
(1,425)	1:14:A:LYS:HE3	1:15:A:PHE:HE1	20	0.1
(1,425)	1:14:A:LYS:HE3	1:15:A:PHE:HE2	20	0.1
(1,308)	1:22:A:CYS:HA	1:29:A:VAL:H	8	0.1
(1,220)	1:33:A:CYS:HA	1:35:A:ASP:H	17	0.1
(1,5)	1:3:A:GLU:H	1:4:A:THR:HG21	17	0.1
(1,5)	1:3:A:GLU:H	1:4:A:THR:HG22	17	0.1
(1,5)	1:3:A:GLU:H	1:4:A:THR:HG23	17	0.1

10 Dihedral-angle violation analysis

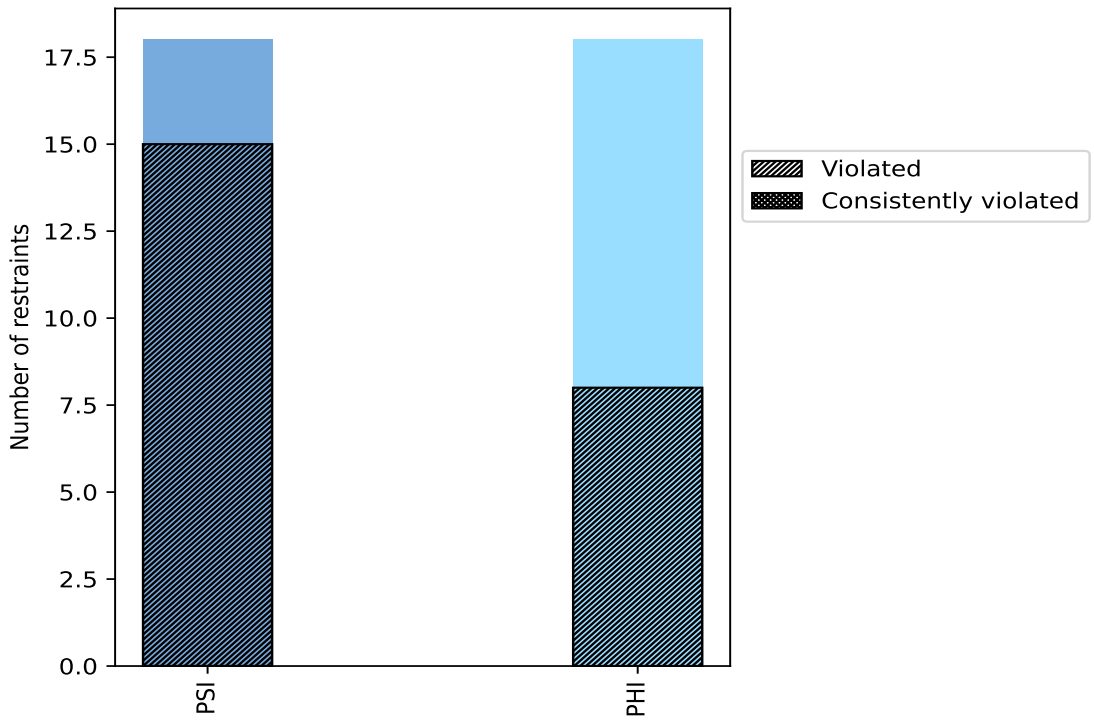
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	18	50.0	15	83.3	41.7	0	0.0	0.0
PHI	18	50.0	8	44.4	22.2	0	0.0	0.0
Total	36	100.0	23	63.9	63.9	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



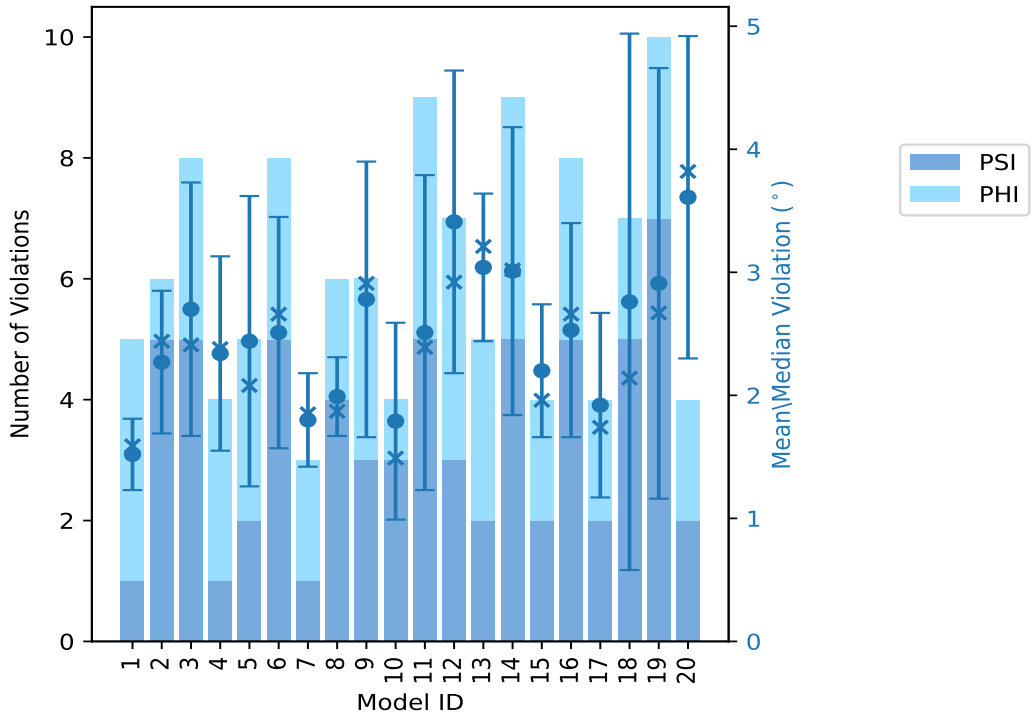
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	1	4	5	1.52	1.84	0.29	1.59
2	5	1	6	2.27	3.09	0.58	2.44
3	5	3	8	2.7	4.37	1.03	2.41
4	1	3	4	2.34	3.27	0.79	2.38
5	2	3	5	2.44	4.22	1.18	2.08
6	5	3	8	2.51	3.69	0.94	2.66
7	1	2	3	1.8	2.23	0.38	1.85
8	4	2	6	1.99	2.67	0.32	1.87
9	3	3	6	2.78	4.39	1.12	2.91
10	3	1	4	1.79	3.13	0.8	1.49
11	5	4	9	2.51	5.03	1.28	2.39
12	3	4	7	3.41	5.61	1.23	2.92
13	2	3	5	3.04	3.86	0.6	3.21
14	5	4	9	3.01	4.4	1.17	3.02
15	2	2	4	2.2	3.12	0.54	1.96
16	5	3	8	2.53	3.91	0.87	2.66
17	2	2	4	1.92	3.12	0.75	1.74
18	5	2	7	2.76	7.91	2.18	2.14
19	7	3	10	2.91	5.68	1.75	2.67
20	2	2	4	3.61	5.21	1.31	3.82

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
2	1	3	1	5.0
5	1	6	2	10.0
3	1	4	3	15.0
0	2	2	4	20.0
1	0	1	5	25.0
0	0	0	6	30.0
1	0	1	7	35.0
0	1	1	8	40.0
0	0	0	9	45.0
2	0	2	10	50.0
0	0	0	11	55.0

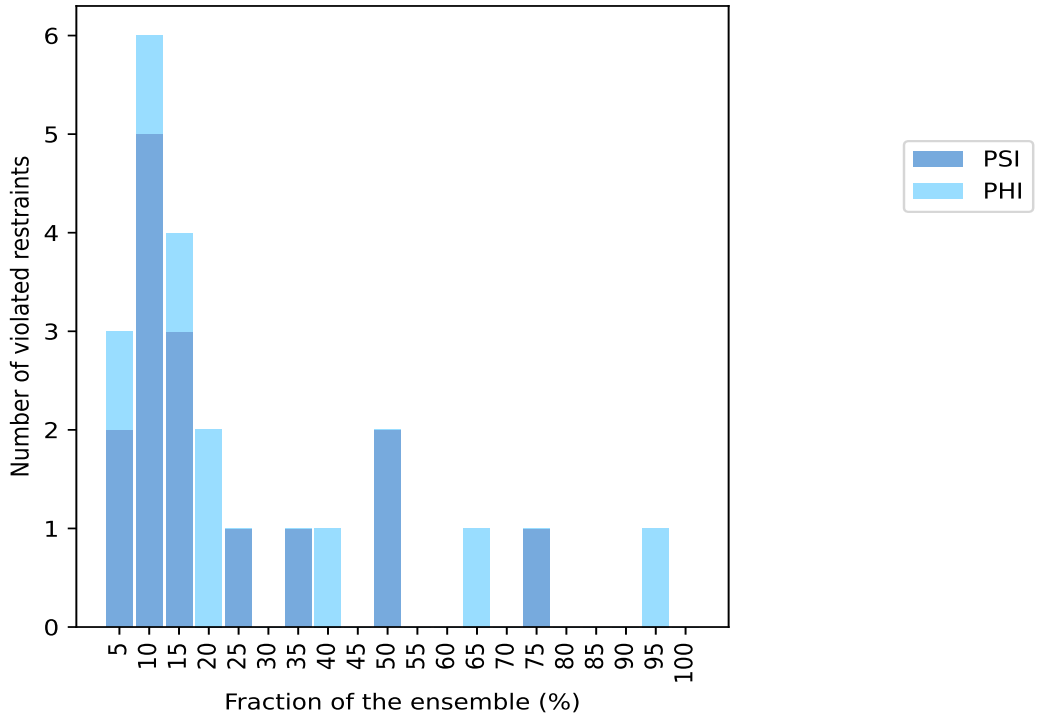
Continued on next page...

Continued from previous page...

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
0	1	1	13	65.0
0	0	0	14	70.0
1	0	1	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	1	1	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

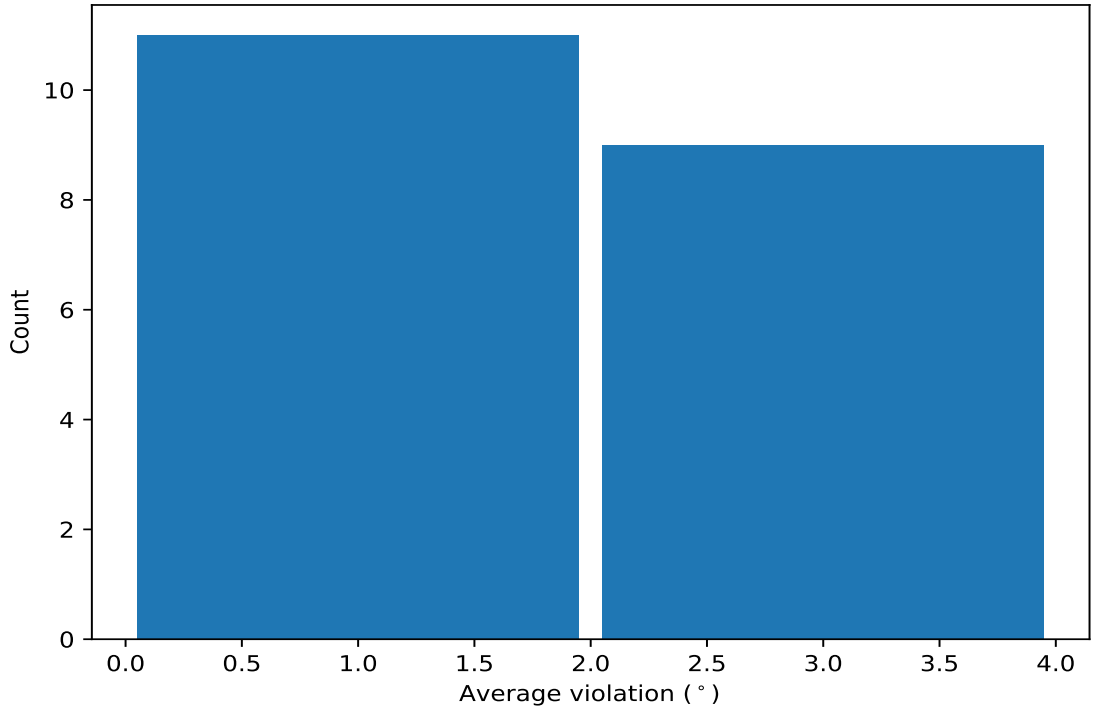


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

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

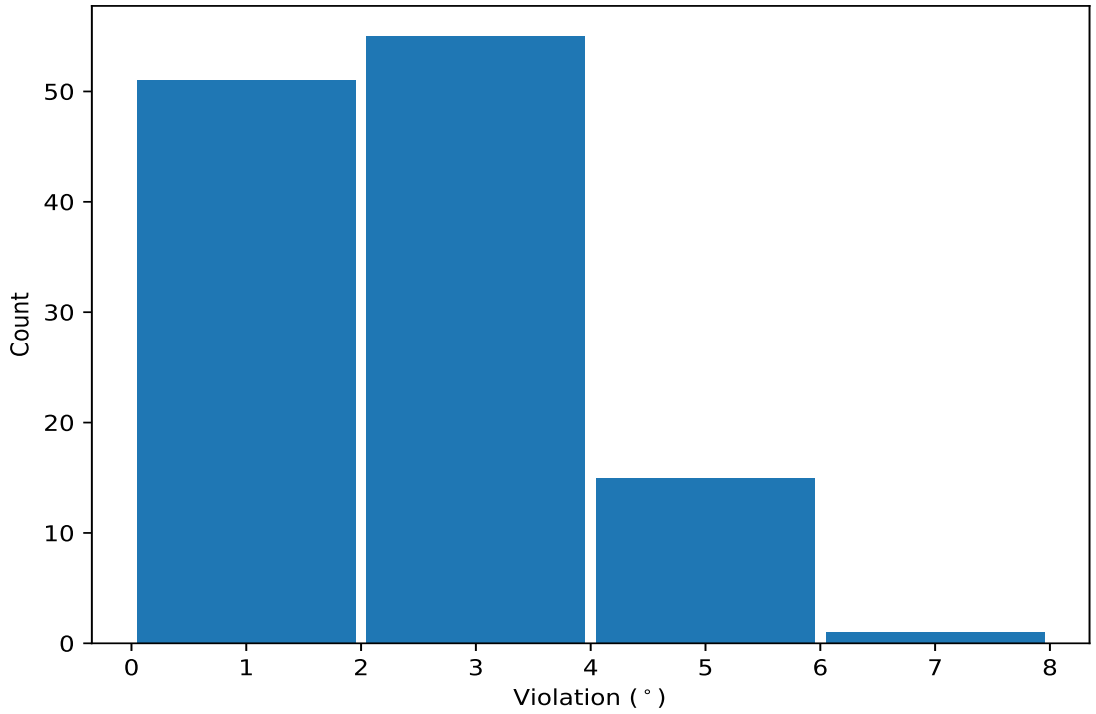
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	19	3.01	1.01	3.12
(1,32)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:ARG:N	15	3.97	1.53	3.37
(1,31)	1:30:A:GLU:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	13	2.72	1.05	2.43
(1,28)	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	1:30:A:GLU:N	10	2.77	1.05	2.93
(1,22)	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	1:21:A:ARG:N	10	2.09	0.89	1.75
(1,27)	1:28:A:CYS:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	8	2.87	0.95	2.76
(1,2)	1:4:A:THR:N	1:4:A:THR:CA	1:4:A:THR:C	1:5:A:ARG:N	7	2.72	1.29	3.02
(1,30)	1:30:A:GLU:N	1:30:A:GLU:CA	1:30:A:GLU:C	1:31:A:VAL:N	5	1.54	0.79	1.18
(1,1)	1:3:A:GLU:C	1:4:A:THR:N	1:4:A:THR:CA	1:4:A:THR:C	4	2.51	1.16	2.34
(1,15)	1:10:A:GLU:C	1:11:A:MET:N	1:11:A:MET:CA	1:11:A:MET:C	4	1.74	0.69	1.37
(1,34)	1:38:A:TYR:N	1:38:A:TYR:CA	1:38:A:TYR:C	1:39:A:THR:N	3	1.82	0.16	1.85
(1,20)	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	1:14:A:LYS:N	3	1.74	0.53	1.8
(1,33)	1:37:A:LYS:C	1:38:A:TYR:N	1:38:A:TYR:CA	1:38:A:TYR:C	3	1.67	0.2	1.77
(1,36)	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	1:40:A:LEU:N	3	1.49	0.48	1.31
(1,10)	1:8:A:CYS:N	1:8:A:CYS:CA	1:8:A:CYS:C	1:9:A:THR:N	2	2.12	0.4	2.12
(1,4)	1:5:A:ARG:N	1:5:A:ARG:CA	1:5:A:ARG:C	1:6:A:LYS:N	2	1.94	0.6	1.94
(1,18)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:LYS:N	2	1.92	0.2	1.92
(1,16)	1:11:A:MET:N	1:11:A:MET:CA	1:11:A:MET:C	1:12:A:LYS:N	2	1.91	0.89	1.91
(1,24)	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	1:22:A:CYS:N	2	1.85	0.27	1.85
(1,3)	1:4:A:THR:C	1:5:A:ARG:N	1:5:A:ARG:CA	1:5:A:ARG:C	2	1.4	0.26	1.4

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,32)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:ARG:N	18	7.91
(1,32)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:ARG:N	19	5.68
(1,32)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:ARG:N	12	5.61
(1,32)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:ARG:N	20	5.21
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	11	5.03
(1,2)	1:4:A:THR:N	1:4:A:THR:CA	1:4:A:THR:C	1:5:A:ARG:N	19	4.91
(1,28)	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	1:30:A:GLU:N	19	4.78
(1,27)	1:28:A:CYS:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	12	4.43
(1,32)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:ARG:N	14	4.4
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	9	4.39
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	3	4.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,31)	1:30:A:GLU:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	14	4.27
(1,1)	1:3:A:GLU:C	1:4:A:THR:N	1:4:A:THR:CA	1:4:A:THR:C	3	4.25
(1,27)	1:28:A:CYS:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	5	4.22
(1,31)	1:30:A:GLU:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	20	4.07
(1,28)	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	1:30:A:GLU:N	14	4.0
(1,22)	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	1:21:A:ARG:N	16	3.91
(1,31)	1:30:A:GLU:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	12	3.89
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	14	3.88
(1,32)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:ARG:N	11	3.87
(1,32)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:ARG:N	13	3.86
(1,31)	1:30:A:GLU:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	19	3.79
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	19	3.76
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	6	3.69
(1,2)	1:4:A:THR:N	1:4:A:THR:CA	1:4:A:THR:C	1:5:A:ARG:N	6	3.68
(1,31)	1:30:A:GLU:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	9	3.58
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	20	3.57
(1,32)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:ARG:N	5	3.37
(1,32)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:ARG:N	9	3.37
(1,32)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:ARG:N	16	3.37
(1,2)	1:4:A:THR:N	1:4:A:THR:CA	1:4:A:THR:C	1:5:A:ARG:N	11	3.33
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	4	3.27
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	13	3.25
(1,28)	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	1:30:A:GLU:N	13	3.21
(1,32)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:ARG:N	6	3.16
(1,32)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:ARG:N	10	3.13
(1,28)	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	1:30:A:GLU:N	15	3.12
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	17	3.12
(1,30)	1:30:A:GLU:N	1:30:A:GLU:CA	1:30:A:GLU:C	1:31:A:VAL:N	2	3.09
(1,2)	1:4:A:THR:N	1:4:A:THR:CA	1:4:A:THR:C	1:5:A:ARG:N	14	3.02
(1,28)	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	1:30:A:GLU:N	18	2.98
(1,27)	1:28:A:CYS:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	14	2.97
(1,31)	1:30:A:GLU:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	16	2.96
(1,22)	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	1:21:A:ARG:N	3	2.95
(1,15)	1:10:A:GLU:C	1:11:A:MET:N	1:11:A:MET:CA	1:11:A:MET:C	4	2.94
(1,22)	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	1:21:A:ARG:N	12	2.92
(1,28)	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	1:30:A:GLU:N	6	2.88
(1,27)	1:28:A:CYS:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	13	2.85
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	12	2.83
(1,16)	1:11:A:MET:N	1:11:A:MET:CA	1:11:A:MET:C	1:12:A:LYS:N	16	2.8
(1,1)	1:3:A:GLU:C	1:4:A:THR:N	1:4:A:THR:CA	1:4:A:THR:C	11	2.74
(1,27)	1:28:A:CYS:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	8	2.67
(1,32)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:ARG:N	2	2.64
(1,4)	1:5:A:ARG:N	1:5:A:ARG:CA	1:5:A:ARG:C	1:6:A:LYS:N	12	2.54
(1,10)	1:8:A:CYS:N	1:8:A:CYS:CA	1:8:A:CYS:C	1:9:A:THR:N	3	2.53
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	2	2.52
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	16	2.52
(1,22)	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	1:21:A:ARG:N	9	2.45
(1,31)	1:30:A:GLU:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	6	2.43
(1,27)	1:28:A:CYS:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	11	2.39
(1,20)	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	1:14:A:LYS:N	2	2.35
(1,32)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:ARG:N	3	2.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,31)	1:30:A:GLU:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	7	2.23
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	18	2.17
(1,36)	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	1:40:A:LEU:N	18	2.14
(1,18)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:LYS:N	16	2.13
(1,24)	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	1:22:A:CYS:N	3	2.12
(1,28)	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	1:30:A:GLU:N	5	2.08
(1,31)	1:30:A:GLU:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	13	2.04
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	8	2.01
(1,34)	1:38:A:TYR:N	1:38:A:TYR:CA	1:38:A:TYR:C	1:39:A:THR:N	15	2.0
(1,1)	1:3:A:GLU:C	1:4:A:THR:N	1:4:A:THR:CA	1:4:A:THR:C	14	1.94
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	15	1.91
(1,22)	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	1:21:A:ARG:N	8	1.89
(1,27)	1:28:A:CYS:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	17	1.87
(1,34)	1:38:A:TYR:N	1:38:A:TYR:CA	1:38:A:TYR:C	1:39:A:THR:N	8	1.85
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	7	1.85
(1,33)	1:37:A:LYS:C	1:38:A:TYR:N	1:38:A:TYR:CA	1:38:A:TYR:C	1	1.84
(1,31)	1:30:A:GLU:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	4	1.83
(1,31)	1:30:A:GLU:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	18	1.8
(1,20)	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	1:14:A:LYS:N	8	1.8
(1,33)	1:37:A:LYS:C	1:38:A:TYR:N	1:38:A:TYR:CA	1:38:A:TYR:C	15	1.77
(1,35)	1:38:A:TYR:C	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	1	1.73
(1,18)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:LYS:N	3	1.72
(1,10)	1:8:A:CYS:N	1:8:A:CYS:CA	1:8:A:CYS:C	1:9:A:THR:N	9	1.72
(1,32)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:ARG:N	8	1.71
(1,3)	1:4:A:THR:C	1:5:A:ARG:N	1:5:A:ARG:CA	1:5:A:ARG:C	12	1.66
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	10	1.62
(1,34)	1:38:A:TYR:N	1:38:A:TYR:CA	1:38:A:TYR:C	1:39:A:THR:N	14	1.61
(1,22)	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	1:21:A:ARG:N	17	1.61
(1,22)	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	1:21:A:ARG:N	20	1.6
(1,28)	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	1:30:A:GLU:N	1	1.59
(1,24)	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	1:22:A:CYS:N	19	1.58
(1,27)	1:28:A:CYS:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	6	1.57
(1,28)	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	1:30:A:GLU:N	11	1.53
(1,2)	1:4:A:THR:N	1:4:A:THR:CA	1:4:A:THR:C	1:5:A:ARG:N	2	1.52
(1,28)	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	1:30:A:GLU:N	2	1.49
(1,31)	1:30:A:GLU:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	11	1.48
(1,21)	1:19:A:GLU:C	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	1	1.44
(1,30)	1:30:A:GLU:N	1:30:A:GLU:CA	1:30:A:GLU:C	1:31:A:VAL:N	6	1.4
(1,33)	1:37:A:LYS:C	1:38:A:TYR:N	1:38:A:TYR:CA	1:38:A:TYR:C	5	1.39
(1,15)	1:10:A:GLU:C	1:11:A:MET:N	1:11:A:MET:CA	1:11:A:MET:C	3	1.38
(1,15)	1:10:A:GLU:C	1:11:A:MET:N	1:11:A:MET:CA	1:11:A:MET:C	16	1.36
(1,2)	1:4:A:THR:N	1:4:A:THR:CA	1:4:A:THR:C	1:5:A:ARG:N	10	1.36
(1,6)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LYS:N	4	1.33
(1,4)	1:5:A:ARG:N	1:5:A:ARG:CA	1:5:A:ARG:C	1:6:A:LYS:N	18	1.33
(1,36)	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	1:40:A:LEU:N	7	1.31
(1,15)	1:10:A:GLU:C	1:11:A:MET:N	1:11:A:MET:CA	1:11:A:MET:C	19	1.29
(1,22)	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	1:21:A:ARG:N	19	1.26
(1,22)	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	1:21:A:ARG:N	6	1.24
(1,2)	1:4:A:THR:N	1:4:A:THR:CA	1:4:A:THR:C	1:5:A:ARG:N	16	1.22
(1,30)	1:30:A:GLU:N	1:30:A:GLU:CA	1:30:A:GLU:C	1:31:A:VAL:N	11	1.18
(1,3)	1:4:A:THR:C	1:5:A:ARG:N	1:5:A:ARG:CA	1:5:A:ARG:C	9	1.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1)	1:3:A:GLU:C	1:4:A:THR:N	1:4:A:THR:CA	1:4:A:THR:C	5	1.12
(1,22)	1:20:A:VAL:N	1:20:A:VAL:CA	1:20:A:VAL:C	1:21:A:ARG:N	11	1.07
(1,8)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:CYS:N	19	1.07
(1,20)	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	1:14:A:LYS:N	17	1.06
(1,30)	1:30:A:GLU:N	1:30:A:GLU:CA	1:30:A:GLU:C	1:31:A:VAL:N	10	1.05
(1,16)	1:11:A:MET:N	1:11:A:MET:CA	1:11:A:MET:C	1:12:A:LYS:N	19	1.02
(1,36)	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	1:40:A:LEU:N	14	1.01
(1,31)	1:30:A:GLU:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1	1.0
(1,30)	1:30:A:GLU:N	1:30:A:GLU:CA	1:30:A:GLU:C	1:31:A:VAL:N	18	1.0