Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 10:57 PM EDT

PDB ID	:	2M1H
BMRB ID	:	18474
Title	:	Solution structure of a PWWP domain from Trypanosoma brucei
Authors	:	Wang, R.; Fan, K.; Liao, S.; Zhang, J.; Tu, X.
Deposited on	:	2012-11-28

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 (1)) were used in the production of this report:

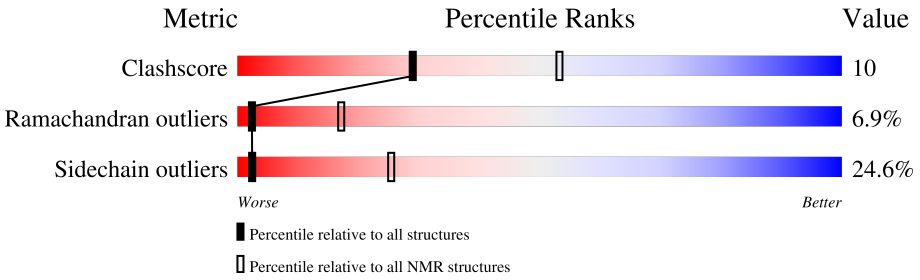
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 71%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	118	39% 23% • • 27% 7%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:7-A:16, A:22-A:37, A:41-A:74, A:86-A:103 (78)	0.34	4

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

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

The models can be grouped into 2 clusters and 6 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1681 atoms, of which 824 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	110	1681	532	824	148	176	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	LEU	-	expression tag	UNP Q586X9
A	112	GLU	-	expression tag	UNP Q586X9
A	113	HIS	-	expression tag	UNP Q586X9
A	114	HIS	-	expression tag	UNP Q586X9
A	115	HIS	-	expression tag	UNP Q586X9
A	116	HIS	-	expression tag	UNP Q586X9
A	117	HIS	-	expression tag	UNP Q586X9
A	118	HIS	-	expression tag	UNP Q586X9

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Transcription elongation factor S-II

Chain A: 39% 23% • • 27% 7%

M1 L2 Q3 E4 R5 V6 D11 R12 V13 W14 L15 K16 T17 G18 A19 N20 T21 W22 W23 P24 A25 K26 V27 T28 S29 V30 V33 E34 G38 R39 S40 S41 E42 T43 G44 T45 V50 L51 T52 T61 S67 H68 S69 S70 A71 I72 T73 F74 F75 E76 P77 S78 S79 E80

K81 A82 V83 T84 A85 L89 L90 Q91 A92 A96 S102 N103 A104 L105 R106 F107 E108 P109 T110 LEU GLU HIS HIS HIS HIS HIS HIS

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: Transcription elongation factor S-II

Chain A: 40% 22% • 27% 7%

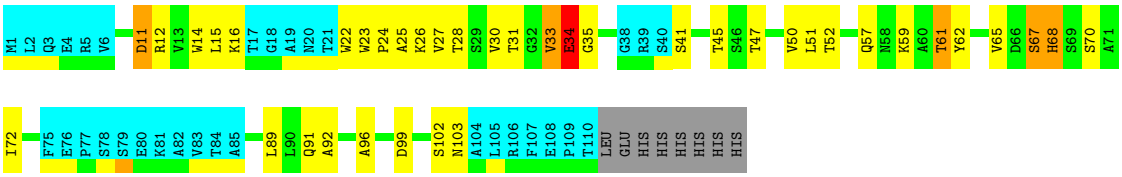
M1 L2 Q3 E4 R5 V6 D11 R12 V13 W14 L15 K16 T17 G18 A19 N20 T21 W22 W23 P24 A25 K26 V27 T28 S29 V30 V33 E34 G38 R39 S40 S41 E42 V50 L51 T52 Q57 N58 K59 A60 T61 V65 D66 S67 H68 I72 T73 F74 F75 E76 P77 S78 S79

E80 K81 A82 V83 T84 A85 A92 A96 S102 N103 A104 L105 R106 F107 E108 P109 T110 LEU GLU HIS HIS HIS HIS HIS HIS

4.2.2 Score per residue for model 2

• Molecule 1: Transcription elongation factor S-II

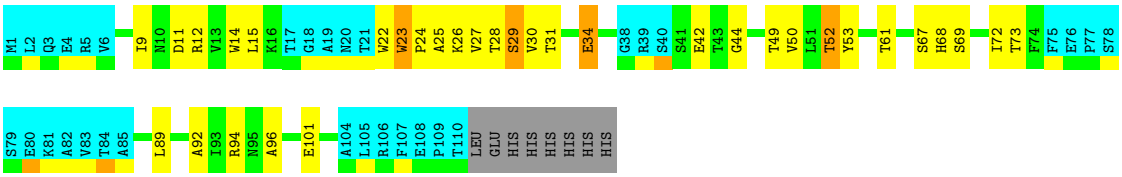
Chain A: 33% 28% • • 27% 7%



4.2.3 Score per residue for model 3

- Molecule 1: Transcription elongation factor S-II

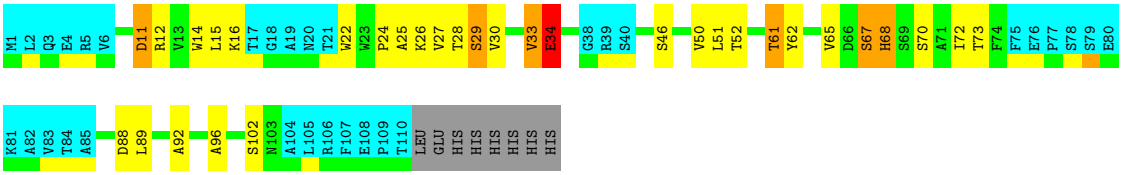
Chain A: 38% 25% • 27% 7%



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Transcription elongation factor S-II

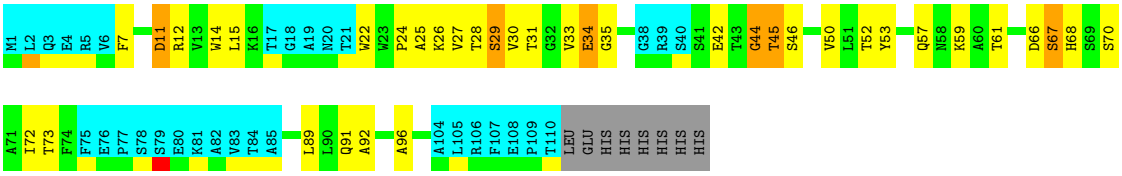
Chain A: 39% 21% 5% • 27% 7%



4.2.5 Score per residue for model 5

- Molecule 1: Transcription elongation factor S-II

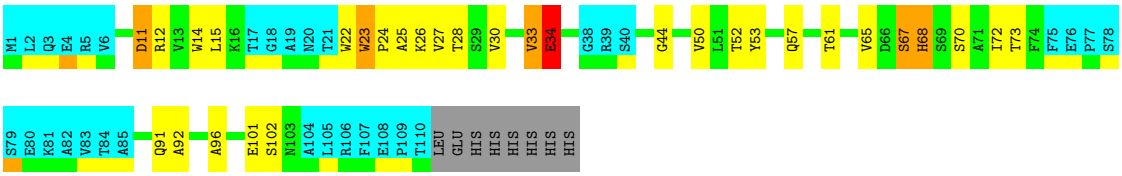
Chain A: 35% 26% 5% 27% 7%



4.2.6 Score per residue for model 6

- Molecule 1: Transcription elongation factor S-II

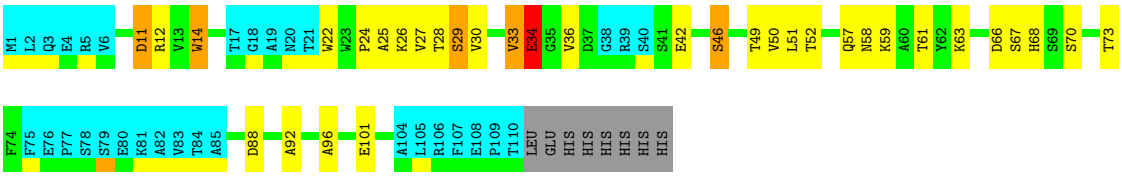
Chain A: 40% 21% • • 27% 7%



4.2.7 Score per residue for model 7

- Molecule 1: Transcription elongation factor S-II

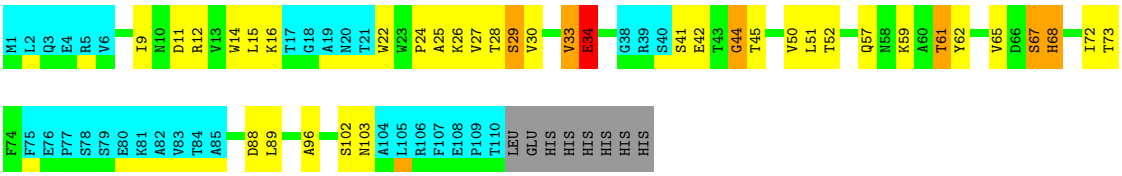
Chain A: 37% 24% • • 27% 7%



4.2.8 Score per residue for model 8

- Molecule 1: Transcription elongation factor S-II

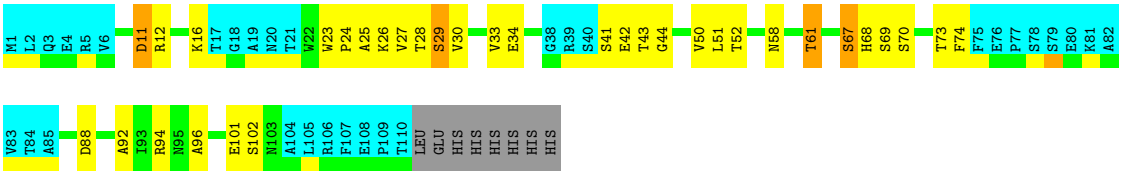
Chain A: 35% 25% 5% • 27% 7%



4.2.9 Score per residue for model 9

- Molecule 1: Transcription elongation factor S-II

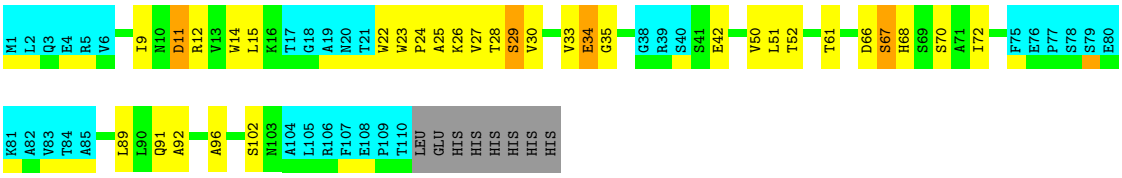
Chain A: 37% 25% • 27% 7%



4.2.10 Score per residue for model 10

- Molecule 1: Transcription elongation factor S-II

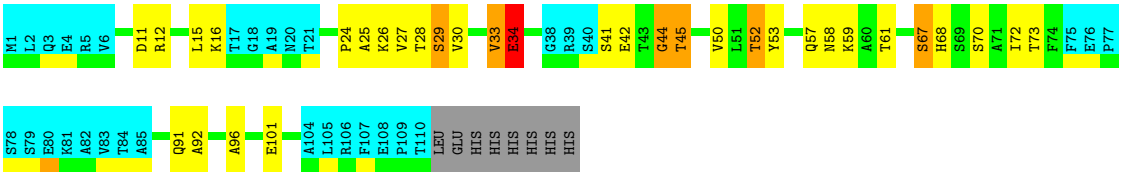
Chain A: 39% 24% • 27% 7%



4.2.11 Score per residue for model 11

- Molecule 1: Transcription elongation factor S-II

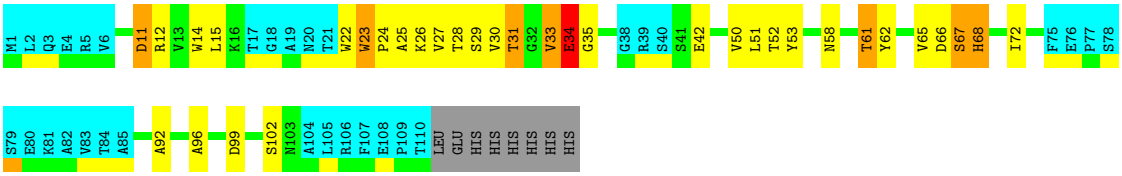
Chain A: 38% 22% 5% • 27% 7%



4.2.12 Score per residue for model 12

- Molecule 1: Transcription elongation factor S-II

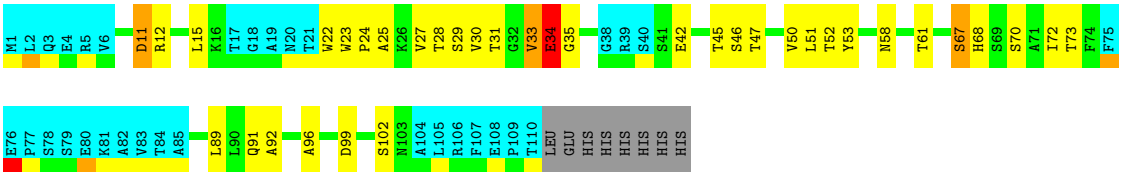
Chain A: 37% 22% 6% • 27% 7%



4.2.13 Score per residue for model 13

- Molecule 1: Transcription elongation factor S-II

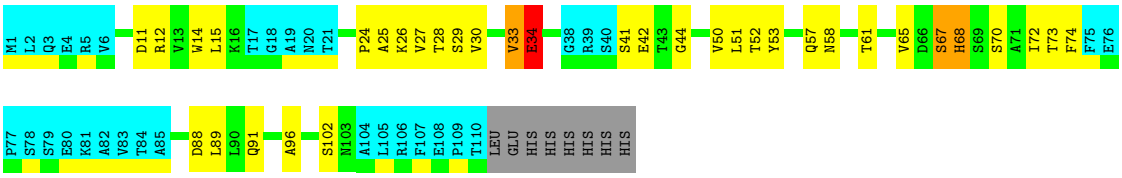
Chain A: 36% 27% • • 27% 7%



4.2.14 Score per residue for model 14

- Molecule 1: Transcription elongation factor S-II

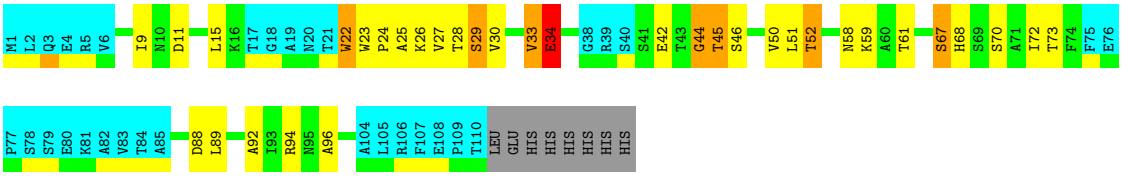
Chain A: 36% 26% • • 27% 7%



4.2.15 Score per residue for model 15

- Molecule 1: Transcription elongation factor S-II

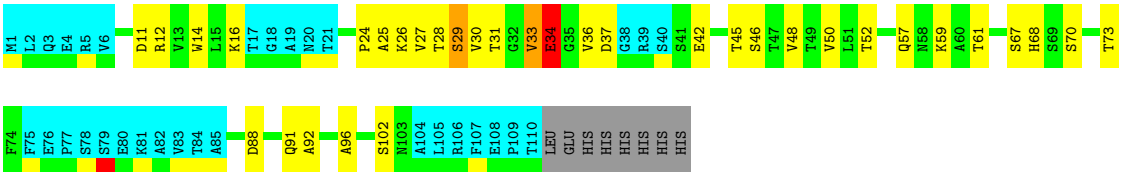
Chain A: 37% 22% 6% • 27% 7%



4.2.16 Score per residue for model 16

- Molecule 1: Transcription elongation factor S-II

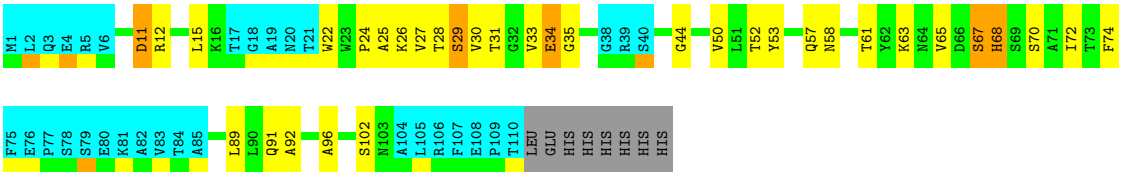
Chain A: 37% 26% • • 27% 7%



4.2.17 Score per residue for model 17

- Molecule 1: Transcription elongation factor S-II

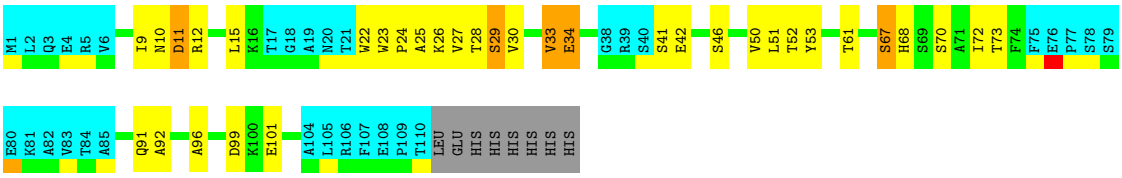
Chain A: 37% 25% • 27% 7%



4.2.18 Score per residue for model 18

- Molecule 1: Transcription elongation factor S-II

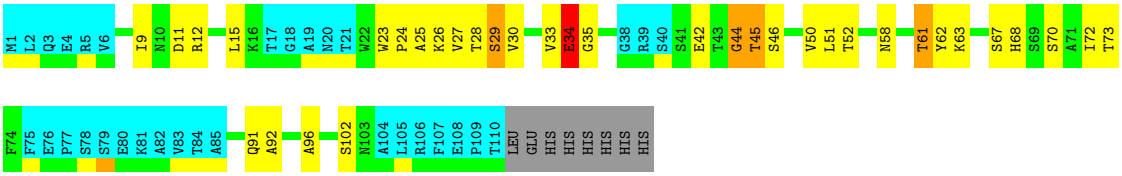
Chain A: 37% 25% • 27% 7%



4.2.19 Score per residue for model 19

- Molecule 1: Transcription elongation factor S-II

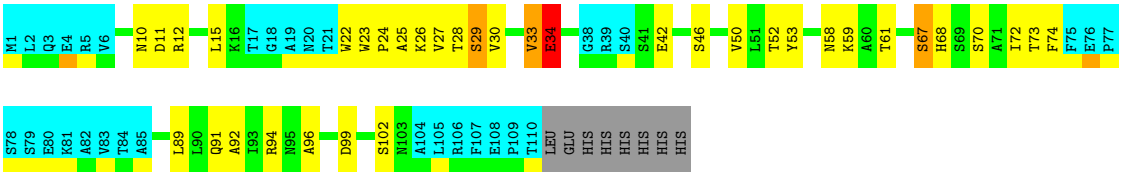
Chain A: 36% 25% • • 27% 7%



4.2.20 Score per residue for model 20

- Molecule 1: Transcription elongation factor S-II

Chain A: 36% 27% • • 27% 7%



5 Refinement protocol and experimental data overview (i)

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

Of the 500 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1017
Number of shifts mapped to atoms	1000
Number of unparsed shifts	0
Number of shifts with mapping errors	17
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	71%

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	614	584	584	12±2
All	All	12280	11680	11680	246

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:VAL:HG13	1:A:50:VAL:HG12	0.84	1.50	17	20
1:A:24:PRO:HD3	1:A:92:ALA:HB1	0.68	1.64	19	13
1:A:36:VAL:HG13	1:A:46:SER:HB2	0.65	1.68	7	1
1:A:24:PRO:CD	1:A:92:ALA:HB1	0.64	2.22	16	14
1:A:22:TRP:CD1	1:A:89:LEU:HD11	0.64	2.28	17	6
1:A:28:THR:HG23	1:A:30:VAL:HG23	0.62	1.71	11	20
1:A:22:TRP:NE1	1:A:89:LEU:HD11	0.62	2.10	5	3
1:A:15:LEU:HA	1:A:72:ILE:HG22	0.61	1.72	14	9
1:A:51:LEU:HD12	1:A:61:THR:O	0.58	1.97	9	8
1:A:33:VAL:HG12	1:A:34:GLU:HG2	0.58	1.76	18	9
1:A:33:VAL:HG22	1:A:34:GLU:HG2	0.58	1.75	13	4
1:A:24:PRO:HB3	1:A:96:ALA:HB2	0.58	1.75	11	20
1:A:22:TRP:CE2	1:A:89:LEU:HD11	0.55	2.35	4	2
1:A:25:ALA:HA	1:A:52:THR:HG22	0.54	1.78	11	20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:VAL:HG22	1:A:34:GLU:CG	0.54	2.33	12	2
1:A:51:LEU:HD13	1:A:62:TYR:HB3	0.54	1.78	8	5
1:A:23:TRP:CZ3	1:A:92:ALA:HB2	0.54	2.38	20	3
1:A:33:VAL:HG12	1:A:34:GLU:CG	0.51	2.36	6	10
1:A:15:LEU:CG	1:A:72:ILE:HG22	0.48	2.38	15	2
1:A:23:TRP:NE1	1:A:92:ALA:HB2	0.48	2.24	6	4
1:A:15:LEU:HG	1:A:72:ILE:HG22	0.48	1.84	15	7
1:A:14:TRP:CH2	1:A:96:ALA:HB1	0.47	2.44	7	1
1:A:15:LEU:HD12	1:A:72:ILE:HG21	0.47	1.86	14	2
1:A:27:VAL:HG12	1:A:29:SER:H	0.47	1.70	5	18
1:A:31:THR:HG21	1:A:35:GLY:H	0.47	1.70	17	3
1:A:36:VAL:HG13	1:A:46:SER:CB	0.46	2.39	7	1
1:A:31:THR:HG21	1:A:35:GLY:HA2	0.46	1.86	2	2
1:A:15:LEU:CB	1:A:72:ILE:HG22	0.45	2.41	19	1
1:A:51:LEU:HD12	1:A:61:THR:C	0.45	2.31	12	6
1:A:44:GLY:O	1:A:45:THR:HG23	0.44	2.12	15	5
1:A:65:VAL:HG21	1:A:68:HIS:HB2	0.44	1.90	8	7
1:A:24:PRO:HD2	1:A:92:ALA:HB1	0.44	1.88	9	1
1:A:23:TRP:CE3	1:A:92:ALA:HB2	0.43	2.48	20	1
1:A:15:LEU:HD12	1:A:72:ILE:CG2	0.43	2.44	19	1
1:A:45:THR:O	1:A:47:THR:HG23	0.42	2.14	13	2
1:A:72:ILE:HD12	1:A:72:ILE:O	0.42	2.14	1	1
1:A:28:THR:HG22	1:A:49:THR:O	0.42	2.15	3	2
1:A:37:ASP:CG	1:A:48:VAL:HG22	0.42	2.35	16	1
1:A:27:VAL:HG22	1:A:50:VAL:HG11	0.42	1.92	4	3
1:A:28:THR:HG23	1:A:30:VAL:CG2	0.41	2.45	11	1
1:A:34:GLU:HG3	1:A:36:VAL:HG23	0.41	1.92	16	1
1:A:31:THR:HG21	1:A:35:GLY:CA	0.41	2.45	2	1
1:A:23:TRP:CE2	1:A:92:ALA:HB2	0.41	2.51	3	1
1:A:33:VAL:HG13	1:A:34:GLU:N	0.40	2.31	16	1
1:A:65:VAL:HG11	1:A:68:HIS:CD2	0.40	2.51	17	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	78/118 (66%)	66±1 (84±2%)	7±1 (9±2%)	5±1 (7±1%)	2 17
All	All	1560/2360 (66%)	1312 (84%)	141 (9%)	107 (7%)	2 17

All 9 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	11	ASP	20
1	A	34	GLU	20
1	A	67	SER	20
1	A	33	VAL	18
1	A	102	SER	12
1	A	44	GLY	10
1	A	52	THR	3
1	A	35	GLY	2
1	A	31	THR	2

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	69/103 (67%)	52±2 (75±3%)	17±2 (25±3%)	2 25
All	All	1380/2060 (67%)	1040 (75%)	340 (25%)	2 25

All 38 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	68	HIS	20
1	A	12	ARG	19
1	A	26	LYS	19
1	A	34	GLU	18
1	A	61	THR	18
1	A	42	GLU	16
1	A	67	SER	16
1	A	70	SER	16
1	A	29	SER	15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	73	THR	15
1	A	14	TRP	12
1	A	91	GLN	12
1	A	11	ASP	11
1	A	57	GLN	10
1	A	53	TYR	10
1	A	58	ASN	10
1	A	59	LYS	9
1	A	46	SER	9
1	A	23	TRP	8
1	A	16	LYS	7
1	A	41	SER	7
1	A	88	ASP	7
1	A	9	ILE	6
1	A	101	GLU	6
1	A	22	TRP	5
1	A	74	PHE	5
1	A	99	ASP	5
1	A	45	THR	5
1	A	94	ARG	4
1	A	66	ASP	4
1	A	51	LEU	4
1	A	63	LYS	3
1	A	103	ASN	2
1	A	69	SER	2
1	A	10	ASN	2
1	A	102	SER	1
1	A	31	THR	1
1	A	7	PHE	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 71% for the well-defined parts and 69% 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	1017
Number of shifts mapped to atoms	1000
Number of unparsed shifts	0
Number of shifts with mapping errors	17
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

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

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

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	111	LEU	CA	55.293	0.057	1
1	A	111	LEU	CB	42.249	0.065	1
1	A	111	LEU	CG	24.433	2.329	1
1	A	111	LEU	HA	4.26	0.006	1
1	A	111	LEU	HB2	1.486	0.006	2
1	A	111	LEU	HB3	1.486	0.006	2
1	A	111	LEU	HD11	0.798	0.007	2
1	A	111	LEU	HD12	0.798	0.007	2
1	A	111	LEU	HD13	0.798	0.007	2
1	A	111	LEU	HD21	0.798	0.007	2
1	A	111	LEU	HD22	0.798	0.007	2
1	A	111	LEU	HD23	0.798	0.007	2
1	A	111	LEU	N	124.482	0.008	1
1	A	111	LEU	H	8.225	0.005	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	112	GLU	CB	30.297	0.000	1
1	A	112	GLU	N	121.399	0.023	1
1	A	112	GLU	H	8.273	0.004	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	109	-0.13 ± 0.12	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	105	0.10 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	107	-0.48 ± 0.20	None needed (< 0.5 ppm)

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 71%, i.e. 721 atoms were assigned a chemical shift out of a possible 1020. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	309/390 (79%)	155/158 (98%)	78/156 (50%)	76/76 (100%)
Sidechain	412/542 (76%)	282/350 (81%)	130/173 (75%)	0/19 (0%)
Aromatic	0/88 (0%)	0/44 (0%)	0/39 (0%)	0/5 (0%)
Overall	721/1020 (71%)	437/552 (79%)	208/368 (57%)	76/100 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 69%, i.e. 1000 atoms were assigned a chemical shift out of a possible 1439. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	426/548 (78%)	213/222 (96%)	108/220 (49%)	105/106 (99%)
Sidechain	574/783 (73%)	391/506 (77%)	183/246 (74%)	0/31 (0%)
Aromatic	0/108 (0%)	0/54 (0%)	0/49 (0%)	0/5 (0%)
Overall	1000/1439 (69%)	604/782 (77%)	291/515 (57%)	105/142 (74%)

7.1.4 Statistically unusual chemical shifts (i)

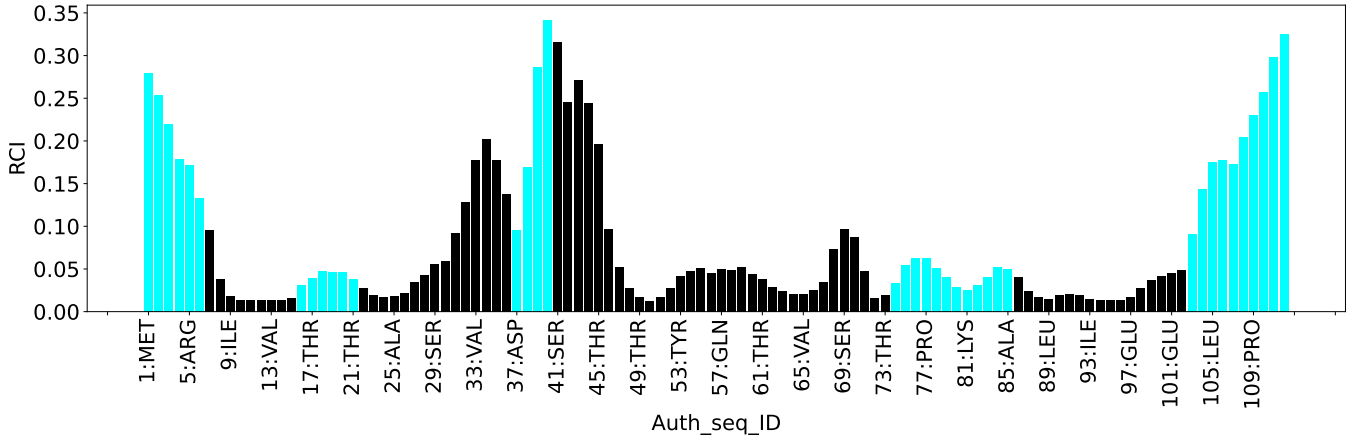
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	16	LYS	HG2	0.08	0.13 – 2.61	-5.2
1	A	96	ALA	HB1	0.10	0.14 – 2.58	-5.2
1	A	96	ALA	HB2	0.10	0.14 – 2.58	-5.2
1	A	96	ALA	HB3	0.10	0.14 – 2.58	-5.2

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 (i)

8.1 Conformationally restricting restraints (i)

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	1223
Intra-residue (|i-j|=0)	181
Sequential (|i-j|=1)	482
Medium range (|i-j|>1 and |i-j|<5)	235
Long range (|i-j|≥5)	311
Inter-chain	0
Hydrogen bond restraints	14
Disulfide bond restraints	0
Total dihedral-angle restraints	109
Number of unmapped restraints	0
Number of restraints per residue	11.3
Number of long range restraints per residue[1]	2.6

[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 (i)

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 (i)

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)	5.5	0.2
0.2-0.5 (Medium)	1.3	0.35
>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)	17.7	5.0
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

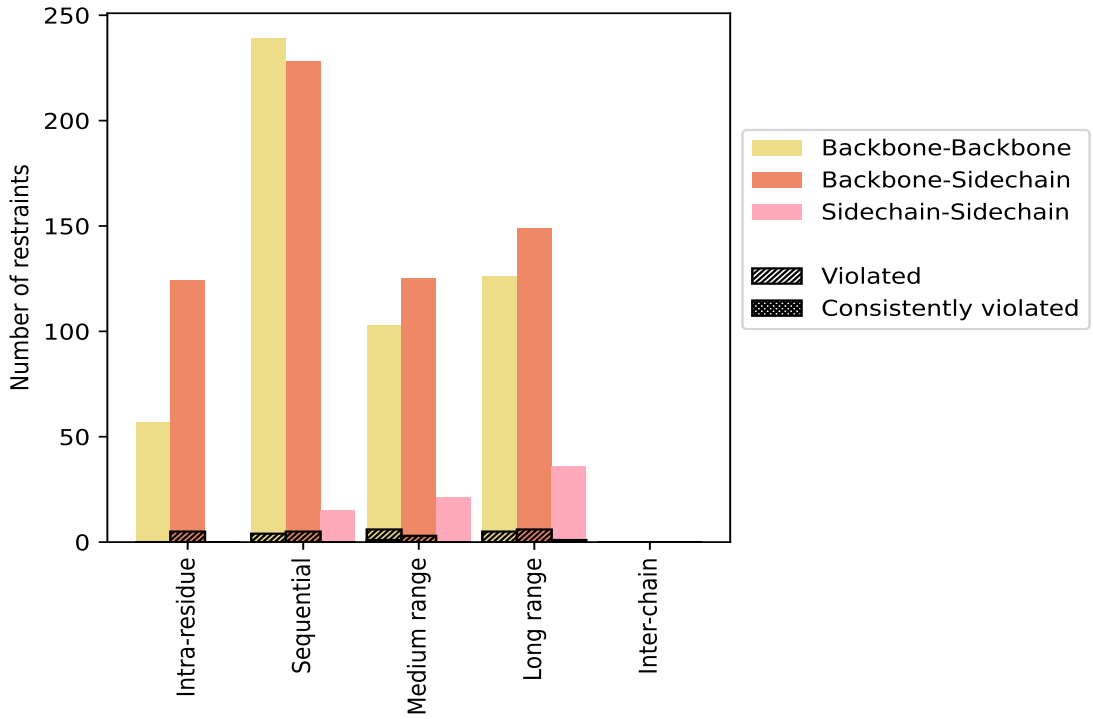
9.1 Summary of distance violations (i)

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)	181	14.8	5	2.8	0.4	0	0.0	0.0
Backbone-Backbone	57	4.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	124	10.1	5	4.0	0.4	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	482	39.4	9	1.9	0.7	0	0.0	0.0
Backbone-Backbone	239	19.5	4	1.7	0.3	0	0.0	0.0
Backbone-Sidechain	228	18.6	5	2.2	0.4	0	0.0	0.0
Sidechain-Sidechain	15	1.2	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	235	19.2	5	2.1	0.4	0	0.0	0.0
Backbone-Backbone	89	7.3	2	2.2	0.2	0	0.0	0.0
Backbone-Sidechain	125	10.2	3	2.4	0.2	0	0.0	0.0
Sidechain-Sidechain	21	1.7	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	311	25.4	12	3.9	1.0	0	0.0	0.0
Backbone-Backbone	126	10.3	5	4.0	0.4	0	0.0	0.0
Backbone-Sidechain	149	12.2	6	4.0	0.5	0	0.0	0.0
Sidechain-Sidechain	36	2.9	1	2.8	0.1	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	14	1.1	4	28.6	0.3	1	7.1	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1223	100.0	35	2.9	2.9	1	0.1	0.1
Backbone-Backbone	525	42.9	15	2.9	1.2	1	0.2	0.1
Backbone-Sidechain	626	51.2	19	3.0	1.6	0	0.0	0.0
Sidechain-Sidechain	72	5.9	1	1.4	0.1	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 disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	1	0	3	0	0	4	0.14	0.23	0.05	0.12
2	0	1	5	2	0	8	0.14	0.24	0.05	0.12
3	1	1	3	4	0	9	0.15	0.22	0.04	0.12
4	1	1	3	2	0	7	0.18	0.35	0.09	0.11
5	1	0	3	2	0	6	0.16	0.26	0.05	0.15
6	0	1	1	1	0	3	0.17	0.22	0.04	0.18
7	2	1	2	4	0	9	0.15	0.23	0.04	0.15
8	0	0	4	2	0	6	0.15	0.28	0.06	0.12
9	0	0	4	3	0	7	0.14	0.22	0.04	0.13
10	0	2	4	0	0	6	0.18	0.26	0.06	0.17
11	0	1	4	4	0	9	0.14	0.24	0.04	0.12

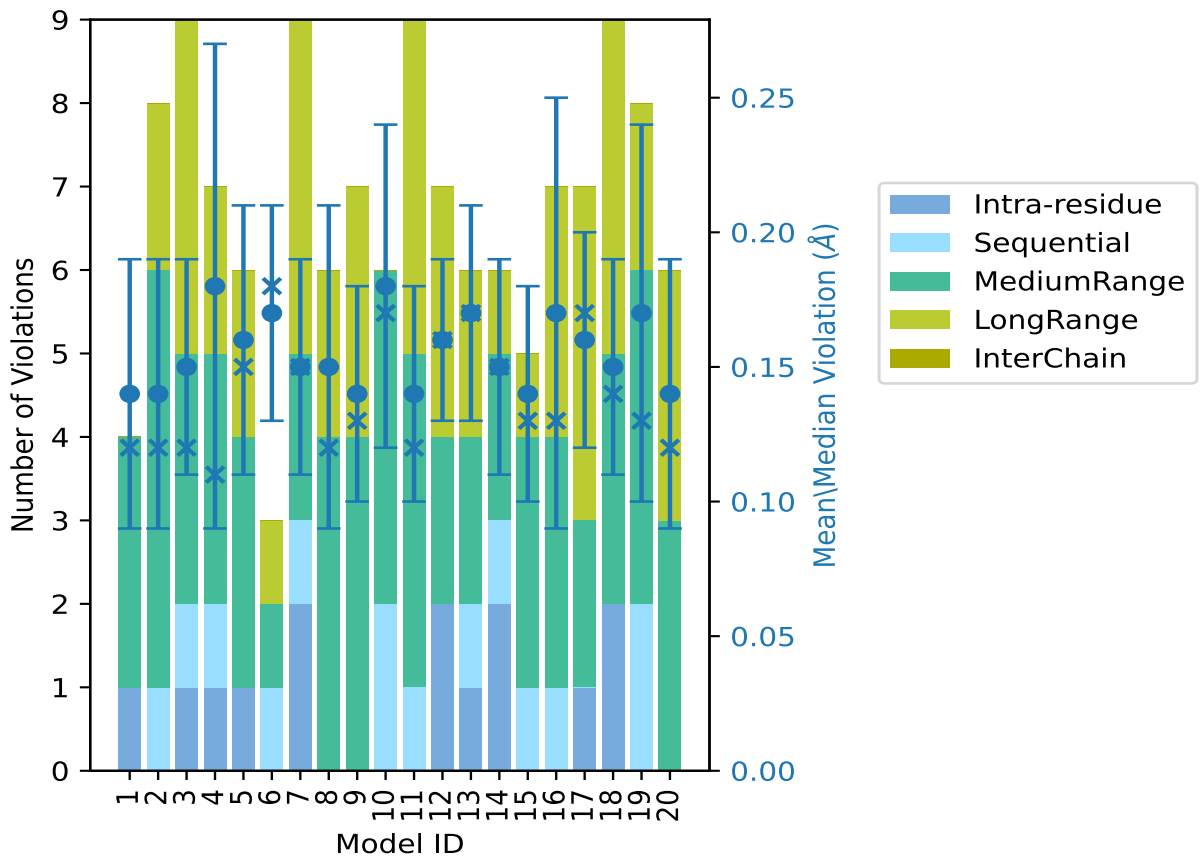
Continued on next page...

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				
12	2	0	2	3	0	7	0.16	0.22	0.03	0.16
13	1	1	2	2	0	6	0.17	0.25	0.04	0.17
14	2	1	2	1	0	6	0.15	0.22	0.04	0.15
15	0	1	3	1	0	5	0.14	0.23	0.04	0.13
16	0	1	3	3	0	7	0.17	0.35	0.08	0.13
17	1	0	2	4	0	7	0.16	0.23	0.04	0.17
18	2	0	3	4	0	9	0.15	0.25	0.04	0.14
19	0	2	4	2	0	8	0.17	0.28	0.07	0.13
20	0	0	3	3	0	6	0.14	0.25	0.05	0.12

[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 (i)



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

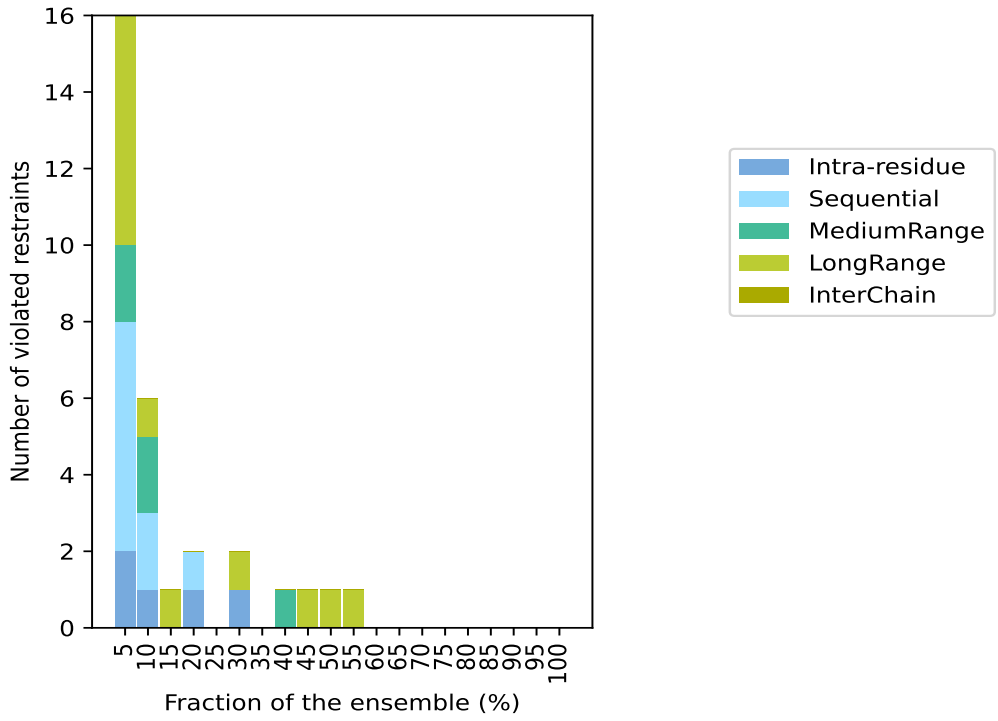
9.3 Distance violation statistics for the ensemble (i)

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, 1178(IR:176, SQ:473, MR:230, LR:299, 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]	%
2	6	2	6	0	16	1	5.0
1	2	2	1	0	6	2	10.0
0	0	0	1	0	1	3	15.0
1	1	0	0	0	2	4	20.0
0	0	0	0	0	0	5	25.0
1	0	0	1	0	2	6	30.0
0	0	0	0	0	0	7	35.0
0	0	1	0	0	1	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	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

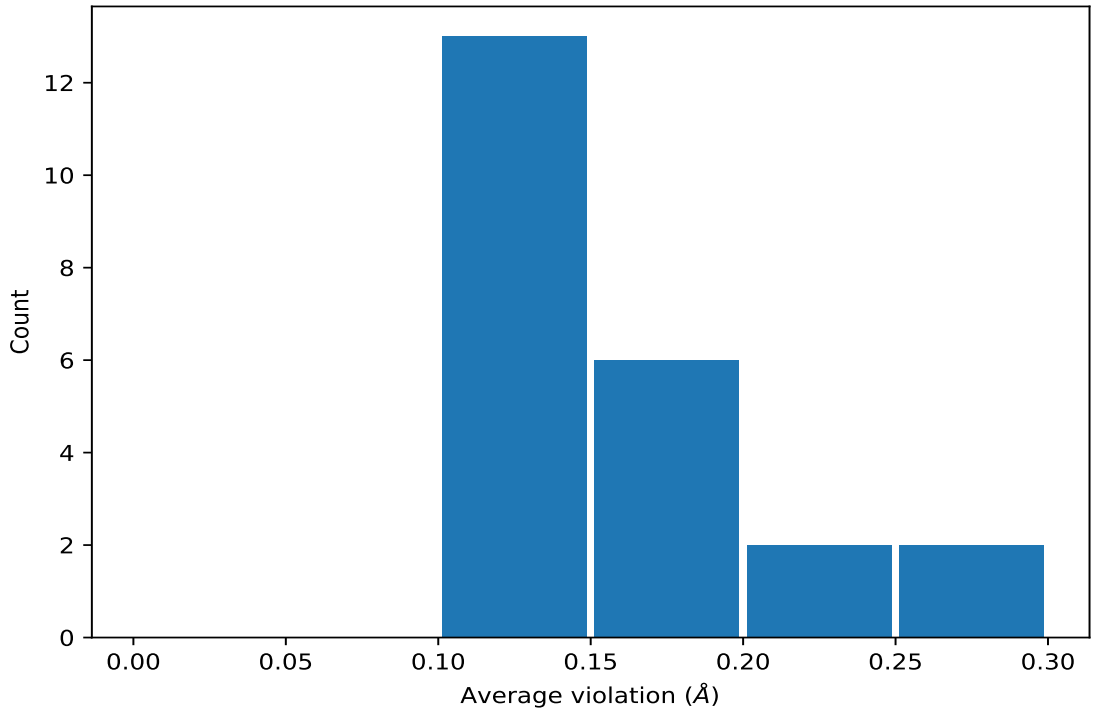
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	20	0.24	0.02	0.24
(2,10)	1:A:93:ILE:N	1:A:89:LEU:O	13	0.12	0.01	0.11
(1,1070)	1:A:96:ALA:H	1:A:53:TYR:H	11	0.13	0.02	0.12
(1,334)	1:A:30:VAL:H	1:A:50:VAL:HB	10	0.13	0.02	0.14
(1,481)	1:A:47:THR:H	1:A:31:THR:H	9	0.11	0.01	0.11
(1,1128)	1:A:100:LYS:H	1:A:97:GLU:HA	8	0.13	0.02	0.12
(2,7)	1:A:94:ARG:H	1:A:90:LEU:O	8	0.12	0.01	0.12
(1,270)	1:A:26:LYS:HB2	1:A:11:ASP:HB2	6	0.18	0.01	0.18
(1,270)	1:A:26:LYS:HB3	1:A:11:ASP:HB2	6	0.18	0.01	0.18
(1,64)	1:A:11:ASP:H	1:A:11:ASP:HB3	6	0.17	0.0	0.17
(2,1)	1:A:98:GLU:H	1:A:94:ARG:O	5	0.12	0.01	0.12
(1,383)	1:A:35:GLY:H	1:A:34:GLU:HA	4	0.2	0.0	0.2
(1,433)	1:A:40:SER:H	1:A:40:SER:HB2	4	0.12	0.0	0.12
(1,433)	1:A:40:SER:H	1:A:40:SER:HB3	4	0.12	0.0	0.12
(1,501)	1:A:48:VAL:H	1:A:31:THR:HB	3	0.14	0.03	0.13
(1,169)	1:A:17:THR:H	1:A:16:LYS:HG2	2	0.25	0.1	0.25

Continued on next page...

Continued from previous page...

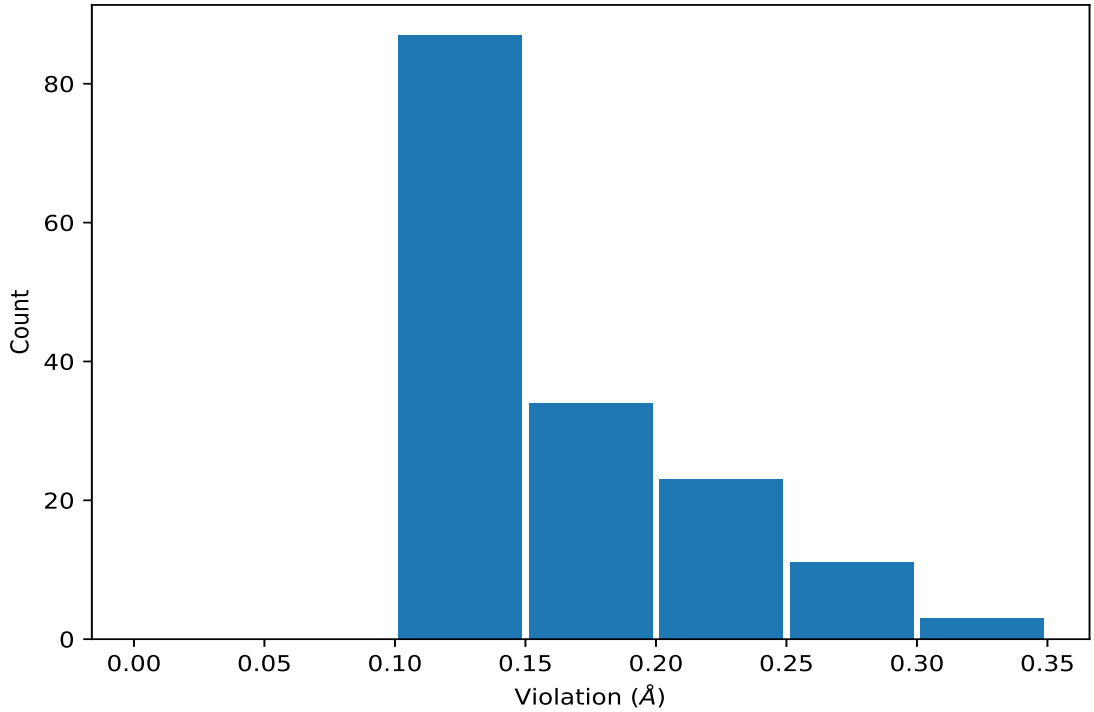
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,169)	1:A:17:THR:H	1:A:16:LYS:HG3	2	0.25	0.1	0.25
(1,1205)	1:A:110:THR:H	1:A:109:PRO:HA	2	0.18	0.0	0.18
(1,855)	1:A:79:SER:H	1:A:79:SER:HB2	2	0.16	0.0	0.16
(1,855)	1:A:79:SER:H	1:A:79:SER:HB3	2	0.16	0.0	0.16
(1,908)	1:A:85:ALA:H	1:A:83:VAL:H	2	0.14	0.01	0.14
(1,206)	1:A:22:TRP:H	1:A:20:ASN:HB3	2	0.12	0.0	0.12
(1,266)	1:A:26:LYS:H	1:A:51:LEU:H	2	0.12	0.0	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)
(1,19)	1:A:6:VAL:H	1:A:5:ARG:HD3	16	0.35
(1,169)	1:A:17:THR:H	1:A:16:LYS:HG2	4	0.35
(1,169)	1:A:17:THR:H	1:A:16:LYS:HG3	4	0.35
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	8	0.28
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	19	0.28
(1,13)	1:A:5:ARG:H	1:A:4:GLU:HB2	19	0.27
(1,13)	1:A:5:ARG:H	1:A:4:GLU:HB3	19	0.27
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	4	0.26
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	5	0.26
(1,17)	1:A:6:VAL:H	1:A:5:ARG:HA	10	0.26
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	10	0.25
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	13	0.25
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	18	0.25
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	20	0.25
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	2	0.24
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	11	0.24
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	16	0.24
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	1	0.23
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	7	0.23
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	15	0.23
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	17	0.23
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	3	0.22
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	6	0.22
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	9	0.22
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	12	0.22
(2,4)	1:A:97:GLU:N	1:A:93:ILE:O	14	0.22
(1,343)	1:A:31:THR:H	1:A:31:THR:HG21	3	0.22
(1,343)	1:A:31:THR:H	1:A:31:THR:HG22	3	0.22
(1,343)	1:A:31:THR:H	1:A:31:THR:HG23	3	0.22
(1,383)	1:A:35:GLY:H	1:A:34:GLU:HA	10	0.21
(1,383)	1:A:35:GLY:H	1:A:34:GLU:HA	2	0.2
(1,383)	1:A:35:GLY:H	1:A:34:GLU:HA	13	0.2
(1,383)	1:A:35:GLY:H	1:A:34:GLU:HA	19	0.2
(1,270)	1:A:26:LYS:HB2	1:A:11:ASP:HB2	5	0.2
(1,270)	1:A:26:LYS:HB3	1:A:11:ASP:HB2	5	0.2
(1,150)	1:A:16:LYS:H	1:A:16:LYS:HE2	4	0.2
(1,150)	1:A:16:LYS:H	1:A:16:LYS:HE3	4	0.2
(1,270)	1:A:26:LYS:HB2	1:A:11:ASP:HB2	18	0.19
(1,270)	1:A:26:LYS:HB3	1:A:11:ASP:HB2	18	0.19
(1,501)	1:A:48:VAL:H	1:A:31:THR:HB	3	0.18
(1,270)	1:A:26:LYS:HB2	1:A:11:ASP:HB2	17	0.18
(1,270)	1:A:26:LYS:HB3	1:A:11:ASP:HB2	17	0.18
(1,1205)	1:A:110:THR:H	1:A:109:PRO:HA	6	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1205)	1:A:110:THR:H	1:A:109:PRO:HA	14	0.18
(1,64)	1:A:11:ASP:H	1:A:11:ASP:HB3	5	0.17
(1,64)	1:A:11:ASP:H	1:A:11:ASP:HB3	7	0.17
(1,64)	1:A:11:ASP:H	1:A:11:ASP:HB3	12	0.17
(1,64)	1:A:11:ASP:H	1:A:11:ASP:HB3	13	0.17
(1,64)	1:A:11:ASP:H	1:A:11:ASP:HB3	17	0.17
(1,64)	1:A:11:ASP:H	1:A:11:ASP:HB3	18	0.17
(1,541)	1:A:50:VAL:H	1:A:63:LYS:HB2	17	0.17
(1,541)	1:A:50:VAL:H	1:A:63:LYS:HB3	17	0.17
(1,270)	1:A:26:LYS:HB2	1:A:11:ASP:HB2	7	0.17
(1,270)	1:A:26:LYS:HB3	1:A:11:ASP:HB2	7	0.17
(1,270)	1:A:26:LYS:HB2	1:A:11:ASP:HB2	12	0.17
(1,270)	1:A:26:LYS:HB3	1:A:11:ASP:HB2	12	0.17
(1,270)	1:A:26:LYS:HB2	1:A:11:ASP:HB2	13	0.17
(1,270)	1:A:26:LYS:HB3	1:A:11:ASP:HB2	13	0.17
(1,1070)	1:A:96:ALA:H	1:A:53:TYR:H	9	0.17
(1,855)	1:A:79:SER:H	1:A:79:SER:HB2	14	0.16
(1,855)	1:A:79:SER:H	1:A:79:SER:HB3	14	0.16
(1,855)	1:A:79:SER:H	1:A:79:SER:HB2	18	0.16
(1,855)	1:A:79:SER:H	1:A:79:SER:HB3	18	0.16
(1,334)	1:A:30:VAL:H	1:A:50:VAL:HB	7	0.16
(1,1128)	1:A:100:LYS:H	1:A:97:GLU:HA	12	0.16
(2,7)	1:A:94:ARG:H	1:A:90:LEU:O	8	0.15
(1,908)	1:A:85:ALA:H	1:A:83:VAL:H	11	0.15
(1,334)	1:A:30:VAL:H	1:A:50:VAL:HB	12	0.15
(1,169)	1:A:17:THR:H	1:A:16:LYS:HG2	11	0.15
(1,169)	1:A:17:THR:H	1:A:16:LYS:HG3	11	0.15
(1,1070)	1:A:96:ALA:H	1:A:53:TYR:H	7	0.15
(1,360)	1:A:32:GLY:HA2	1:A:31:THR:HG21	3	0.14
(1,360)	1:A:32:GLY:HA2	1:A:31:THR:HG22	3	0.14
(1,360)	1:A:32:GLY:HA2	1:A:31:THR:HG23	3	0.14
(1,334)	1:A:30:VAL:H	1:A:50:VAL:HB	13	0.14
(1,334)	1:A:30:VAL:H	1:A:50:VAL:HB	17	0.14
(1,334)	1:A:30:VAL:H	1:A:50:VAL:HB	18	0.14
(1,1128)	1:A:100:LYS:H	1:A:97:GLU:HA	7	0.14
(1,1128)	1:A:100:LYS:H	1:A:97:GLU:HA	15	0.14
(2,7)	1:A:94:ARG:H	1:A:90:LEU:O	9	0.13
(2,7)	1:A:94:ARG:H	1:A:90:LEU:O	10	0.13
(2,10)	1:A:93:ILE:N	1:A:89:LEU:O	8	0.13
(2,10)	1:A:93:ILE:N	1:A:89:LEU:O	19	0.13
(2,1)	1:A:98:GLU:H	1:A:94:ARG:O	9	0.13
(1,908)	1:A:85:ALA:H	1:A:83:VAL:H	19	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:A:48:VAL:H	1:A:31:THR:HB	12	0.13
(1,481)	1:A:47:THR:H	1:A:31:THR:H	18	0.13
(1,433)	1:A:40:SER:H	1:A:40:SER:HB2	14	0.13
(1,433)	1:A:40:SER:H	1:A:40:SER:HB3	14	0.13
(1,334)	1:A:30:VAL:H	1:A:50:VAL:HB	5	0.13
(1,334)	1:A:30:VAL:H	1:A:50:VAL:HB	16	0.13
(1,236)	1:A:24:PRO:HA	1:A:14:TRP:HA	11	0.13
(1,193)	1:A:18:GLY:H	1:A:22:TRP:HB2	15	0.13
(1,193)	1:A:18:GLY:H	1:A:22:TRP:HB3	15	0.13
(1,179)	1:A:17:THR:H	1:A:23:TRP:HB2	9	0.13
(1,179)	1:A:17:THR:H	1:A:23:TRP:HB3	9	0.13
(1,1128)	1:A:100:LYS:H	1:A:97:GLU:HA	2	0.13
(1,1070)	1:A:96:ALA:H	1:A:53:TYR:H	2	0.13
(1,1070)	1:A:96:ALA:H	1:A:53:TYR:H	16	0.13
(2,7)	1:A:94:ARG:H	1:A:90:LEU:O	16	0.12
(2,7)	1:A:94:ARG:H	1:A:90:LEU:O	20	0.12
(2,10)	1:A:93:ILE:N	1:A:89:LEU:O	10	0.12
(2,10)	1:A:93:ILE:N	1:A:89:LEU:O	11	0.12
(2,10)	1:A:93:ILE:N	1:A:89:LEU:O	20	0.12
(2,1)	1:A:98:GLU:H	1:A:94:ARG:O	16	0.12
(2,1)	1:A:98:GLU:H	1:A:94:ARG:O	19	0.12
(1,501)	1:A:48:VAL:H	1:A:31:THR:HB	16	0.12
(1,481)	1:A:47:THR:H	1:A:31:THR:H	20	0.12
(1,433)	1:A:40:SER:H	1:A:40:SER:HB2	1	0.12
(1,433)	1:A:40:SER:H	1:A:40:SER:HB3	1	0.12
(1,433)	1:A:40:SER:H	1:A:40:SER:HB2	7	0.12
(1,433)	1:A:40:SER:H	1:A:40:SER:HB3	7	0.12
(1,433)	1:A:40:SER:H	1:A:40:SER:HB2	12	0.12
(1,433)	1:A:40:SER:H	1:A:40:SER:HB3	12	0.12
(1,334)	1:A:30:VAL:H	1:A:50:VAL:HB	2	0.12
(1,266)	1:A:26:LYS:H	1:A:51:LEU:H	11	0.12
(1,217)	1:A:22:TRP:HA	1:A:15:LEU:HB2	17	0.12
(1,206)	1:A:22:TRP:H	1:A:20:ASN:HB3	5	0.12
(1,206)	1:A:22:TRP:H	1:A:20:ASN:HB3	18	0.12
(1,1128)	1:A:100:LYS:H	1:A:97:GLU:HA	3	0.12
(1,1128)	1:A:100:LYS:H	1:A:97:GLU:HA	14	0.12
(1,1070)	1:A:96:ALA:H	1:A:53:TYR:H	3	0.12
(1,1070)	1:A:96:ALA:H	1:A:53:TYR:H	6	0.12
(1,1070)	1:A:96:ALA:H	1:A:53:TYR:H	11	0.12
(2,7)	1:A:94:ARG:H	1:A:90:LEU:O	1	0.11
(2,7)	1:A:94:ARG:H	1:A:90:LEU:O	2	0.11
(2,7)	1:A:94:ARG:H	1:A:90:LEU:O	11	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,10)	1:A:93:ILE:N	1:A:89:LEU:O	1	0.11
(2,10)	1:A:93:ILE:N	1:A:89:LEU:O	2	0.11
(2,10)	1:A:93:ILE:N	1:A:89:LEU:O	3	0.11
(2,10)	1:A:93:ILE:N	1:A:89:LEU:O	4	0.11
(2,10)	1:A:93:ILE:N	1:A:89:LEU:O	5	0.11
(2,10)	1:A:93:ILE:N	1:A:89:LEU:O	13	0.11
(2,10)	1:A:93:ILE:N	1:A:89:LEU:O	17	0.11
(2,10)	1:A:93:ILE:N	1:A:89:LEU:O	18	0.11
(2,1)	1:A:98:GLU:H	1:A:94:ARG:O	2	0.11
(2,1)	1:A:98:GLU:H	1:A:94:ARG:O	10	0.11
(1,833)	1:A:74:PHE:H	1:A:75:PHE:HA	7	0.11
(1,517)	1:A:49:THR:H	1:A:30:VAL:HA	3	0.11
(1,481)	1:A:47:THR:H	1:A:31:THR:H	4	0.11
(1,481)	1:A:47:THR:H	1:A:31:THR:H	7	0.11
(1,481)	1:A:47:THR:H	1:A:31:THR:H	8	0.11
(1,481)	1:A:47:THR:H	1:A:31:THR:H	9	0.11
(1,481)	1:A:47:THR:H	1:A:31:THR:H	11	0.11
(1,481)	1:A:47:THR:H	1:A:31:THR:H	15	0.11
(1,481)	1:A:47:THR:H	1:A:31:THR:H	19	0.11
(1,334)	1:A:30:VAL:H	1:A:50:VAL:HB	19	0.11
(1,334)	1:A:30:VAL:H	1:A:50:VAL:HB	20	0.11
(1,268)	1:A:26:LYS:H	1:A:52:THR:HB	8	0.11
(1,266)	1:A:26:LYS:H	1:A:51:LEU:H	3	0.11
(1,161)	1:A:16:LYS:HE2	1:A:20:ASN:HA	4	0.11
(1,1128)	1:A:100:LYS:H	1:A:97:GLU:HA	8	0.11
(1,1128)	1:A:100:LYS:H	1:A:97:GLU:HA	9	0.11
(1,1126)	1:A:99:ASP:HA	1:A:100:LYS:HE2	15	0.11
(1,1070)	1:A:96:ALA:H	1:A:53:TYR:H	4	0.11
(1,1070)	1:A:96:ALA:H	1:A:53:TYR:H	14	0.11
(1,1070)	1:A:96:ALA:H	1:A:53:TYR:H	18	0.11
(1,1070)	1:A:96:ALA:H	1:A:53:TYR:H	20	0.11

10 Dihedral-angle violation analysis (i)

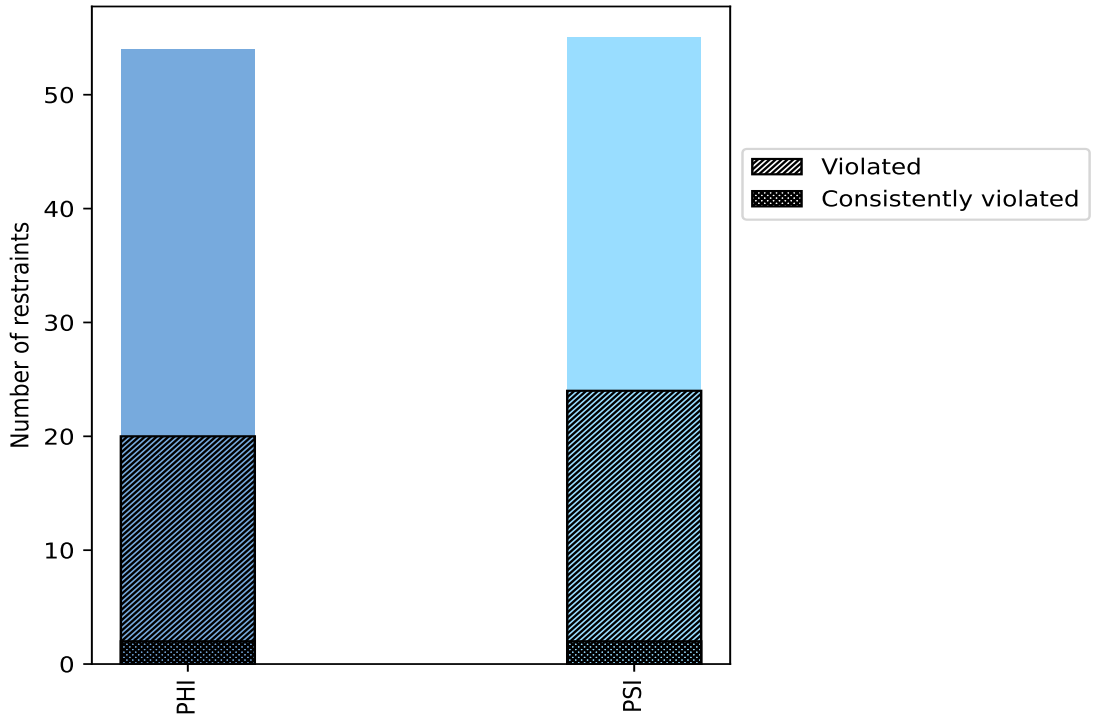
10.1 Summary of dihedral-angle violations (i)

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	54	49.5	20	37.0	18.3	2	3.7	1.8
PSI	55	50.5	24	43.6	22.0	2	3.6	1.8
Total	109	100.0	44	40.4	40.4	4	3.7	3.7

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

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



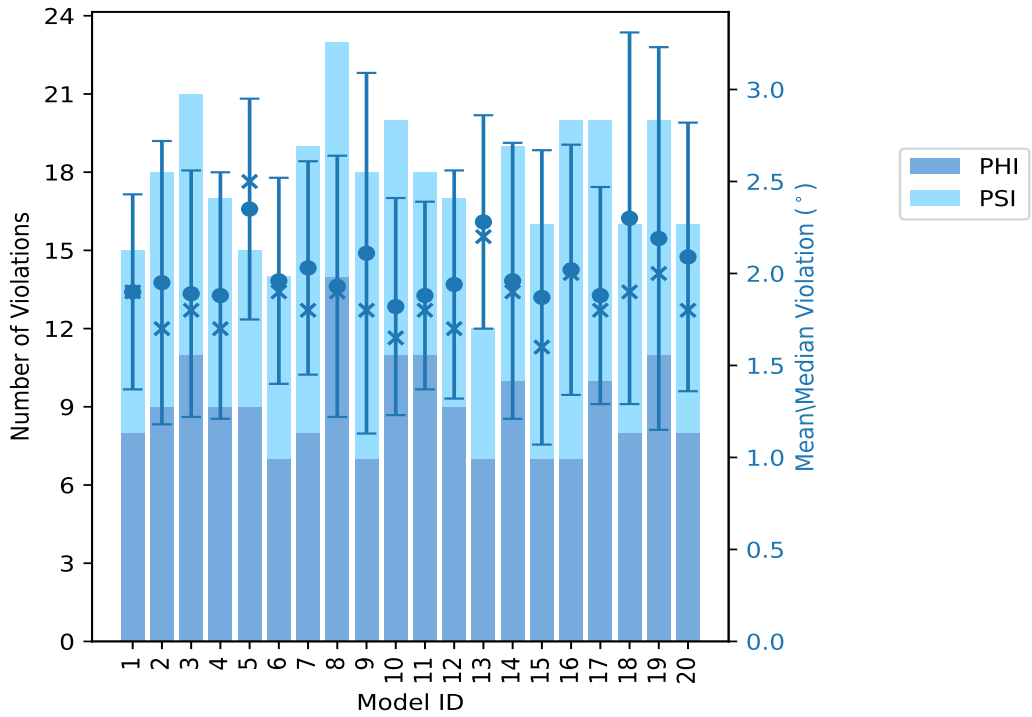
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	8	7	15	1.9	3.1	0.53	1.9
2	9	9	18	1.95	3.5	0.77	1.7
3	11	10	21	1.89	3.4	0.67	1.8
4	9	8	17	1.88	3.5	0.67	1.7
5	9	6	15	2.35	3.4	0.6	2.5
6	7	7	14	1.96	3.2	0.56	1.9
7	8	11	19	2.03	3.3	0.58	1.8
8	14	9	23	1.93	3.8	0.71	1.9
9	7	11	18	2.11	4.6	0.98	1.8
10	11	9	20	1.82	3.1	0.59	1.65
11	11	7	18	1.88	3.1	0.51	1.8
12	9	8	17	1.94	3.3	0.62	1.7
13	7	5	12	2.28	3.3	0.58	2.2
14	10	9	19	1.96	3.9	0.75	1.9
15	7	9	16	1.87	4.0	0.8	1.6
16	7	13	20	2.02	3.5	0.68	2.0
17	10	10	20	1.88	3.4	0.59	1.8
18	8	8	16	2.3	4.5	1.01	1.9
19	11	9	20	2.19	5.0	1.04	2.0
20	8	8	16	2.09	3.8	0.73	1.8

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



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

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

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

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

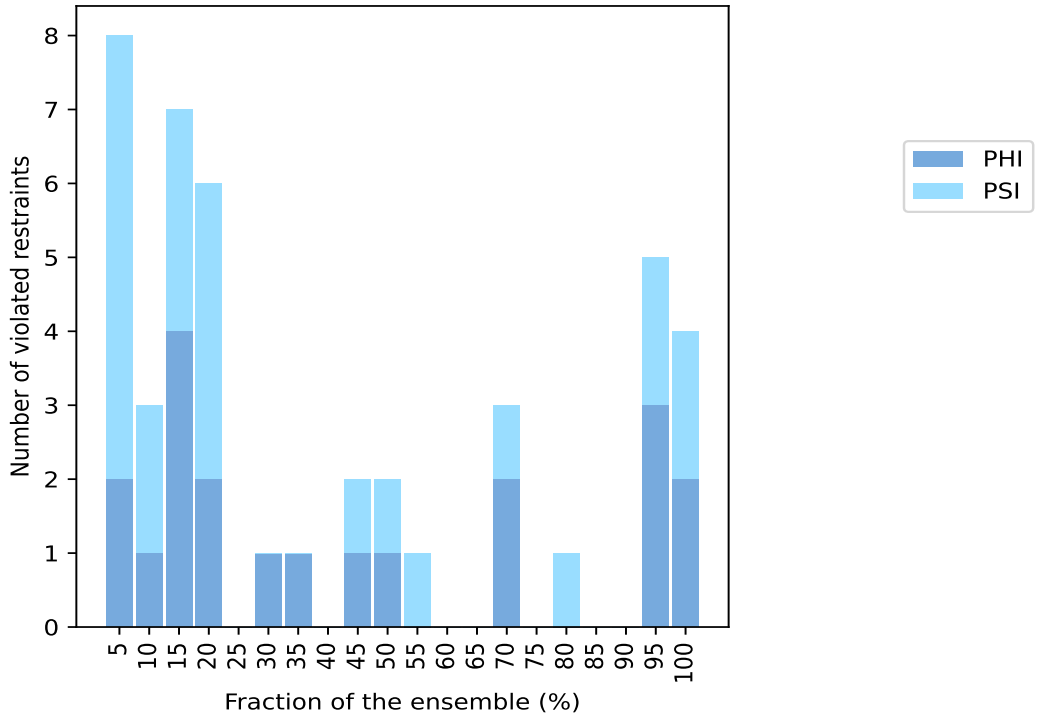
Continued on next page...

Continued from previous page...

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
2	1	3	14	70.0
0	0	0	15	75.0
0	1	1	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
3	2	5	19	95.0
2	2	4	20	100.0

[1] Number of models with violations

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

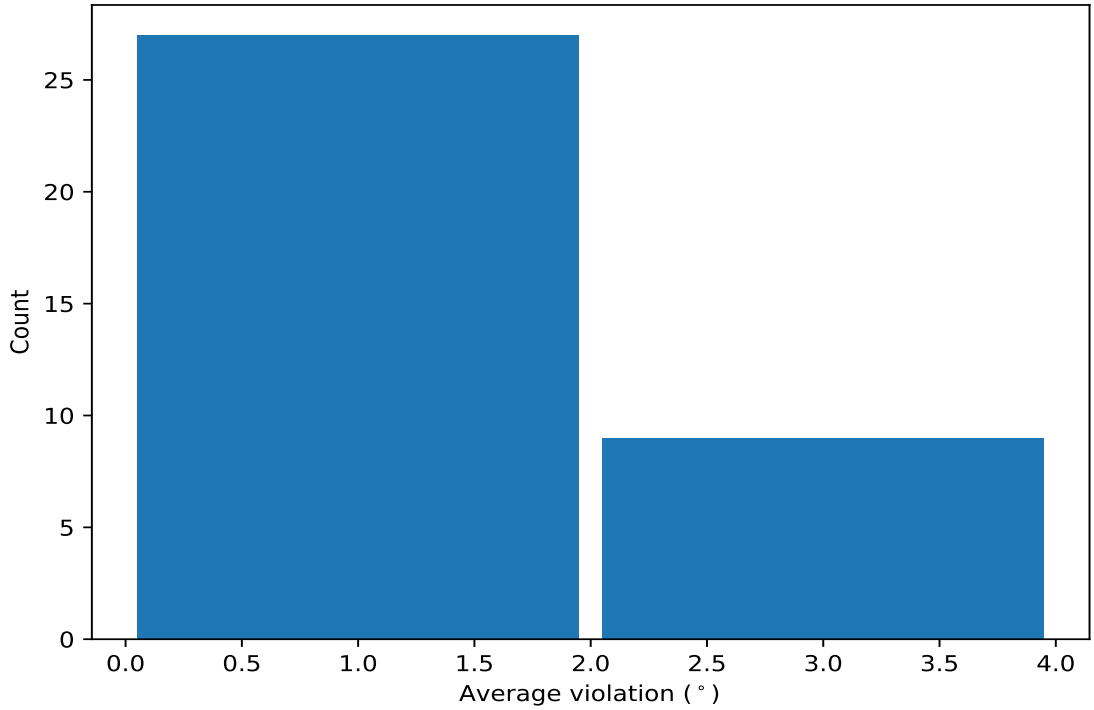


10.4 Most violated dihedral-angle restraints in the ensemble (i)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	20	3.25	0.82	3.2
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	20	3.15	0.3	3.1
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	20	2.85	0.36	2.8
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	20	2.07	0.46	1.9
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	19	2.67	0.76	2.4
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	19	2.07	0.07	2.1
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	19	1.99	0.65	1.7
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	19	1.88	0.27	1.8
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	19	1.77	0.24	1.9
(1,95)	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	1:A:94:ARG:N	16	1.56	0.24	1.55
(1,11)	1:A:11:ASP:C	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	14	1.87	0.32	1.85
(1,29)	1:A:25:ALA:N	1:A:25:ALA:CA	1:A:25:ALA:C	1:A:26:LYS:N	14	1.81	0.42	1.65
(1,9)	1:A:9:ILE:C	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	14	1.51	0.3	1.4
(1,33)	1:A:27:VAL:N	1:A:27:VAL:CA	1:A:27:VAL:C	1:A:28:THR:N	11	1.38	0.21	1.4
(1,70)	1:A:72:ILE:C	1:A:73:THR:N	1:A:73:THR:CA	1:A:73:THR:C	10	1.55	0.4	1.45
(1,27)	1:A:24:PRO:N	1:A:24:PRO:CA	1:A:24:PRO:C	1:A:25:ALA:N	10	1.46	0.19	1.45
(1,16)	1:A:14:TRP:N	1:A:14:TRP:CA	1:A:14:TRP:C	1:A:15:LEU:N	9	1.82	1.02	1.3
(1,42)	1:A:46:SER:C	1:A:47:THR:N	1:A:47:THR:CA	1:A:47:THR:C	9	1.28	0.17	1.2
(1,30)	1:A:25:ALA:C	1:A:26:LYS:N	1:A:26:LYS:CA	1:A:26:LYS:C	7	1.91	0.45	2.0
(1,82)	1:A:85:ALA:C	1:A:86:ASN:N	1:A:86:ASN:CA	1:A:86:ASN:C	6	1.43	0.14	1.5

Continued on next page...

Continued from previous page...

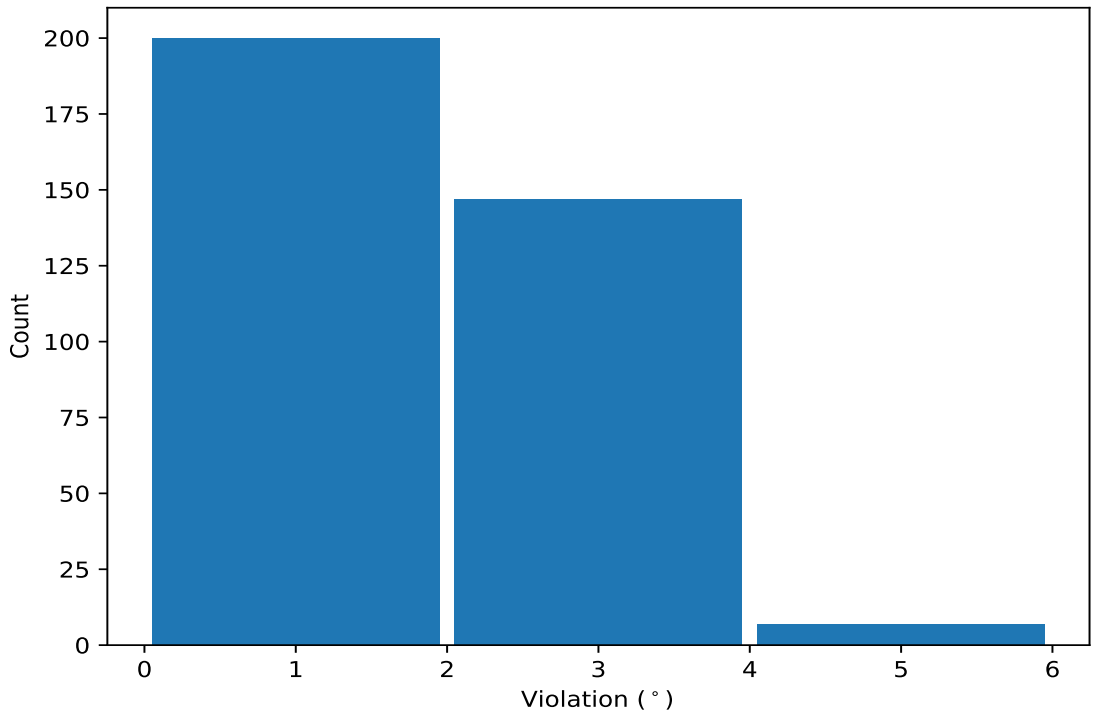
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,76)	1:A:80:GLU:C	1:A:81:LYS:N	1:A:81:LYS:CA	1:A:81:LYS:C	4	2.02	0.18	2.0
(1,14)	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	1:A:14:TRP:N	4	1.55	0.47	1.4
(1,71)	1:A:73:THR:N	1:A:73:THR:CA	1:A:73:THR:C	1:A:74:PHE:N	4	1.38	0.11	1.4
(1,69)	1:A:72:ILE:N	1:A:72:ILE:CA	1:A:72:ILE:C	1:A:73:THR:N	4	1.27	0.11	1.3
(1,77)	1:A:81:LYS:N	1:A:81:LYS:CA	1:A:81:LYS:C	1:A:82:ALA:N	4	1.2	0.12	1.15
(1,38)	1:A:41:SER:C	1:A:42:GLU:N	1:A:42:GLU:CA	1:A:42:GLU:C	4	1.15	0.05	1.15
(1,23)	1:A:21:THR:C	1:A:22:TRP:N	1:A:22:TRP:CA	1:A:22:TRP:C	3	2.17	0.41	2.1
(1,73)	1:A:78:SER:N	1:A:78:SER:CA	1:A:78:SER:C	1:A:79:SER:N	3	1.9	0.36	2.1
(1,35)	1:A:30:VAL:N	1:A:30:VAL:CA	1:A:30:VAL:C	1:A:31:THR:N	3	1.87	0.26	2.0
(1,15)	1:A:13:VAL:C	1:A:14:TRP:N	1:A:14:TRP:CA	1:A:14:TRP:C	3	1.77	0.48	2.0
(1,75)	1:A:80:GLU:N	1:A:80:GLU:CA	1:A:80:GLU:C	1:A:81:LYS:N	3	1.7	0.36	1.5
(1,74)	1:A:79:SER:C	1:A:80:GLU:N	1:A:80:GLU:CA	1:A:80:GLU:C	3	1.33	0.09	1.4
(1,94)	1:A:92:ALA:C	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	3	1.3	0.22	1.2
(1,22)	1:A:21:THR:N	1:A:21:THR:CA	1:A:21:THR:C	1:A:22:TRP:N	2	2.3	0.4	2.3
(1,20)	1:A:16:LYS:N	1:A:16:LYS:CA	1:A:16:LYS:C	1:A:17:THR:N	2	1.65	0.35	1.65
(1,50)	1:A:50:VAL:C	1:A:51:LEU:N	1:A:51:LEU:CA	1:A:51:LEU:C	2	1.6	0.3	1.6

[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 (°)
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	19	5.0
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	19	4.7
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	9	4.6
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	18	4.5
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	9	4.2
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	18	4.1
(1,16)	1:A:14:TRP:N	1:A:14:TRP:CA	1:A:14:TRP:C	1:A:15:LEU:N	15	4.0
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	14	3.9
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	20	3.8
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	8	3.8
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	2	3.5
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	4	3.5
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	16	3.5
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	3	3.4
(1,16)	1:A:14:TRP:N	1:A:14:TRP:CA	1:A:14:TRP:C	1:A:15:LEU:N	17	3.4
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	18	3.4
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	5	3.4
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	15	3.4
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	2	3.4
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	18	3.3
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	7	3.3
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	12	3.3
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	13	3.3
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	19	3.3
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	16	3.3
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	8	3.2
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	14	3.2
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	2	3.2
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	6	3.2
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	9	3.2
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	20	3.1
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	3	3.1
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	10	3.1
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1	3.1
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	8	3.1
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	11	3.1
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	18	3.1
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	19	3.1
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	4	3.0
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	16	3.0
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	5	3.0
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	7	3.0
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	10	3.0
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	13	3.0
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	20	3.0
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	7	3.0
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	9	3.0

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	5	2.9
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	12	2.9
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	3	2.9
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	14	2.9
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	17	2.9
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	20	2.9
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	13	2.8
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	2	2.8
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	16	2.8
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	6	2.8
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	10	2.8
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	11	2.8
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	14	2.8
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	4	2.7
(1,29)	1:A:25:ALA:N	1:A:25:ALA:CA	1:A:25:ALA:C	1:A:26:LYS:N	7	2.7
(1,23)	1:A:21:THR:C	1:A:22:TRP:N	1:A:22:TRP:CA	1:A:22:TRP:C	5	2.7
(1,22)	1:A:21:THR:N	1:A:21:THR:CA	1:A:21:THR:C	1:A:22:TRP:N	5	2.7
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	3	2.7
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	5	2.7
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	13	2.7
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	17	2.7
(1,30)	1:A:25:ALA:C	1:A:26:LYS:N	1:A:26:LYS:CA	1:A:26:LYS:C	5	2.6
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	1	2.6
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	8	2.6
(1,102)	1:A:98:GLU:C	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	12	2.6
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	6	2.6
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	13	2.5
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	16	2.5
(1,29)	1:A:25:ALA:N	1:A:25:ALA:CA	1:A:25:ALA:C	1:A:26:LYS:N	5	2.5
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	4	2.5
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	12	2.5
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	20	2.5
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	1	2.5
(1,70)	1:A:72:ILE:C	1:A:73:THR:N	1:A:73:THR:CA	1:A:73:THR:C	15	2.4
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	3	2.4
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	5	2.4
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	7	2.4
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	10	2.4
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	13	2.4
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	11	2.4
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	17	2.4
(1,11)	1:A:11:ASP:C	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	8	2.4
(1,11)	1:A:11:ASP:C	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	11	2.4
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	12	2.4
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	15	2.4
(1,76)	1:A:80:GLU:C	1:A:81:LYS:N	1:A:81:LYS:CA	1:A:81:LYS:C	8	2.3
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	2	2.3
(1,30)	1:A:25:ALA:C	1:A:26:LYS:N	1:A:26:LYS:CA	1:A:26:LYS:C	7	2.3
(1,14)	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	1:A:14:TRP:N	14	2.3
(1,10)	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1:A:11:ASP:N	4	2.3
(1,75)	1:A:80:GLU:N	1:A:80:GLU:CA	1:A:80:GLU:C	1:A:81:LYS:N	16	2.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,73)	1:A:78:SER:N	1:A:78:SER:CA	1:A:78:SER:C	1:A:79:SER:N	16	2.2
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	6	2.2
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	17	2.2
(1,29)	1:A:25:ALA:N	1:A:25:ALA:CA	1:A:25:ALA:C	1:A:26:LYS:N	12	2.2
(1,15)	1:A:13:VAL:C	1:A:14:TRP:N	1:A:14:TRP:CA	1:A:14:TRP:C	11	2.2
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	1	2.2
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	1	2.2
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	7	2.2
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	5	2.2
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	8	2.2
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	10	2.2
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	19	2.2
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	19	2.1
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	20	2.1
(1,73)	1:A:78:SER:N	1:A:78:SER:CA	1:A:78:SER:C	1:A:79:SER:N	9	2.1
(1,70)	1:A:72:ILE:C	1:A:73:THR:N	1:A:73:THR:CA	1:A:73:THR:C	19	2.1
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	7	2.1
(1,35)	1:A:30:VAL:N	1:A:30:VAL:CA	1:A:30:VAL:C	1:A:31:THR:N	3	2.1
(1,30)	1:A:25:ALA:C	1:A:26:LYS:N	1:A:26:LYS:CA	1:A:26:LYS:C	12	2.1
(1,29)	1:A:25:ALA:N	1:A:25:ALA:CA	1:A:25:ALA:C	1:A:26:LYS:N	16	2.1
(1,23)	1:A:21:THR:C	1:A:22:TRP:N	1:A:22:TRP:CA	1:A:22:TRP:C	17	2.1
(1,11)	1:A:11:ASP:C	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	2	2.1
(1,11)	1:A:11:ASP:C	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	19	2.1
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	2	2.1
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	3	2.1
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	5	2.1
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	8	2.1
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	9	2.1
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	10	2.1
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	15	2.1
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	16	2.1
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	18	2.1
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	19	2.1
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	11	2.1
(1,95)	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	1:A:94:ARG:N	9	2.0
(1,95)	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	1:A:94:ARG:N	19	2.0
(1,9)	1:A:9:ILE:C	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	2	2.0
(1,76)	1:A:80:GLU:C	1:A:81:LYS:N	1:A:81:LYS:CA	1:A:81:LYS:C	3	2.0
(1,76)	1:A:80:GLU:C	1:A:81:LYS:N	1:A:81:LYS:CA	1:A:81:LYS:C	14	2.0
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	19	2.0
(1,35)	1:A:30:VAL:N	1:A:30:VAL:CA	1:A:30:VAL:C	1:A:31:THR:N	16	2.0
(1,30)	1:A:25:ALA:C	1:A:26:LYS:N	1:A:26:LYS:CA	1:A:26:LYS:C	18	2.0
(1,29)	1:A:25:ALA:N	1:A:25:ALA:CA	1:A:25:ALA:C	1:A:26:LYS:N	8	2.0
(1,20)	1:A:16:LYS:N	1:A:16:LYS:CA	1:A:16:LYS:C	1:A:17:THR:N	9	2.0
(1,15)	1:A:13:VAL:C	1:A:14:TRP:N	1:A:14:TRP:CA	1:A:14:TRP:C	14	2.0
(1,11)	1:A:11:ASP:C	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	16	2.0
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	4	2.0
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	12	2.0
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	13	2.0
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	14	2.0
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	17	2.0

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	20	2.0
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	8	2.0
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	10	2.0
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	13	2.0
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	17	2.0
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	6	1.9
(1,9)	1:A:9:ILE:C	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	8	1.9
(1,9)	1:A:9:ILE:C	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	18	1.9
(1,50)	1:A:50:VAL:C	1:A:51:LEU:N	1:A:51:LEU:CA	1:A:51:LEU:C	17	1.9
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	1	1.9
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	9	1.9
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	14	1.9
(1,29)	1:A:25:ALA:N	1:A:25:ALA:CA	1:A:25:ALA:C	1:A:26:LYS:N	13	1.9
(1,22)	1:A:21:THR:N	1:A:21:THR:CA	1:A:21:THR:C	1:A:22:TRP:N	18	1.9
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	6	1.9
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	8	1.9
(1,11)	1:A:11:ASP:C	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	3	1.9
(1,11)	1:A:11:ASP:C	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	6	1.9
(1,109)	1:A:108:GLU:N	1:A:108:GLU:CA	1:A:108:GLU:C	1:A:109:PRO:N	6	1.9
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	1	1.9
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	3	1.9
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	5	1.9
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	7	1.9
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	13	1.9
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	17	1.9
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	20	1.9
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	1	1.9
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	14	1.9
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	3	1.8
(1,95)	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	1:A:94:ARG:N	16	1.8
(1,9)	1:A:9:ILE:C	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	7	1.8
(1,76)	1:A:80:GLU:C	1:A:81:LYS:N	1:A:81:LYS:CA	1:A:81:LYS:C	11	1.8
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	8	1.8
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	11	1.8
(1,27)	1:A:24:PRO:N	1:A:24:PRO:CA	1:A:24:PRO:C	1:A:25:ALA:N	6	1.8
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	11	1.8
(1,11)	1:A:11:ASP:C	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1	1.8
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	4	1.8
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	6	1.8
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	19	1.8
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	3	1.8
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	4	1.8
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	11	1.8
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	1	1.7
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	2	1.7
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	7	1.7
(1,95)	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	1:A:94:ARG:N	2	1.7
(1,95)	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	1:A:94:ARG:N	14	1.7
(1,93)	1:A:92:ALA:N	1:A:92:ALA:CA	1:A:92:ALA:C	1:A:93:ILE:N	8	1.7
(1,9)	1:A:9:ILE:C	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	19	1.7
(1,9)	1:A:9:ILE:C	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	20	1.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,70)	1:A:72:ILE:C	1:A:73:THR:N	1:A:73:THR:CA	1:A:73:THR:C	10	1.7
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	5	1.7
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	10	1.7
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	20	1.7
(1,42)	1:A:46:SER:C	1:A:47:THR:N	1:A:47:THR:CA	1:A:47:THR:C	7	1.7
(1,33)	1:A:27:VAL:N	1:A:27:VAL:CA	1:A:27:VAL:C	1:A:28:THR:N	9	1.7
(1,33)	1:A:27:VAL:N	1:A:27:VAL:CA	1:A:27:VAL:C	1:A:28:THR:N	18	1.7
(1,30)	1:A:25:ALA:C	1:A:26:LYS:N	1:A:26:LYS:CA	1:A:26:LYS:C	13	1.7
(1,29)	1:A:25:ALA:N	1:A:25:ALA:CA	1:A:25:ALA:C	1:A:26:LYS:N	18	1.7
(1,27)	1:A:24:PRO:N	1:A:24:PRO:CA	1:A:24:PRO:C	1:A:25:ALA:N	7	1.7
(1,23)	1:A:21:THR:C	1:A:22:TRP:N	1:A:22:TRP:CA	1:A:22:TRP:C	18	1.7
(1,13)	1:A:12:ARG:C	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	17	1.7
(1,11)	1:A:11:ASP:C	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	4	1.7
(1,11)	1:A:11:ASP:C	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	10	1.7
(1,11)	1:A:11:ASP:C	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	14	1.7
(1,11)	1:A:11:ASP:C	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	15	1.7
(1,11)	1:A:11:ASP:C	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	20	1.7
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	12	1.7
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	9	1.7
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	15	1.7
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	10	1.6
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	12	1.6
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	17	1.6
(1,95)	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	1:A:94:ARG:N	10	1.6
(1,95)	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	1:A:94:ARG:N	11	1.6
(1,95)	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	1:A:94:ARG:N	15	1.6
(1,94)	1:A:92:ALA:C	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	9	1.6
(1,82)	1:A:85:ALA:C	1:A:86:ASN:N	1:A:86:ASN:CA	1:A:86:ASN:C	11	1.6
(1,72)	1:A:77:PRO:C	1:A:78:SER:N	1:A:78:SER:CA	1:A:78:SER:C	19	1.6
(1,70)	1:A:72:ILE:C	1:A:73:THR:N	1:A:73:THR:CA	1:A:73:THR:C	20	1.6
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	4	1.6
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	15	1.6
(1,44)	1:A:47:THR:C	1:A:48:VAL:N	1:A:48:VAL:CA	1:A:48:VAL:C	18	1.6
(1,33)	1:A:27:VAL:N	1:A:27:VAL:CA	1:A:27:VAL:C	1:A:28:THR:N	20	1.6
(1,29)	1:A:25:ALA:N	1:A:25:ALA:CA	1:A:25:ALA:C	1:A:26:LYS:N	3	1.6
(1,27)	1:A:24:PRO:N	1:A:24:PRO:CA	1:A:24:PRO:C	1:A:25:ALA:N	17	1.6
(1,14)	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	1:A:14:TRP:N	11	1.6
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	9	1.6
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	16	1.6
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	2	1.6
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	12	1.6
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	16	1.6
(1,99)	1:A:97:GLU:N	1:A:97:GLU:CA	1:A:97:GLU:C	1:A:98:GLU:N	18	1.5
(1,95)	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	1:A:94:ARG:N	3	1.5
(1,95)	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	1:A:94:ARG:N	7	1.5
(1,95)	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	1:A:94:ARG:N	17	1.5
(1,82)	1:A:85:ALA:C	1:A:86:ASN:N	1:A:86:ASN:CA	1:A:86:ASN:C	4	1.5
(1,82)	1:A:85:ALA:C	1:A:86:ASN:N	1:A:86:ASN:CA	1:A:86:ASN:C	10	1.5
(1,82)	1:A:85:ALA:C	1:A:86:ASN:N	1:A:86:ASN:CA	1:A:86:ASN:C	12	1.5
(1,75)	1:A:80:GLU:N	1:A:80:GLU:CA	1:A:80:GLU:C	1:A:81:LYS:N	7	1.5
(1,71)	1:A:73:THR:N	1:A:73:THR:CA	1:A:73:THR:C	1:A:74:PHE:N	7	1.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,70)	1:A:72:ILE:C	1:A:73:THR:N	1:A:73:THR:CA	1:A:73:THR:C	17	1.5
(1,35)	1:A:30:VAL:N	1:A:30:VAL:CA	1:A:30:VAL:C	1:A:31:THR:N	12	1.5
(1,33)	1:A:27:VAL:N	1:A:27:VAL:CA	1:A:27:VAL:C	1:A:28:THR:N	19	1.5
(1,30)	1:A:25:ALA:C	1:A:26:LYS:N	1:A:26:LYS:CA	1:A:26:LYS:C	8	1.5
(1,29)	1:A:25:ALA:N	1:A:25:ALA:CA	1:A:25:ALA:C	1:A:26:LYS:N	1	1.5
(1,29)	1:A:25:ALA:N	1:A:25:ALA:CA	1:A:25:ALA:C	1:A:26:LYS:N	4	1.5
(1,29)	1:A:25:ALA:N	1:A:25:ALA:CA	1:A:25:ALA:C	1:A:26:LYS:N	17	1.5
(1,29)	1:A:25:ALA:N	1:A:25:ALA:CA	1:A:25:ALA:C	1:A:26:LYS:N	19	1.5
(1,27)	1:A:24:PRO:N	1:A:24:PRO:CA	1:A:24:PRO:C	1:A:25:ALA:N	1	1.5
(1,27)	1:A:24:PRO:N	1:A:24:PRO:CA	1:A:24:PRO:C	1:A:25:ALA:N	12	1.5
(1,16)	1:A:14:TRP:N	1:A:14:TRP:CA	1:A:14:TRP:C	1:A:15:LEU:N	11	1.5
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	14	1.5
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	6	1.5
(1,100)	1:A:97:GLU:C	1:A:98:GLU:N	1:A:98:GLU:CA	1:A:98:GLU:C	7	1.5
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	11	1.4
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	14	1.4
(1,95)	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	1:A:94:ARG:N	1	1.4
(1,95)	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	1:A:94:ARG:N	20	1.4
(1,9)	1:A:9:ILE:C	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	10	1.4
(1,9)	1:A:9:ILE:C	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	11	1.4
(1,9)	1:A:9:ILE:C	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	16	1.4
(1,77)	1:A:81:LYS:N	1:A:81:LYS:CA	1:A:81:LYS:C	1:A:82:ALA:N	16	1.4
(1,75)	1:A:80:GLU:N	1:A:80:GLU:CA	1:A:80:GLU:C	1:A:81:LYS:N	9	1.4
(1,74)	1:A:79:SER:C	1:A:80:GLU:N	1:A:80:GLU:CA	1:A:80:GLU:C	3	1.4
(1,74)	1:A:79:SER:C	1:A:80:GLU:N	1:A:80:GLU:CA	1:A:80:GLU:C	8	1.4
(1,73)	1:A:78:SER:N	1:A:78:SER:CA	1:A:78:SER:C	1:A:79:SER:N	7	1.4
(1,71)	1:A:73:THR:N	1:A:73:THR:CA	1:A:73:THR:C	1:A:74:PHE:N	9	1.4
(1,71)	1:A:73:THR:N	1:A:73:THR:CA	1:A:73:THR:C	1:A:74:PHE:N	16	1.4
(1,70)	1:A:72:ILE:C	1:A:73:THR:N	1:A:73:THR:CA	1:A:73:THR:C	8	1.4
(1,69)	1:A:72:ILE:N	1:A:72:ILE:CA	1:A:72:ILE:C	1:A:73:THR:N	15	1.4
(1,42)	1:A:46:SER:C	1:A:47:THR:N	1:A:47:THR:CA	1:A:47:THR:C	19	1.4
(1,33)	1:A:27:VAL:N	1:A:27:VAL:CA	1:A:27:VAL:C	1:A:28:THR:N	2	1.4
(1,33)	1:A:27:VAL:N	1:A:27:VAL:CA	1:A:27:VAL:C	1:A:28:THR:N	7	1.4
(1,29)	1:A:25:ALA:N	1:A:25:ALA:CA	1:A:25:ALA:C	1:A:26:LYS:N	6	1.4
(1,27)	1:A:24:PRO:N	1:A:24:PRO:CA	1:A:24:PRO:C	1:A:25:ALA:N	15	1.4
(1,16)	1:A:14:TRP:N	1:A:14:TRP:CA	1:A:14:TRP:C	1:A:15:LEU:N	20	1.4
(1,12)	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	1:A:13:VAL:N	15	1.4
(1,104)	1:A:102:SER:C	1:A:103:ASN:N	1:A:103:ASN:CA	1:A:103:ASN:C	8	1.4
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	2	1.4
(1,95)	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	1:A:94:ARG:N	6	1.3
(1,9)	1:A:9:ILE:C	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	12	1.3
(1,9)	1:A:9:ILE:C	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	14	1.3
(1,82)	1:A:85:ALA:C	1:A:86:ASN:N	1:A:86:ASN:CA	1:A:86:ASN:C	5	1.3
(1,79)	1:A:82:ALA:N	1:A:82:ALA:CA	1:A:82:ALA:C	1:A:83:VAL:N	15	1.3
(1,69)	1:A:72:ILE:N	1:A:72:ILE:CA	1:A:72:ILE:C	1:A:73:THR:N	10	1.3
(1,69)	1:A:72:ILE:N	1:A:72:ILE:CA	1:A:72:ILE:C	1:A:73:THR:N	19	1.3
(1,50)	1:A:50:VAL:C	1:A:51:LEU:N	1:A:51:LEU:CA	1:A:51:LEU:C	3	1.3
(1,42)	1:A:46:SER:C	1:A:47:THR:N	1:A:47:THR:CA	1:A:47:THR:C	10	1.3
(1,33)	1:A:27:VAL:N	1:A:27:VAL:CA	1:A:27:VAL:C	1:A:28:THR:N	4	1.3
(1,29)	1:A:25:ALA:N	1:A:25:ALA:CA	1:A:25:ALA:C	1:A:26:LYS:N	2	1.3
(1,27)	1:A:24:PRO:N	1:A:24:PRO:CA	1:A:24:PRO:C	1:A:25:ALA:N	4	1.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,27)	1:A:24:PRO:N	1:A:24:PRO:CA	1:A:24:PRO:C	1:A:25:ALA:N	11	1.3
(1,27)	1:A:24:PRO:N	1:A:24:PRO:CA	1:A:24:PRO:C	1:A:25:ALA:N	16	1.3
(1,20)	1:A:16:LYS:N	1:A:16:LYS:CA	1:A:16:LYS:C	1:A:17:THR:N	17	1.3
(1,16)	1:A:14:TRP:N	1:A:14:TRP:CA	1:A:14:TRP:C	1:A:15:LEU:N	10	1.3
(1,16)	1:A:14:TRP:N	1:A:14:TRP:CA	1:A:14:TRP:C	1:A:15:LEU:N	19	1.3
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	16	1.2
(1,95)	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	1:A:94:ARG:N	4	1.2
(1,94)	1:A:92:ALA:C	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	8	1.2
(1,9)	1:A:9:ILE:C	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	6	1.2
(1,82)	1:A:85:ALA:C	1:A:86:ASN:N	1:A:86:ASN:CA	1:A:86:ASN:C	1	1.2
(1,77)	1:A:81:LYS:N	1:A:81:LYS:CA	1:A:81:LYS:C	1:A:82:ALA:N	14	1.2
(1,74)	1:A:79:SER:C	1:A:80:GLU:N	1:A:80:GLU:CA	1:A:80:GLU:C	14	1.2
(1,71)	1:A:73:THR:N	1:A:73:THR:CA	1:A:73:THR:C	1:A:74:PHE:N	15	1.2
(1,70)	1:A:72:ILE:C	1:A:73:THR:N	1:A:73:THR:CA	1:A:73:THR:C	2	1.2
(1,70)	1:A:72:ILE:C	1:A:73:THR:N	1:A:73:THR:CA	1:A:73:THR:C	4	1.2
(1,70)	1:A:72:ILE:C	1:A:73:THR:N	1:A:73:THR:CA	1:A:73:THR:C	5	1.2
(1,70)	1:A:72:ILE:C	1:A:73:THR:N	1:A:73:THR:CA	1:A:73:THR:C	11	1.2
(1,42)	1:A:46:SER:C	1:A:47:THR:N	1:A:47:THR:CA	1:A:47:THR:C	3	1.2
(1,42)	1:A:46:SER:C	1:A:47:THR:N	1:A:47:THR:CA	1:A:47:THR:C	8	1.2
(1,42)	1:A:46:SER:C	1:A:47:THR:N	1:A:47:THR:CA	1:A:47:THR:C	15	1.2
(1,42)	1:A:46:SER:C	1:A:47:THR:N	1:A:47:THR:CA	1:A:47:THR:C	17	1.2
(1,42)	1:A:46:SER:C	1:A:47:THR:N	1:A:47:THR:CA	1:A:47:THR:C	18	1.2
(1,38)	1:A:41:SER:C	1:A:42:GLU:N	1:A:42:GLU:CA	1:A:42:GLU:C	10	1.2
(1,38)	1:A:41:SER:C	1:A:42:GLU:N	1:A:42:GLU:CA	1:A:42:GLU:C	13	1.2
(1,37)	1:A:41:SER:N	1:A:41:SER:CA	1:A:41:SER:C	1:A:42:GLU:N	10	1.2
(1,33)	1:A:27:VAL:N	1:A:27:VAL:CA	1:A:27:VAL:C	1:A:28:THR:N	8	1.2
(1,33)	1:A:27:VAL:N	1:A:27:VAL:CA	1:A:27:VAL:C	1:A:28:THR:N	10	1.2
(1,30)	1:A:25:ALA:C	1:A:26:LYS:N	1:A:26:LYS:CA	1:A:26:LYS:C	17	1.2
(1,27)	1:A:24:PRO:N	1:A:24:PRO:CA	1:A:24:PRO:C	1:A:25:ALA:N	3	1.2
(1,16)	1:A:14:TRP:N	1:A:14:TRP:CA	1:A:14:TRP:C	1:A:15:LEU:N	9	1.2
(1,16)	1:A:14:TRP:N	1:A:14:TRP:CA	1:A:14:TRP:C	1:A:15:LEU:N	14	1.2
(1,14)	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	1:A:14:TRP:N	2	1.2
(1,96)	1:A:93:ILE:C	1:A:94:ARG:N	1:A:94:ARG:CA	1:A:94:ARG:C	15	1.1
(1,95)	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	1:A:94:ARG:N	12	1.1
(1,94)	1:A:92:ALA:C	1:A:93:ILE:N	1:A:93:ILE:CA	1:A:93:ILE:C	19	1.1
(1,9)	1:A:9:ILE:C	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	1	1.1
(1,9)	1:A:9:ILE:C	1:A:10:ASN:N	1:A:10:ASN:CA	1:A:10:ASN:C	3	1.1
(1,89)	1:A:90:LEU:N	1:A:90:LEU:CA	1:A:90:LEU:C	1:A:91:GLN:N	8	1.1
(1,77)	1:A:81:LYS:N	1:A:81:LYS:CA	1:A:81:LYS:C	1:A:82:ALA:N	3	1.1
(1,77)	1:A:81:LYS:N	1:A:81:LYS:CA	1:A:81:LYS:C	1:A:82:ALA:N	8	1.1
(1,69)	1:A:72:ILE:N	1:A:72:ILE:CA	1:A:72:ILE:C	1:A:73:THR:N	20	1.1
(1,49)	1:A:50:VAL:N	1:A:50:VAL:CA	1:A:50:VAL:C	1:A:51:LEU:N	17	1.1
(1,42)	1:A:46:SER:C	1:A:47:THR:N	1:A:47:THR:CA	1:A:47:THR:C	9	1.1
(1,38)	1:A:41:SER:C	1:A:42:GLU:N	1:A:42:GLU:CA	1:A:42:GLU:C	2	1.1
(1,38)	1:A:41:SER:C	1:A:42:GLU:N	1:A:42:GLU:CA	1:A:42:GLU:C	12	1.1
(1,33)	1:A:27:VAL:N	1:A:27:VAL:CA	1:A:27:VAL:C	1:A:28:THR:N	14	1.1
(1,33)	1:A:27:VAL:N	1:A:27:VAL:CA	1:A:27:VAL:C	1:A:28:THR:N	16	1.1
(1,16)	1:A:14:TRP:N	1:A:14:TRP:CA	1:A:14:TRP:C	1:A:15:LEU:N	2	1.1
(1,15)	1:A:13:VAL:C	1:A:14:TRP:N	1:A:14:TRP:CA	1:A:14:TRP:C	4	1.1
(1,14)	1:A:13:VAL:N	1:A:13:VAL:CA	1:A:13:VAL:C	1:A:14:TRP:N	3	1.1
(1,11)	1:A:11:ASP:C	1:A:12:ARG:N	1:A:12:ARG:CA	1:A:12:ARG:C	9	1.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,103)	1:A:99:ASP:N	1:A:99:ASP:CA	1:A:99:ASP:C	1:A:100:LYS:N	18	1.1