Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 05:49 AM EDT

PDB ID	:	2MHS
BMRB ID	:	19654
Title	:	NMR Structure of human Mcl-1
Authors	:	Liu, G.; Poppe, L.; Aoki, K.; Yamane, H.; Lewis, J.; Szyperski, T.
Deposited on	:	2013-12-04

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:

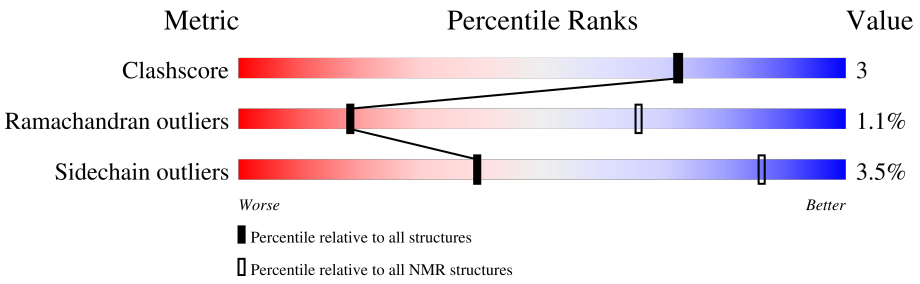
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 84%.

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	164	77% 5% 18%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 10 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:3-A:23, A:34-A:85, A:92-A:152 (134)	0.61	10

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

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

The models can be grouped into 6 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2651 atoms, of which 1323 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Induced myeloid leukemia cell differentiation protein Mcl-1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	164	2651	829	1323	249	246	4	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q07820
A	117	SER	CYS	engineered mutation	UNP Q07820
A	159	HIS	-	expression tag	UNP Q07820
A	160	HIS	-	expression tag	UNP Q07820
A	161	HIS	-	expression tag	UNP Q07820
A	162	HIS	-	expression tag	UNP Q07820
A	163	HIS	-	expression tag	UNP Q07820
A	164	HIS	-	expression tag	UNP Q07820

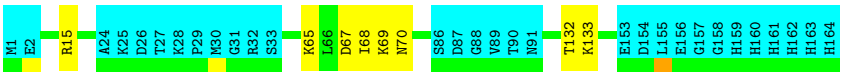
4 Residue-property plots (i)

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: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain A: 77% 5% 18%



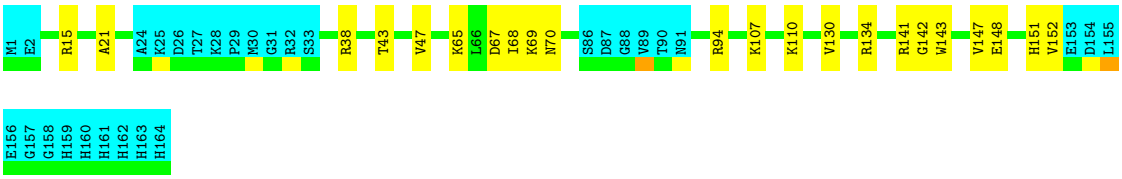
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

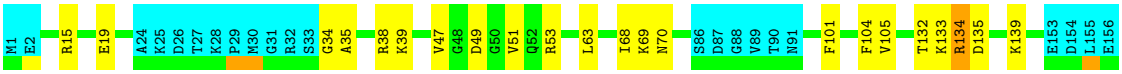
Chain A: 68% 13% 18%

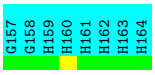


4.2.2 Score per residue for model 2

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain A: 68% 13% • 18%





4.2.3 Score per residue for model 3

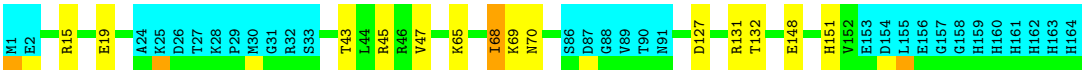
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain A:

4.2.4 Score per residue for model 4

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

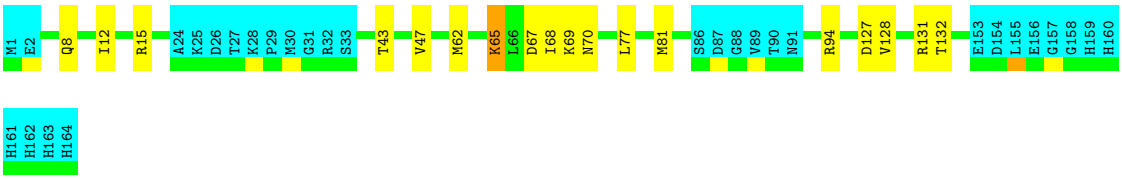
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

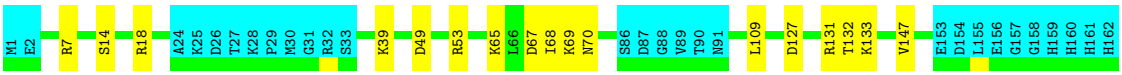
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

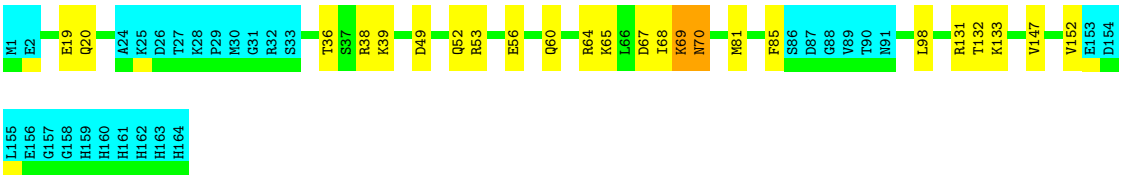
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

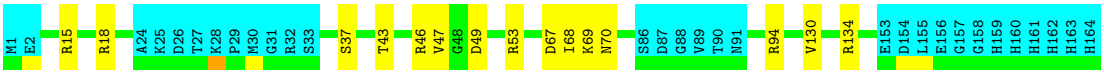
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

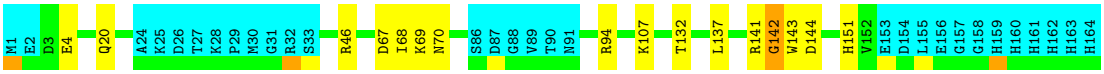
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain A:



4.2.10 Score per residue for model 10 (medoid)

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain A:

4.2.11 Score per residue for model 11

- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain A: 70% 10% • 18%

M1 E2 R15 E19 A24 K25 D26 T27 K28 P29 M30 G31 R32 S33 S37 Q60 R64 K65 I68 K69 N70 E71 K75 F85 S86 D87 G88 V89 T90 N91 L98 D127 V128 L129 V130 R131 T132 K133 R134 D135 K139 E153 D154 L155 E156 G157 G158

H159 H160 H161 H162 H163 H164

4.2.12 Score per residue for model 12

- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain A: 71% 11% 18%

M1 E2 A24 K25 D26 T27 K28 P29 M30 G31 R32 S33 G34 A35 K39 A40 L41 H55 E56 F59 D67 I68 K69 N70 L77 M81 V84 F85 S86 D87 G88 V89 T90 N91 R94 F104 V105 L109 E148 E153 D154 L155 E156 G157 G158 H159 H160

H161 H162 H163 H164

4.2.13 Score per residue for model 13

- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain A: 66% 14% • 18%

M1 E2 R7 R15 E19 Q20 A24 K25 D26 T27 K28 P29 M30 G31 R32 S33 K39 T43 L44 R45 R46 V47 G48 D49 R53 M62 K65 L66 D67 I68 K69 N70 M81 F85 S86 D87 G88 V89 T90 N91 L98 H108 I112 D127

R131 T132 K133 E153 D154 L155 E156 G157 G158 H159 H160 H161 H162 H163 H164

4.2.14 Score per residue for model 14

- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain A: 68% 13% • 18%

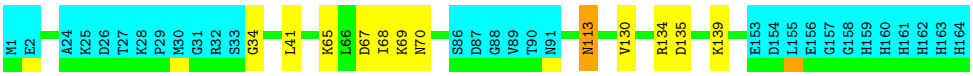
M1 E2 Q8 E11 S14 R15 R18 E19 Q20 A24 K25 D26 T27 K28 P29 M30 G31 R32 S33 S37 D49 R53 Q60 R64 D67 I68 K69 N70 S86 D87 G88 V89 T90 N91 R94 K107 E119 T132 K133 E148 F149 E153

D154 L155 E156 G157 G158 H159 H160 H161 H162 H163 H164

4.2.15 Score per residue for model 15

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

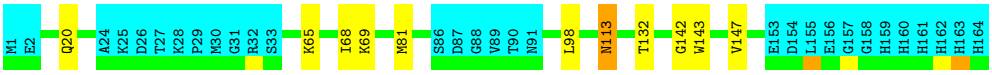
Chain A: 74% 7% • 18%



4.2.16 Score per residue for model 16

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

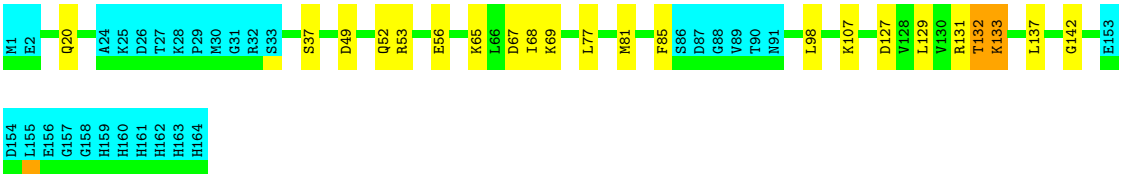
Chain A: 75% 6% • 18%



4.2.17 Score per residue for model 17

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

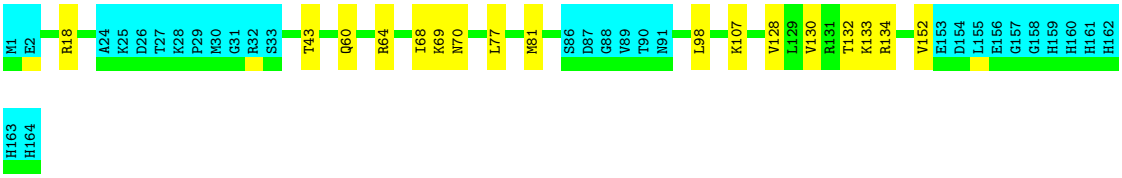
Chain A: 68% 12% • 18%



4.2.18 Score per residue for model 18

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

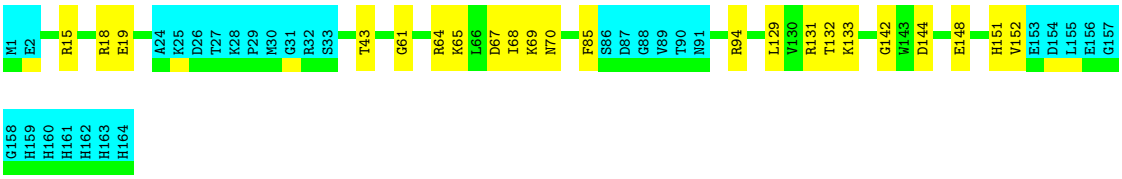
Chain A: 71% 10% 18%



4.2.19 Score per residue for model 19

- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

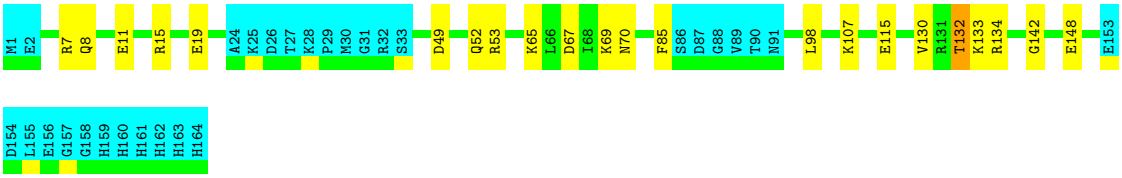
Chain A: 68% 13% 18%



4.2.20 Score per residue for model 20

- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain A: 68% 13% • 18%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry, molecular dynamics, simulated annealing, torsion angle 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**
AutoStructure	structure solution	
CYANA	structure solution	
CNS	structure solution	
CNS	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	1876
Number of shifts mapped to atoms	1876
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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	1094	1112	1108	7±2
All	All	21880	22240	22160	149

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:LYS:HB3	1:A:133:LYS:HZ2	0.68	1.49	17	1
1:A:94:ARG:HE	1:A:94:ARG:HA	0.58	1.59	8	3
1:A:132:THR:HG23	1:A:133:LYS:HD2	0.57	1.76	6	6
1:A:134:ARG:HG3	1:A:135:ASP:N	0.55	2.17	2	1
1:A:8:GLN:O	1:A:11:GLU:HG2	0.54	2.03	14	1
1:A:49:ASP:O	1:A:53:ARG:HG2	0.54	2.02	7	7
1:A:127:ASP:O	1:A:131:ARG:HB2	0.53	2.03	6	7
1:A:15:ARG:O	1:A:19:GLU:HG2	0.53	2.04	3	5
1:A:113:ASN:HD22	1:A:113:ASN:N	0.52	2.02	15	2
1:A:35:ALA:O	1:A:39:LYS:HG3	0.51	2.06	12	3
1:A:60:GLN:O	1:A:64:ARG:HG3	0.51	2.05	7	5
1:A:128:VAL:O	1:A:132:THR:HG22	0.50	2.06	18	2
1:A:81:MET:SD	1:A:98:LEU:HD11	0.50	2.46	16	1
1:A:7:ARG:O	1:A:11:GLU:HB2	0.50	2.06	20	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:MET:SD	1:A:98:LEU:CD1	0.50	3.00	16	1
1:A:56:GLU:HG3	1:A:104:PHE:CE1	0.49	2.43	12	1
1:A:20:GLN:HG3	1:A:107:LYS:HE2	0.49	1.85	14	1
1:A:36:THR:HA	1:A:39:LYS:NZ	0.48	2.23	7	1
1:A:43:THR:O	1:A:47:VAL:HG22	0.48	2.09	1	5
1:A:49:ASP:O	1:A:53:ARG:HG3	0.47	2.09	13	3
1:A:85:PHE:CZ	1:A:98:LEU:HD22	0.47	2.45	11	5
1:A:132:THR:HG23	1:A:133:LYS:HD3	0.47	1.84	11	1
1:A:130:VAL:O	1:A:134:ARG:HB2	0.47	2.09	1	5
1:A:132:THR:HG23	1:A:133:LYS:HG2	0.46	1.86	2	1
1:A:81:MET:SD	1:A:98:LEU:HD12	0.46	2.51	18	3
1:A:18:ARG:NH2	1:A:119:GLU:HG2	0.46	2.26	14	1
1:A:62:MET:O	1:A:65:LYS:HG3	0.46	2.11	5	2
1:A:77:LEU:O	1:A:81:MET:HG2	0.46	2.10	18	5
1:A:39:LYS:HG3	1:A:147:VAL:HG21	0.45	1.87	7	2
1:A:105:VAL:O	1:A:109:LEU:HG	0.45	2.10	12	1
1:A:132:THR:OG1	1:A:133:LYS:HD3	0.45	2.12	19	1
1:A:43:THR:HA	1:A:46:ARG:NE	0.45	2.27	8	1
1:A:55:HIS:HB3	1:A:59:PHE:CE2	0.45	2.47	12	1
1:A:68:ILE:HD12	1:A:68:ILE:N	0.45	2.27	10	12
1:A:52:GLN:O	1:A:56:GLU:N	0.45	2.50	3	2
1:A:143:TRP:O	1:A:147:VAL:HG23	0.44	2.13	16	1
1:A:63:LEU:HD22	1:A:104:PHE:CE2	0.44	2.47	2	1
1:A:85:PHE:HA	1:A:94:ARG:NH2	0.44	2.27	19	1
1:A:135:ASP:O	1:A:139:LYS:HG2	0.44	2.13	2	3
1:A:20:GLN:HB3	1:A:107:LYS:HE3	0.44	1.90	17	2
1:A:85:PHE:HZ	1:A:98:LEU:HD22	0.44	1.73	11	1
1:A:15:ARG:O	1:A:19:GLU:HG3	0.43	2.12	2	1
1:A:19:GLU:HG3	1:A:20:GLN:N	0.43	2.28	7	1
1:A:43:THR:OG1	1:A:152:VAL:HG21	0.43	2.14	19	1
1:A:52:GLN:OE1	1:A:107:LYS:NZ	0.43	2.52	20	1
1:A:141:ARG:O	1:A:143:TRP:N	0.43	2.52	1	2
1:A:14:SER:O	1:A:18:ARG:HG2	0.43	2.14	6	2
1:A:52:GLN:O	1:A:56:GLU:HB2	0.43	2.14	7	1
1:A:14:SER:OG	1:A:18:ARG:NH1	0.42	2.52	14	1
1:A:21:ALA:O	1:A:110:LYS:HD3	0.42	2.14	1	1
1:A:84:VAL:O	1:A:94:ARG:HD3	0.42	2.15	3	2
1:A:108:HIS:O	1:A:112:ILE:HG12	0.42	2.15	13	1
1:A:71:GLU:O	1:A:75:LYS:HG3	0.42	2.15	11	1
1:A:70:ASN:HD22	1:A:70:ASN:N	0.41	2.13	14	1
1:A:19:GLU:OE2	1:A:45:ARG:HD3	0.41	2.15	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:LYS:HD3	1:A:70:ASN:ND2	0.41	2.30	7	2
1:A:3:ASP:O	1:A:7:ARG:HG2	0.41	2.16	3	1
1:A:101:PHE:O	1:A:105:VAL:HG23	0.41	2.15	2	1
1:A:8:GLN:O	1:A:12:ILE:HG13	0.41	2.16	5	1
1:A:129:LEU:HG	1:A:137:LEU:HD11	0.41	1.91	17	1
1:A:43:THR:HG23	1:A:152:VAL:HG21	0.41	1.91	18	1
1:A:61:GLY:HA2	1:A:64:ARG:NH1	0.41	2.30	19	1
1:A:48:GLY:O	1:A:52:GLN:HG3	0.41	2.16	3	1
1:A:94:ARG:HA	1:A:94:ARG:NE	0.41	2.30	8	1
1:A:137:LEU:O	1:A:142:GLY:N	0.41	2.54	9	1
1:A:144:ASP:O	1:A:148:GLU:HG3	0.41	2.15	19	1
1:A:141:ARG:HB3	1:A:144:ASP:HB2	0.40	1.92	9	1
1:A:68:ILE:N	1:A:68:ILE:HD12	0.40	2.31	17	2
1:A:36:THR:HA	1:A:39:LYS:HZ3	0.40	1.76	7	1
1:A:129:LEU:O	1:A:133:LYS:HB2	0.40	2.17	11	2
1:A:21:ALA:HA	1:A:107:LYS:HA	0.40	1.92	1	1
1:A:147:VAL:HG13	1:A:152:VAL:HB	0.40	1.94	1	1
1:A:47:VAL:O	1:A:51:VAL:HG23	0.40	2.16	2	1
1:A:10:LEU:HD11	1:A:123:GLU:HG2	0.40	1.93	3	1
1:A:68:ILE:HB	1:A:109:LEU:HD21	0.40	1.92	6	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	134/164 (82%)	126±1 (94±1%)	7±1 (5±1%)	2±1 (1±0%)	18	66
All	All	2680/3280 (82%)	2514 (94%)	136 (5%)	30 (1%)	18	66

All 6 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	67	ASP	14
1	A	142	GLY	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	68	ILE	6
1	A	34	GLY	2
1	A	152	VAL	1
1	A	151	HIS	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	118/143 (83%)	114±1 (96±1%)	4±1 (4±1%)	39 86
All	All	2360/2860 (83%)	2277 (96%)	83 (4%)	39 86

All 18 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	69	LYS	20
1	A	70	ASN	17
1	A	65	LYS	14
1	A	132	THR	8
1	A	38	ARG	3
1	A	133	LYS	3
1	A	18	ARG	3
1	A	7	ARG	2
1	A	131	ARG	2
1	A	20	GLN	2
1	A	113	ASN	2
1	A	134	ARG	1
1	A	4	GLU	1
1	A	46	ARG	1
1	A	148	GLU	1
1	A	39	LYS	1
1	A	107	LYS	1
1	A	115	GLU	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 84% for the well-defined parts and 81% 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	1876
Number of shifts mapped to atoms	1876
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	159	-0.61 ± 0.07	Should be checked
$^{13}C_{\beta}$	146	0.43 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	155	0.38 ± 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 84%, i.e. 1629 atoms were assigned a chemical shift out of a possible 1940. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	543/677 (80%)	276/276 (100%)	134/268 (50%)	133/133 (100%)
Sidechain	971/1107 (88%)	659/716 (92%)	295/335 (88%)	17/56 (30%)

Continued on next page...

Continued from previous page...

	Total	^{1}H	^{13}C	^{15}N
Aromatic	115/156 (74%)	65/77 (84%)	48/68 (71%)	2/11 (18%)
Overall	1629/1940 (84%)	1000/1069 (94%)	477/671 (71%)	152/200 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1874 atoms were assigned a chemical shift out of a possible 2316. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	643/829 (78%)	329/339 (97%)	159/328 (48%)	155/162 (96%)
Sidechain	1114/1283 (87%)	756/828 (91%)	340/393 (87%)	18/62 (29%)
Aromatic	117/204 (57%)	66/101 (65%)	49/80 (61%)	2/23 (9%)
Overall	1874/2316 (81%)	1151/1268 (91%)	548/801 (68%)	175/247 (71%)

7.1.4 Statistically unusual chemical shifts (i)

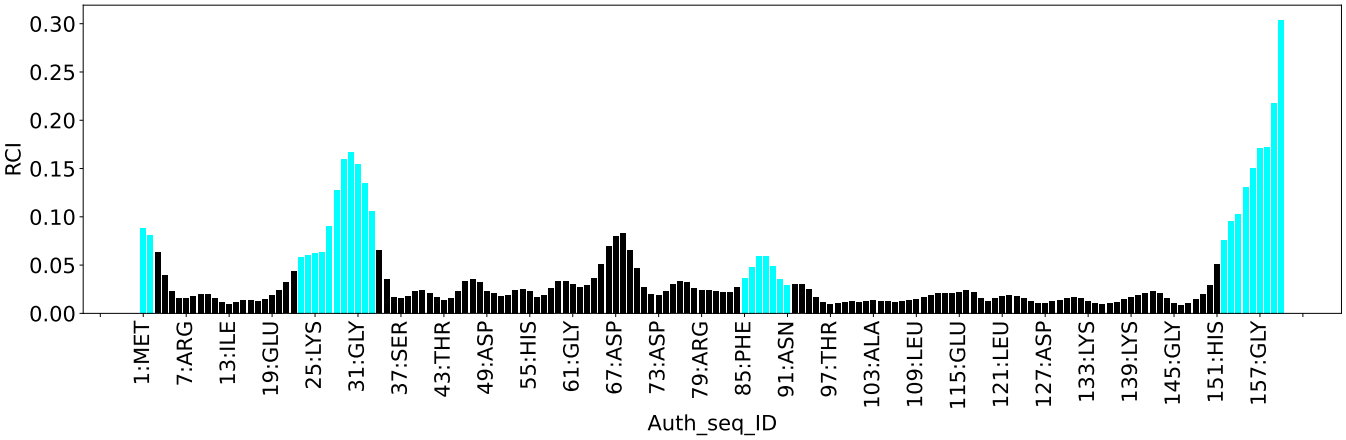
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	140	GLN	HG3	-0.05	0.91 – 3.68	-8.5
1	A	90	THR	HG21	-0.49	0.08 – 2.19	-7.7
1	A	90	THR	HG22	-0.49	0.08 – 2.19	-7.7
1	A	90	THR	HG23	-0.49	0.08 – 2.19	-7.7
1	A	140	GLN	HG2	0.93	1.01 – 3.62	-5.3

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:


RCI
0.30
0.25
0.20
0.15
0.10
0.05
0.00
1:MET
7:ARG
13:ILE
19:GLU
25:LYS
31:GLY
37:SER
43:THR
49:ASP
55:HIS
61:GLY
67:ASP
73:ASP
79:ARG
85:PHE
91:ASN
97:THR
103:ALA
109:LEU
115:GLU
121:LEU
127:ASP
133:LYS
139:LYS
145:GLY
151:HIS
157:GLY
Auth_seq_ID

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	4485
Intra-residue (|i-j|=0)	1052
Sequential (|i-j|=1)	1062
Medium range (|i-j|>1 and |i-j|<5)	1197
Long range (|i-j|≥5)	1058
Inter-chain	0
Hydrogen bond restraints	116
Disulfide bond restraints	0
Total dihedral-angle restraints	226
Number of unmapped restraints	0
Number of restraints per residue	28.7
Number of long range restraints per residue[1]	6.5

[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)	2.9	0.2
0.2-0.5 (Medium)	0.6	0.4
>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)	9.1	7.3
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

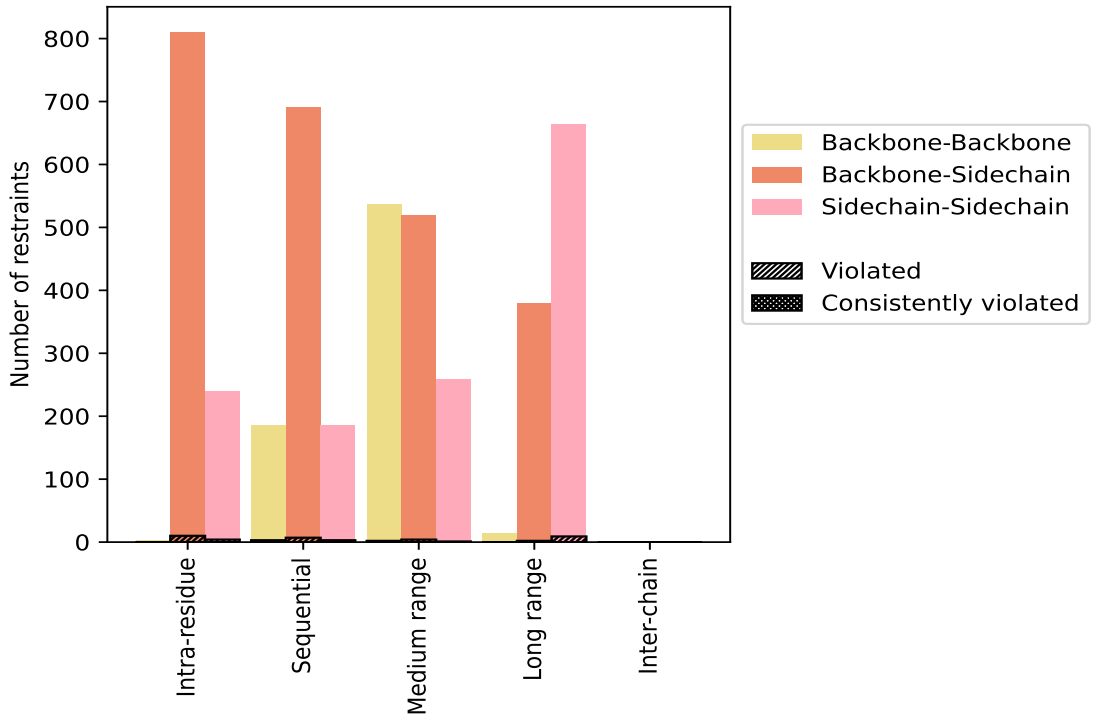
9.1 Summary of distance violations (i)

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)	1052	23.5	14	1.3	0.3	0	0.0	0.0
Backbone-Backbone	3	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	810	18.1	10	1.2	0.2	0	0.0	0.0
Sidechain-Sidechain	239	5.3	4	1.7	0.1	0	0.0	0.0
Sequential (|i-j|=1)	1062	23.7	13	1.2	0.3	0	0.0	0.0
Backbone-Backbone	185	4.1	3	1.6	0.1	0	0.0	0.0
Backbone-Sidechain	691	15.4	7	1.0	0.2	0	0.0	0.0
Sidechain-Sidechain	186	4.1	3	1.6	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	1197	26.7	5	0.4	0.1	0	0.0	0.0
Backbone-Backbone	420	9.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	519	11.6	4	0.8	0.1	0	0.0	0.0
Sidechain-Sidechain	258	5.8	1	0.4	0.0	0	0.0	0.0
Long range (|i-j|≥5)	1058	23.6	11	1.0	0.2	0	0.0	0.0
Backbone-Backbone	14	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	380	8.5	2	0.5	0.0	0	0.0	0.0
Sidechain-Sidechain	664	14.8	9	1.4	0.2	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	116	2.6	2	1.7	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	4485	100.0	45	1.0	1.0	0	0.0	0.0
Backbone-Backbone	738	16.5	5	0.7	0.1	0	0.0	0.0
Backbone-Sidechain	2400	53.5	23	1.0	0.5	0	0.0	0.0
Sidechain-Sidechain	1347	30.0	17	1.3	0.4	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	2	1	0	0	0	3	0.29	0.4	0.1	0.3
2	2	3	0	1	0	6	0.17	0.27	0.06	0.16
3	0	2	0	0	0	2	0.2	0.26	0.06	0.2
4	1	2	0	1	0	4	0.18	0.25	0.05	0.18
5	1	0	0	1	0	2	0.12	0.12	0.0	0.12
6	0	1	0	1	0	2	0.14	0.16	0.02	0.14
7	2	2	0	1	0	5	0.13	0.16	0.02	0.14
8	1	2	0	0	0	3	0.23	0.37	0.1	0.17
9	0	1	3	0	0	4	0.13	0.15	0.01	0.14
10	1	1	0	0	0	2	0.12	0.12	0.0	0.12
11	0	2	1	0	0	3	0.18	0.27	0.07	0.16

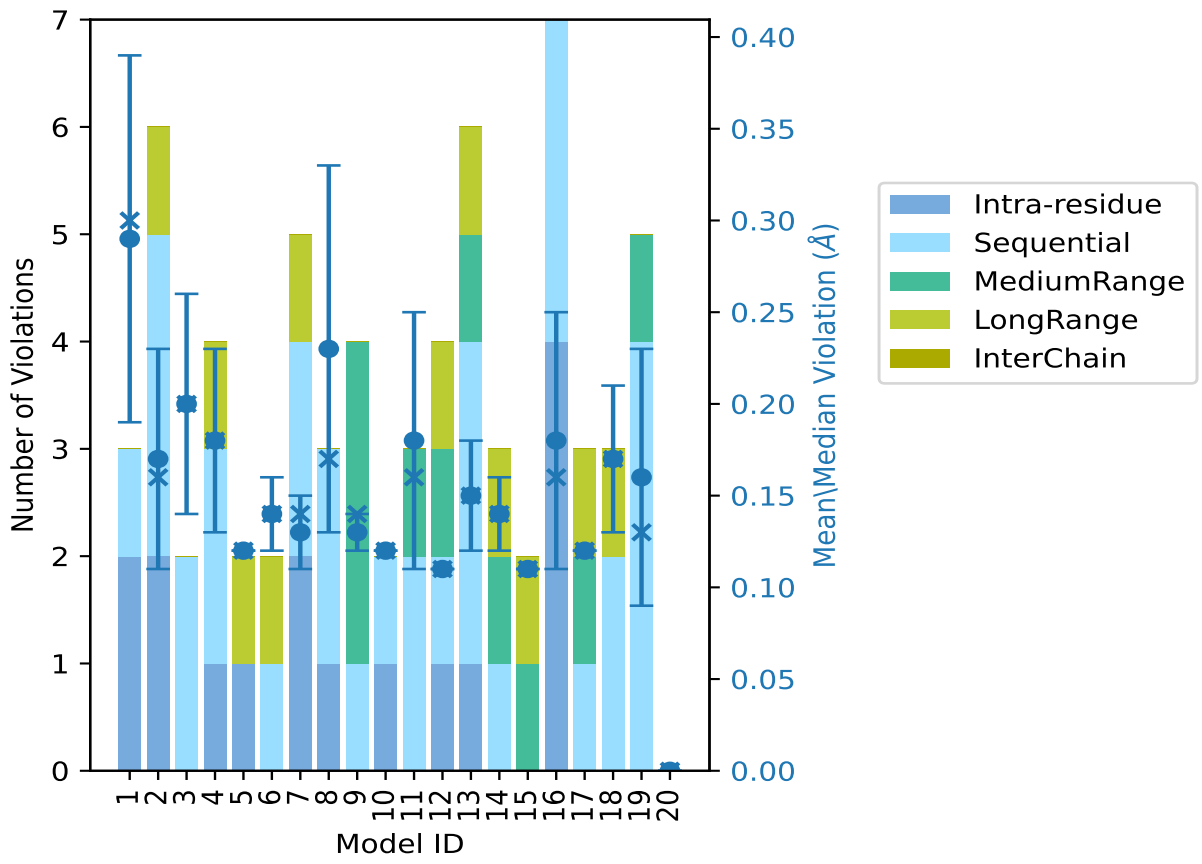
Continued on next page...

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	1	1	1	1	0	4	0.11	0.11	0.0	0.11
13	1	3	1	1	0	6	0.15	0.2	0.03	0.15
14	0	1	1	1	0	3	0.14	0.17	0.02	0.14
15	0	0	1	1	0	2	0.11	0.11	0.0	0.11
16	4	3	0	0	0	7	0.18	0.28	0.07	0.16
17	0	1	1	1	0	3	0.12	0.12	0.0	0.12
18	0	2	0	1	0	3	0.17	0.21	0.04	0.17
19	0	4	1	0	0	5	0.16	0.3	0.07	0.13
20	0	0	0	0	0	0	0.0	0.0	0.0	0.0

[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

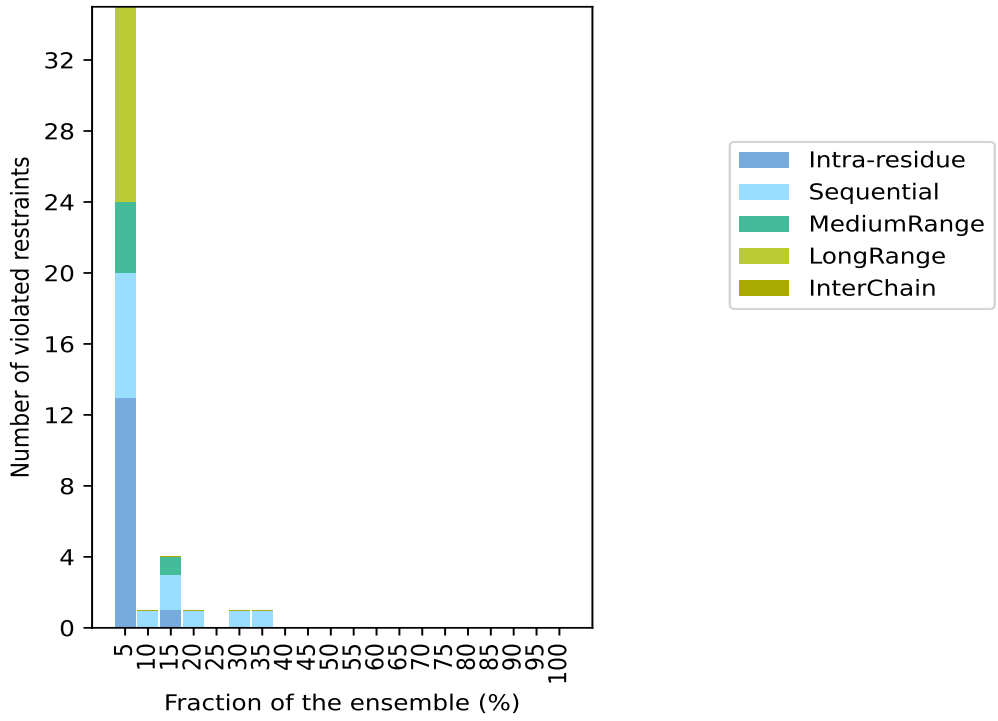
9.3 Distance violation statistics for the ensemble (i)

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, 4326(IR:1038, SQ:1049, MR:1192, LR:1047, 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]	%
13	7	4	11	0	35	1	5.0
0	1	0	0	0	1	2	10.0
1	2	1	0	0	4	3	15.0
0	1	0	0	0	1	4	20.0
0	0	0	0	0	0	5	25.0
0	1	0	0	0	1	6	30.0
0	1	0	0	0	1	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	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

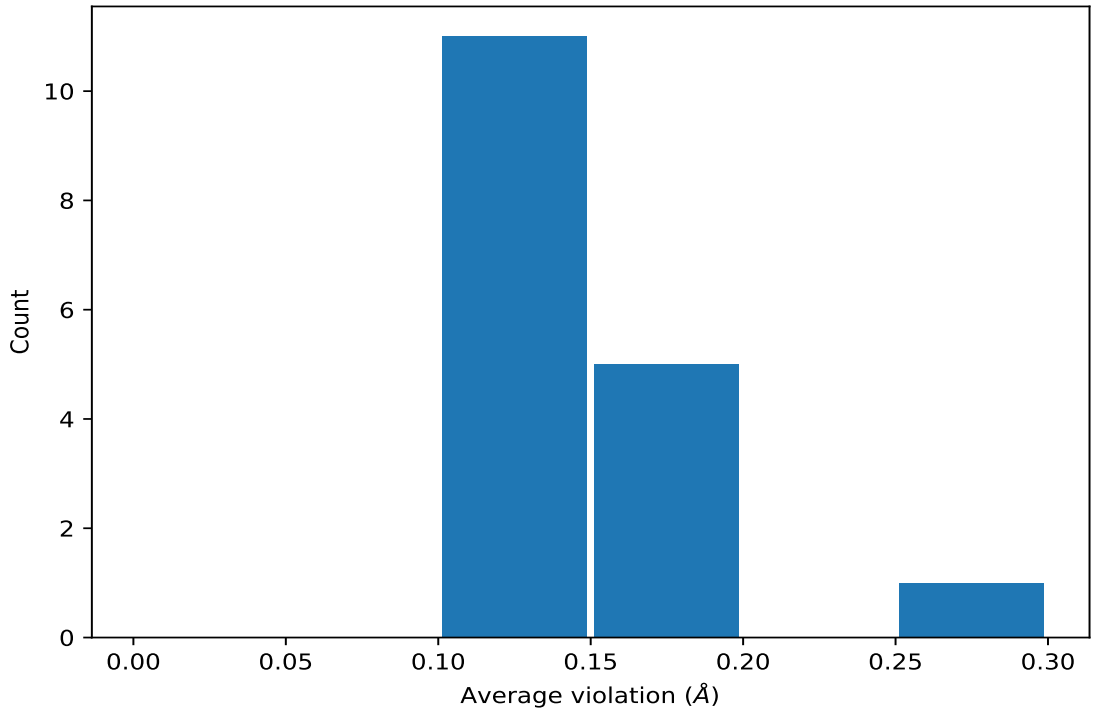
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD11	7	0.16	0.01	0.16
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD12	7	0.16	0.01	0.16
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD13	7	0.16	0.01	0.16
(1,2744)	1:A:67:ASP:HA	1:A:68:ILE:H	6	0.25	0.04	0.26
(1,3941)	1:A:33:SER:HB2	1:A:34:GLY:H	4	0.14	0.03	0.13
(1,3941)	1:A:33:SER:HB3	1:A:34:GLY:H	4	0.14	0.03	0.13
(1,3302)	1:A:142:GLY:H	1:A:143:TRP:H	3	0.14	0.01	0.13
(1,1883)	1:A:140:GLN:HA	1:A:141:ARG:HG2	3	0.14	0.03	0.12
(1,436)	1:A:81:MET:HA	1:A:81:MET:HE1	3	0.12	0.0	0.12
(1,436)	1:A:81:MET:HA	1:A:81:MET:HE2	3	0.12	0.0	0.12
(1,436)	1:A:81:MET:HA	1:A:81:MET:HE3	3	0.12	0.0	0.12
(1,1773)	1:A:126:THR:HA	1:A:129:LEU:HD11	3	0.11	0.0	0.11
(1,1773)	1:A:126:THR:HA	1:A:129:LEU:HD12	3	0.11	0.0	0.11
(1,1773)	1:A:126:THR:HA	1:A:129:LEU:HD13	3	0.11	0.0	0.11
(1,1820)	1:A:134:ARG:HG3	1:A:135:ASP:HB2	2	0.16	0.04	0.16
(1,1820)	1:A:134:ARG:HG3	1:A:135:ASP:HB3	2	0.16	0.04	0.16

Continued on next page...

Continued from previous page...

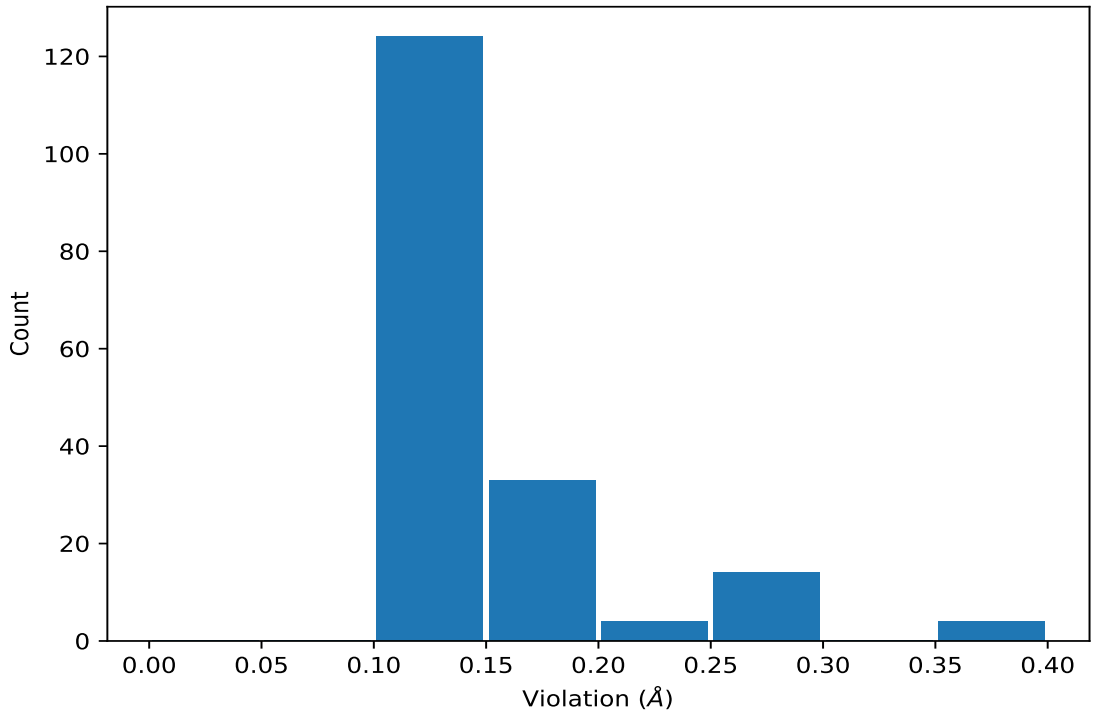
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,23)	1:A:14:SER:O	1:A:18:ARG:H	2	0.13	0.01	0.13

[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)
(1,366)	1:A:69:LYS:HB3	1:A:69:LYS:HE2	1	0.4
(1,366)	1:A:69:LYS:HB3	1:A:69:LYS:HE3	1	0.4
(1,3990)	1:A:45:ARG:H	1:A:45:ARG:HG2	8	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3990)	1:A:45:ARG:H	1:A:45:ARG:HG3	8	0.37
(1,4090)	1:A:69:LYS:HB2	1:A:69:LYS:HE2	1	0.3
(1,4090)	1:A:69:LYS:HB2	1:A:69:LYS:HE3	1	0.3
(1,4090)	1:A:69:LYS:HB3	1:A:69:LYS:HE2	1	0.3
(1,4090)	1:A:69:LYS:HB3	1:A:69:LYS:HE3	1	0.3
(1,1817)	1:A:132:THR:HG21	1:A:133:LYS:HA	19	0.3
(1,1817)	1:A:132:THR:HG22	1:A:133:LYS:HA	19	0.3
(1,1817)	1:A:132:THR:HG23	1:A:133:LYS:HA	19	0.3
(1,3871)	1:A:18:ARG:HA	1:A:18:ARG:HD2	16	0.28
(1,3871)	1:A:18:ARG:HA	1:A:18:ARG:HD3	16	0.28
(1,2744)	1:A:67:ASP:HA	1:A:68:ILE:H	16	0.28
(1,2744)	1:A:67:ASP:HA	1:A:68:ILE:H	2	0.27
(1,2744)	1:A:67:ASP:HA	1:A:68:ILE:H	11	0.27
(1,2744)	1:A:67:ASP:HA	1:A:68:ILE:H	3	0.26
(1,2744)	1:A:67:ASP:HA	1:A:68:ILE:H	4	0.25
(1,3240)	1:A:134:ARG:HB3	1:A:135:ASP:H	2	0.21
(1,2434)	1:A:20:GLN:HE21	1:A:21:ALA:H	18	0.21
(1,1820)	1:A:134:ARG:HG3	1:A:135:ASP:HB2	13	0.2
(1,1820)	1:A:134:ARG:HG3	1:A:135:ASP:HB3	13	0.2
(1,3941)	1:A:33:SER:HB2	1:A:34:GLY:H	4	0.19
(1,3941)	1:A:33:SER:HB3	1:A:34:GLY:H	4	0.19
(1,3710)	1:A:16:TYR:HA	1:A:45:ARG:HE	4	0.18
(1,1883)	1:A:140:GLN:HA	1:A:141:ARG:HG2	13	0.18
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD11	2	0.18
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD12	2	0.18
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD13	2	0.18
(1,3409)	1:A:156:GLU:H	1:A:157:GLY:H	14	0.17
(1,2744)	1:A:67:ASP:HA	1:A:68:ILE:H	18	0.17
(1,2472)	1:A:30:MET:HE1	1:A:31:GLY:H	8	0.17
(1,2472)	1:A:30:MET:HE2	1:A:31:GLY:H	8	0.17
(1,2472)	1:A:30:MET:HE3	1:A:31:GLY:H	8	0.17
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD11	16	0.17
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD12	16	0.17
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD13	16	0.17
(2,17)	1:A:11:GLU:O	1:A:15:ARG:H	11	0.16
(1,4291)	1:A:131:ARG:HG2	1:A:132:THR:HG21	7	0.16
(1,4291)	1:A:131:ARG:HG2	1:A:132:THR:HG22	7	0.16
(1,4291)	1:A:131:ARG:HG2	1:A:132:THR:HG23	7	0.16
(1,4291)	1:A:131:ARG:HG3	1:A:132:THR:HG21	7	0.16
(1,4291)	1:A:131:ARG:HG3	1:A:132:THR:HG22	7	0.16
(1,4291)	1:A:131:ARG:HG3	1:A:132:THR:HG23	7	0.16
(1,3776)	1:A:7:ARG:H	1:A:7:ARG:HG2	16	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3776)	1:A:7:ARG:H	1:A:7:ARG:HG3	16	0.16
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD11	1	0.16
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD12	1	0.16
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD13	1	0.16
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD11	6	0.16
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD12	6	0.16
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD13	6	0.16
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD11	13	0.16
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD12	13	0.16
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD13	13	0.16
(1,3941)	1:A:33:SER:HB2	1:A:34:GLY:H	3	0.15
(1,3941)	1:A:33:SER:HB3	1:A:34:GLY:H	3	0.15
(1,3302)	1:A:142:GLY:H	1:A:143:TRP:H	9	0.15
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD11	7	0.15
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD12	7	0.15
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD13	7	0.15
(2,23)	1:A:14:SER:O	1:A:18:ARG:H	14	0.14
(1,796)	1:A:2:GLU:HG2	1:A:6:TYR:H	9	0.14
(1,796)	1:A:2:GLU:HG3	1:A:6:TYR:H	9	0.14
(1,173)	1:A:39:LYS:H	1:A:39:LYS:HD2	7	0.14
(1,173)	1:A:39:LYS:H	1:A:39:LYS:HD3	7	0.14
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD11	8	0.14
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD12	8	0.14
(1,1250)	1:A:62:MET:H	1:A:63:LEU:HD13	8	0.14
(1,3940)	1:A:33:SER:H	1:A:37:SER:HB2	19	0.13
(1,3940)	1:A:33:SER:H	1:A:37:SER:HB3	19	0.13
(1,3302)	1:A:142:GLY:H	1:A:143:TRP:H	16	0.13
(1,3302)	1:A:142:GLY:H	1:A:143:TRP:H	19	0.13
(1,2466)	1:A:30:MET:H	1:A:30:MET:HG2	2	0.13
(1,1793)	1:A:138:VAL:HG21	1:A:141:ARG:HG2	9	0.13
(1,1793)	1:A:138:VAL:HG22	1:A:141:ARG:HG2	9	0.13
(1,1793)	1:A:138:VAL:HG23	1:A:141:ARG:HG2	9	0.13
(1,1029)	1:A:36:THR:HG21	1:A:147:VAL:HB	13	0.13
(1,1029)	1:A:36:THR:HG22	1:A:147:VAL:HB	13	0.13
(1,1029)	1:A:36:THR:HG23	1:A:147:VAL:HB	13	0.13
(2,23)	1:A:14:SER:O	1:A:18:ARG:H	17	0.12
(1,436)	1:A:81:MET:HA	1:A:81:MET:HE1	10	0.12
(1,436)	1:A:81:MET:HA	1:A:81:MET:HE2	10	0.12
(1,436)	1:A:81:MET:HA	1:A:81:MET:HE3	10	0.12
(1,436)	1:A:81:MET:HA	1:A:81:MET:HE1	16	0.12
(1,436)	1:A:81:MET:HA	1:A:81:MET:HE2	16	0.12
(1,436)	1:A:81:MET:HA	1:A:81:MET:HE3	16	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3399)	1:A:155:LEU:H	1:A:155:LEU:HD11	16	0.12
(1,3399)	1:A:155:LEU:H	1:A:155:LEU:HD12	16	0.12
(1,3399)	1:A:155:LEU:H	1:A:155:LEU:HD13	16	0.12
(1,2748)	1:A:68:ILE:H	1:A:68:ILE:HB	4	0.12
(1,2284)	1:A:8:GLN:H	1:A:32:ARG:HD2	5	0.12
(1,2284)	1:A:8:GLN:H	1:A:32:ARG:HD3	5	0.12
(1,1883)	1:A:140:GLN:HA	1:A:141:ARG:HG2	10	0.12
(1,1820)	1:A:134:ARG:HG3	1:A:135:ASP:HB2	17	0.12
(1,1820)	1:A:134:ARG:HG3	1:A:135:ASP:HB3	17	0.12
(1,1651)	1:A:22:THR:HG21	1:A:115:GLU:HG2	18	0.12
(1,1651)	1:A:22:THR:HG21	1:A:115:GLU:HG3	18	0.12
(1,1651)	1:A:22:THR:HG22	1:A:115:GLU:HG2	18	0.12
(1,1651)	1:A:22:THR:HG22	1:A:115:GLU:HG3	18	0.12
(1,1651)	1:A:22:THR:HG23	1:A:115:GLU:HG2	18	0.12
(1,1651)	1:A:22:THR:HG23	1:A:115:GLU:HG3	18	0.12
(1,564)	1:A:25:LYS:HB2	1:A:25:LYS:HE2	7	0.11
(1,564)	1:A:25:LYS:HB2	1:A:25:LYS:HE3	7	0.11
(1,564)	1:A:25:LYS:HB3	1:A:25:LYS:HE2	7	0.11
(1,564)	1:A:25:LYS:HB3	1:A:25:LYS:HE3	7	0.11
(1,436)	1:A:81:MET:HA	1:A:81:MET:HE1	2	0.11
(1,436)	1:A:81:MET:HA	1:A:81:MET:HE2	2	0.11
(1,436)	1:A:81:MET:HA	1:A:81:MET:HE3	2	0.11
(1,4353)	1:A:153:GLU:H	1:A:153:GLU:HG2	12	0.11
(1,4353)	1:A:153:GLU:H	1:A:153:GLU:HG3	12	0.11
(1,4160)	1:A:89:VAL:HG11	1:A:94:ARG:HD2	2	0.11
(1,4160)	1:A:89:VAL:HG11	1:A:94:ARG:HD3	2	0.11
(1,4160)	1:A:89:VAL:HG12	1:A:94:ARG:HD2	2	0.11
(1,4160)	1:A:89:VAL:HG12	1:A:94:ARG:HD3	2	0.11
(1,4160)	1:A:89:VAL:HG13	1:A:94:ARG:HD2	2	0.11
(1,4160)	1:A:89:VAL:HG13	1:A:94:ARG:HD3	2	0.11
(1,4160)	1:A:89:VAL:HG21	1:A:94:ARG:HD2	2	0.11
(1,4160)	1:A:89:VAL:HG21	1:A:94:ARG:HD3	2	0.11
(1,4160)	1:A:89:VAL:HG22	1:A:94:ARG:HD2	2	0.11
(1,4160)	1:A:89:VAL:HG22	1:A:94:ARG:HD3	2	0.11
(1,4160)	1:A:89:VAL:HG23	1:A:94:ARG:HD2	2	0.11
(1,4160)	1:A:89:VAL:HG23	1:A:94:ARG:HD3	2	0.11
(1,4133)	1:A:81:MET:HB3	1:A:124:SER:HB2	6	0.11
(1,4133)	1:A:81:MET:HB3	1:A:124:SER:HB3	6	0.11
(1,4092)	1:A:69:LYS:HB2	1:A:70:ASN:HD21	19	0.11
(1,4092)	1:A:69:LYS:HB3	1:A:70:ASN:HD21	19	0.11
(1,3970)	1:A:39:LYS:HE2	1:A:153:GLU:HB2	15	0.11
(1,3970)	1:A:39:LYS:HE2	1:A:153:GLU:HB3	15	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3970)	1:A:39:LYS:HE3	1:A:153:GLU:HB2	15	0.11
(1,3970)	1:A:39:LYS:HE3	1:A:153:GLU:HB3	15	0.11
(1,3963)	1:A:39:LYS:HB2	1:A:39:LYS:HE2	5	0.11
(1,3963)	1:A:39:LYS:HB2	1:A:39:LYS:HE3	5	0.11
(1,3963)	1:A:39:LYS:HB3	1:A:39:LYS:HE2	5	0.11
(1,3963)	1:A:39:LYS:HB3	1:A:39:LYS:HE3	5	0.11
(1,3941)	1:A:33:SER:HB2	1:A:34:GLY:H	12	0.11
(1,3941)	1:A:33:SER:HB3	1:A:34:GLY:H	12	0.11
(1,3941)	1:A:33:SER:HB2	1:A:34:GLY:H	19	0.11
(1,3941)	1:A:33:SER:HB3	1:A:34:GLY:H	19	0.11
(1,2427)	1:A:20:GLN:HA	1:A:20:GLN:HE21	13	0.11
(1,2172)	1:A:39:LYS:HG2	1:A:147:VAL:HG21	7	0.11
(1,2172)	1:A:39:LYS:HG2	1:A:147:VAL:HG22	7	0.11
(1,2172)	1:A:39:LYS:HG2	1:A:147:VAL:HG23	7	0.11
(1,2172)	1:A:39:LYS:HG3	1:A:147:VAL:HG21	7	0.11
(1,2172)	1:A:39:LYS:HG3	1:A:147:VAL:HG22	7	0.11
(1,2172)	1:A:39:LYS:HG3	1:A:147:VAL:HG23	7	0.11
(1,2019)	1:A:4:GLU:HG2	1:A:32:ARG:HG2	14	0.11
(1,2019)	1:A:4:GLU:HG2	1:A:32:ARG:HG3	14	0.11
(1,2019)	1:A:4:GLU:HG3	1:A:32:ARG:HG2	14	0.11
(1,2019)	1:A:4:GLU:HG3	1:A:32:ARG:HG3	14	0.11
(1,1883)	1:A:140:GLN:HA	1:A:141:ARG:HG2	11	0.11
(1,1773)	1:A:126:THR:HA	1:A:129:LEU:HD11	12	0.11
(1,1773)	1:A:126:THR:HA	1:A:129:LEU:HD12	12	0.11
(1,1773)	1:A:126:THR:HA	1:A:129:LEU:HD13	12	0.11
(1,1773)	1:A:126:THR:HA	1:A:129:LEU:HD11	13	0.11
(1,1773)	1:A:126:THR:HA	1:A:129:LEU:HD12	13	0.11
(1,1773)	1:A:126:THR:HA	1:A:129:LEU:HD13	13	0.11
(1,1773)	1:A:126:THR:HA	1:A:129:LEU:HD11	15	0.11
(1,1773)	1:A:126:THR:HA	1:A:129:LEU:HD12	15	0.11
(1,1773)	1:A:126:THR:HA	1:A:129:LEU:HD13	15	0.11
(1,1610)	1:A:66:LEU:HD11	1:A:105:VAL:HG11	12	0.11
(1,1610)	1:A:66:LEU:HD11	1:A:105:VAL:HG12	12	0.11
(1,1610)	1:A:66:LEU:HD11	1:A:105:VAL:HG13	12	0.11
(1,1610)	1:A:66:LEU:HD12	1:A:105:VAL:HG11	12	0.11
(1,1610)	1:A:66:LEU:HD12	1:A:105:VAL:HG12	12	0.11
(1,1610)	1:A:66:LEU:HD12	1:A:105:VAL:HG13	12	0.11
(1,1610)	1:A:66:LEU:HD13	1:A:105:VAL:HG11	12	0.11
(1,1610)	1:A:66:LEU:HD13	1:A:105:VAL:HG12	12	0.11
(1,1610)	1:A:66:LEU:HD13	1:A:105:VAL:HG13	12	0.11
(1,1130)	1:A:47:VAL:HG11	1:A:96:VAL:HG21	17	0.11
(1,1130)	1:A:47:VAL:HG11	1:A:96:VAL:HG22	17	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1130)	1:A:47:VAL:HG11	1:A:96:VAL:HG23	17	0.11
(1,1130)	1:A:47:VAL:HG12	1:A:96:VAL:HG21	17	0.11
(1,1130)	1:A:47:VAL:HG12	1:A:96:VAL:HG22	17	0.11
(1,1130)	1:A:47:VAL:HG12	1:A:96:VAL:HG23	17	0.11
(1,1130)	1:A:47:VAL:HG13	1:A:96:VAL:HG21	17	0.11
(1,1130)	1:A:47:VAL:HG13	1:A:96:VAL:HG22	17	0.11
(1,1130)	1:A:47:VAL:HG13	1:A:96:VAL:HG23	17	0.11
(1,102)	1:A:16:TYR:HA	1:A:19:GLU:HG2	9	0.11

10 Dihedral-angle violation analysis (i)

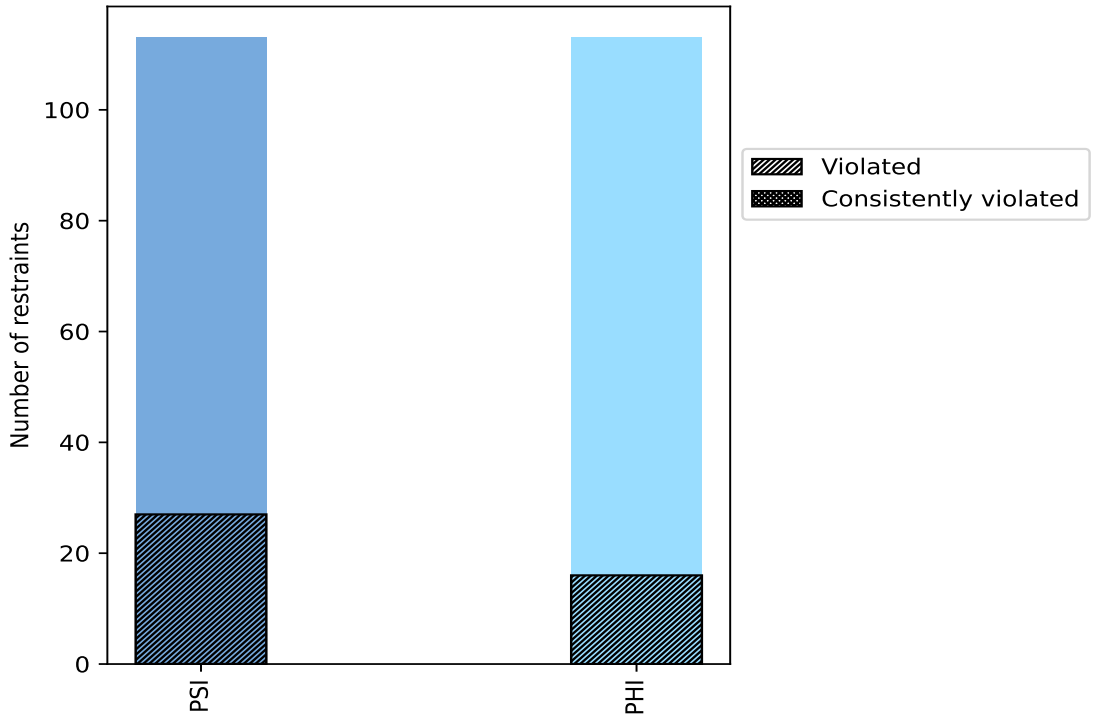
10.1 Summary of dihedral-angle violations (i)

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]
PSI	113	50.0	27	23.9	11.9	0	0.0	0.0
PHI	113	50.0	16	14.2	7.1	0	0.0	0.0
Total	226	100.0	43	19.0	19.0	0	0.0	0.0

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

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



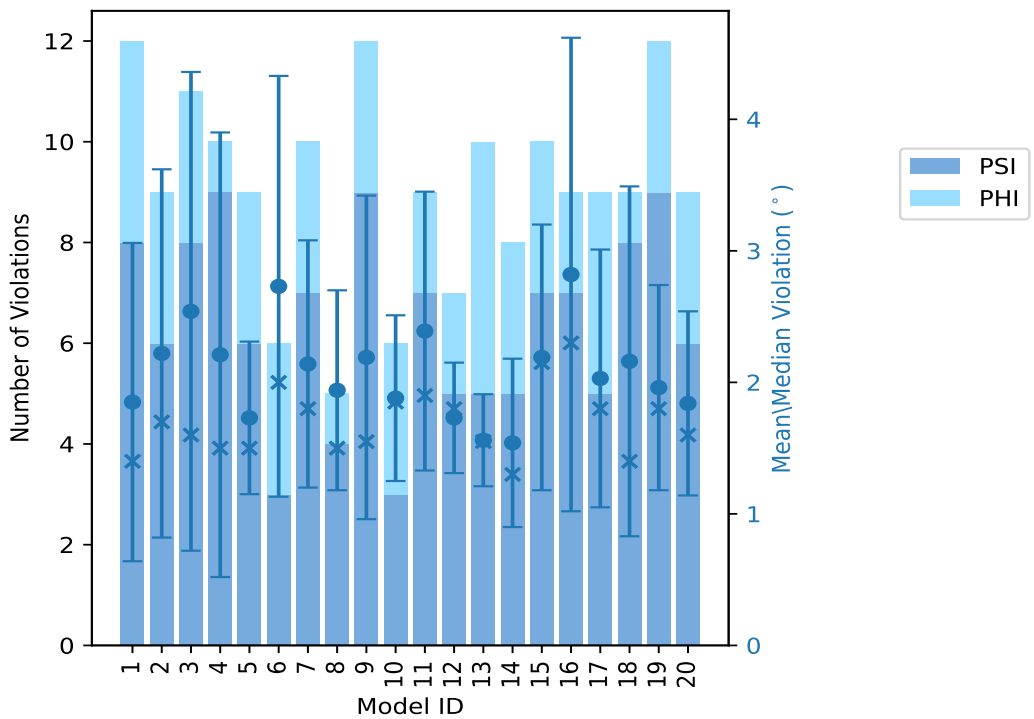
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	8	4	12	1.85	5.4	1.21	1.4
2	6	3	9	2.22	5.5	1.4	1.7
3	8	3	11	2.54	7.3	1.82	1.6
4	9	1	10	2.21	6.3	1.69	1.5
5	6	3	9	1.73	2.9	0.58	1.5
6	3	3	6	2.73	6.0	1.6	2.0
7	7	3	10	2.14	4.6	0.94	1.8
8	4	1	5	1.94	3.0	0.76	1.5
9	9	3	12	2.19	4.7	1.23	1.55
10	3	3	6	1.88	2.9	0.63	1.85
11	7	2	9	2.39	4.8	1.06	1.9
12	5	2	7	1.73	2.4	0.42	1.8
13	5	5	10	1.56	2.2	0.35	1.55
14	5	3	8	1.54	3.1	0.64	1.3
15	7	3	10	2.19	4.6	1.01	2.15
16	7	2	9	2.82	6.8	1.8	2.3
17	5	4	9	2.03	4.5	0.98	1.8
18	8	1	9	2.16	4.8	1.33	1.4
19	9	3	12	1.96	3.9	0.78	1.8
20	6	3	9	1.84	3.2	0.7	1.6

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	
PSI	PHI	Total	Count[1]	%
11	10	21	1	5.0
3	2	5	2	10.0
2	0	2	3	15.0
1	0	1	4	20.0
1	1	2	5	25.0
1	0	1	6	30.0
2	0	2	7	35.0
0	1	1	8	40.0
2	0	2	9	45.0
1	1	2	10	50.0
1	0	1	11	55.0

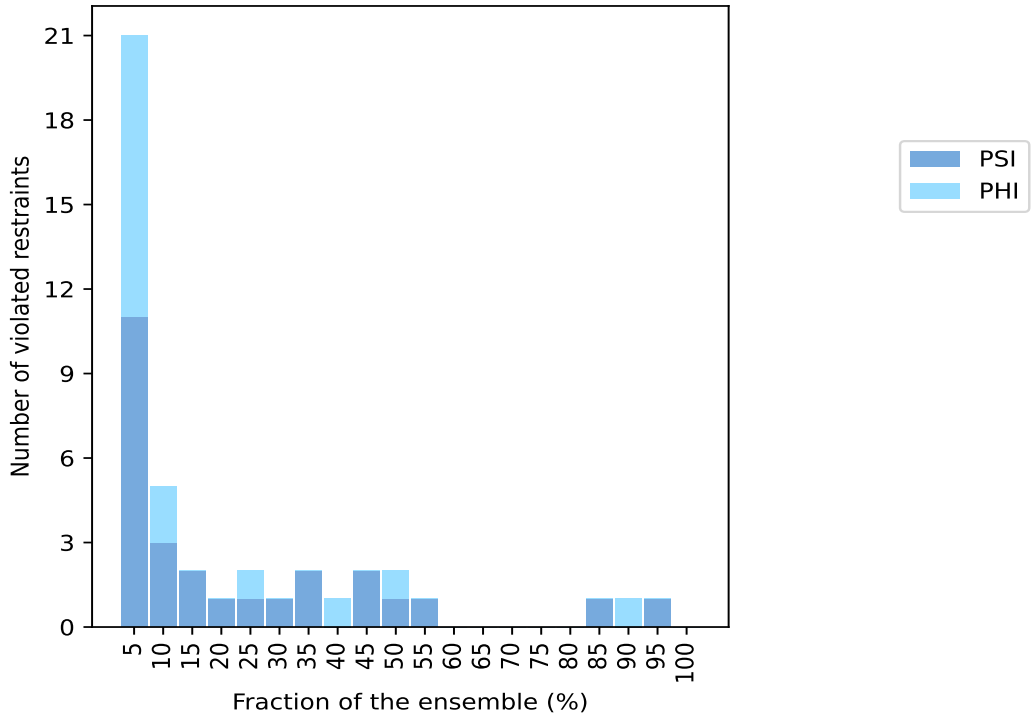
Continued on next page...

Continued from previous page...

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

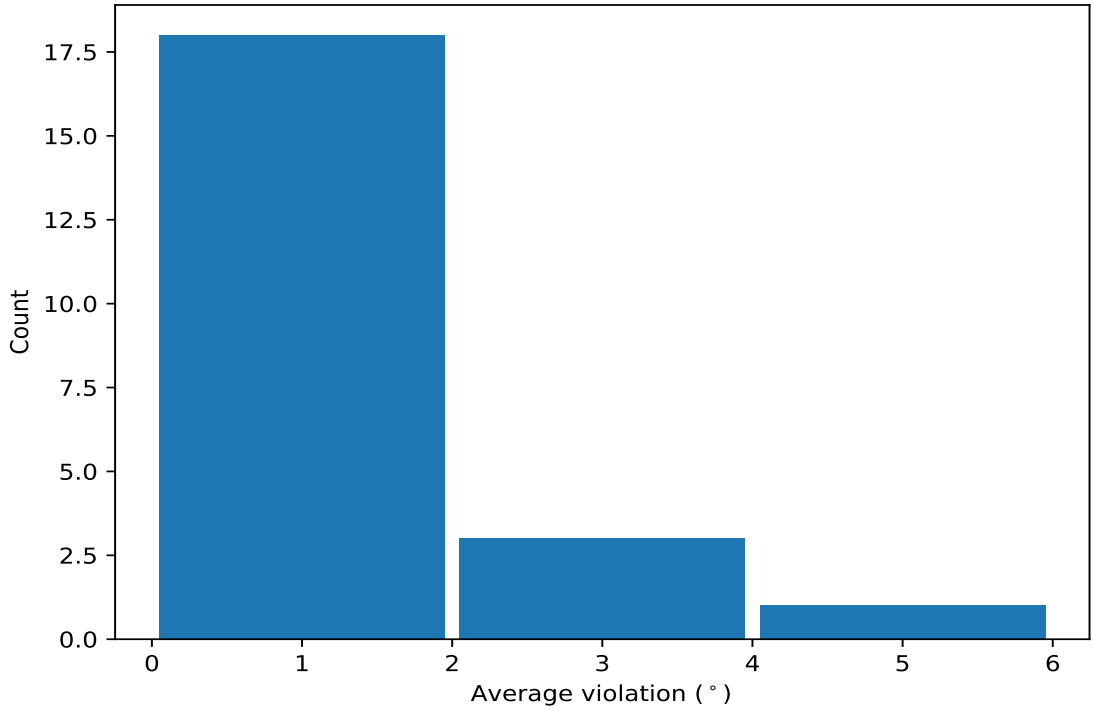


10.4 Most violated dihedral-angle restraints in the ensemble (i)

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
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	19	2.29	0.55	2.2
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	18	2.97	1.18	2.9
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	17	4.37	1.79	4.7
(1,186)	1:A:127:ASP:N	1:A:127:ASP:CA	1:A:127:ASP:C	1:A:128:VAL:N	11	1.66	0.38	1.6
(1,225)	1:A:149:PHE:C	1:A:150:PHE:N	1:A:150:PHE:CA	1:A:150:PHE:C	10	2.12	1.16	1.65
(1,160)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:LYS:N	10	1.5	0.26	1.4
(1,122)	1:A:83:HIS:N	1:A:83:HIS:CA	1:A:83:HIS:C	1:A:84:VAL:N	9	1.74	0.71	1.5
(1,40)	1:A:35:ALA:N	1:A:35:ALA:CA	1:A:35:ALA:C	1:A:36:THR:N	9	1.72	0.66	1.6
(1,205)	1:A:137:LEU:C	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	8	1.52	0.34	1.5
(1,190)	1:A:129:LEU:N	1:A:129:LEU:CA	1:A:129:LEU:C	1:A:130:VAL:N	7	1.39	0.31	1.3
(1,138)	1:A:98:LEU:N	1:A:98:LEU:CA	1:A:98:LEU:C	1:A:99:ILE:N	7	1.33	0.28	1.2
(1,224)	1:A:149:PHE:N	1:A:149:PHE:CA	1:A:149:PHE:C	1:A:150:PHE:N	6	1.85	0.68	1.85
(1,16)	1:A:11:GLU:N	1:A:11:GLU:CA	1:A:11:GLU:C	1:A:12:ILE:N	5	1.98	0.55	1.9
(1,91)	1:A:61:GLY:C	1:A:62:MET:N	1:A:62:MET:CA	1:A:62:MET:C	5	1.54	0.29	1.6
(1,2)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	1:A:5:LEU:N	4	1.92	0.78	1.9
(1,64)	1:A:47:VAL:N	1:A:47:VAL:CA	1:A:47:VAL:C	1:A:48:GLY:N	3	1.47	0.29	1.5
(1,62)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:VAL:N	3	1.23	0.09	1.3
(1,37)	1:A:21:ALA:C	1:A:22:THR:N	1:A:22:THR:CA	1:A:22:THR:C	2	1.65	0.55	1.65
(1,10)	1:A:8:GLN:N	1:A:8:GLN:CA	1:A:8:GLN:C	1:A:9:SER:N	2	1.5	0.2	1.5
(1,25)	1:A:15:ARG:C	1:A:16:TYR:N	1:A:16:TYR:CA	1:A:16:TYR:C	2	1.3	0.2	1.3

Continued on next page...

Continued from previous page...

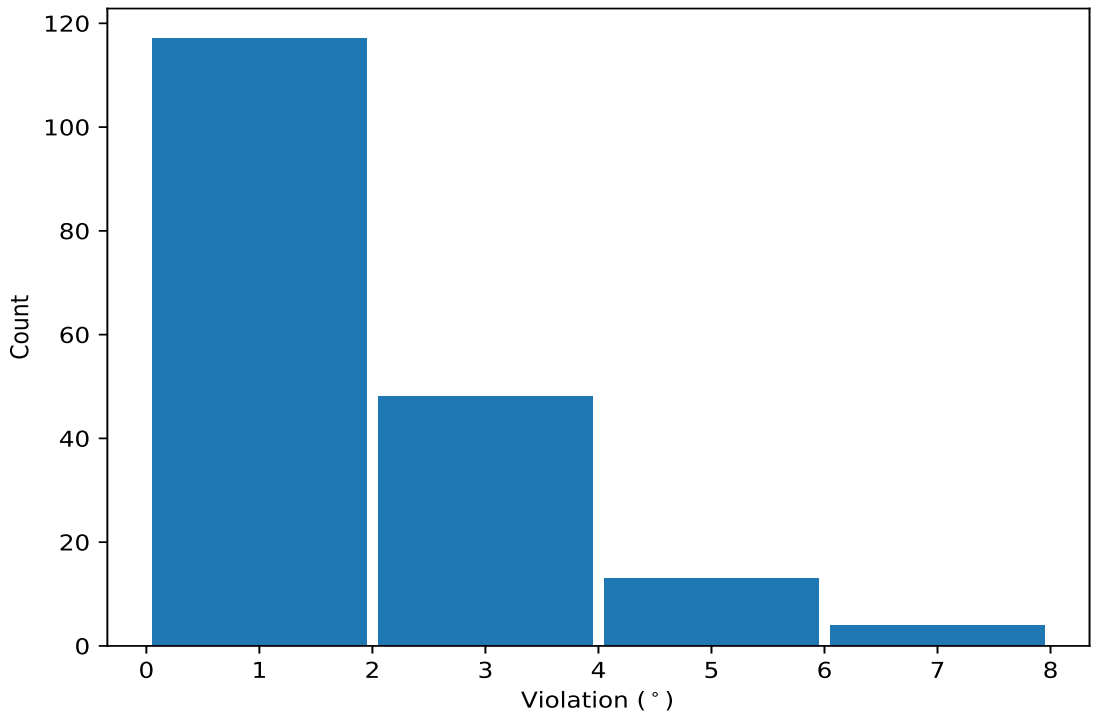
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,46)	1:A:38:ARG:N	1:A:38:ARG:CA	1:A:38:ARG:C	1:A:39:LYS:N	2	1.3	0.2	1.3
(1,202)	1:A:136:TRP:N	1:A:136:TRP:CA	1:A:136:TRP:C	1:A:137:LEU:N	2	1.25	0.05	1.25

[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 (°)
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	3	7.3
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	16	6.8
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	4	6.3
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	6	6.0
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	2	5.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	1	5.4
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	16	5.1
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	11	4.8
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	18	4.8
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	3	4.7
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	4	4.7
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	9	4.7
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	15	4.6
(1,225)	1:A:149:PHE:C	1:A:150:PHE:N	1:A:150:PHE:CA	1:A:150:PHE:C	7	4.6
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	17	4.5
(1,225)	1:A:149:PHE:C	1:A:150:PHE:N	1:A:150:PHE:CA	1:A:150:PHE:C	9	4.2
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	18	4.1
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	19	3.9
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	2	3.8
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	6	3.4
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	1	3.3
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	15	3.2
(1,40)	1:A:35:ALA:N	1:A:35:ALA:CA	1:A:35:ALA:C	1:A:36:THR:N	3	3.2
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	9	3.2
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	20	3.2
(1,122)	1:A:83:HIS:N	1:A:83:HIS:CA	1:A:83:HIS:C	1:A:84:VAL:N	11	3.2
(1,222)	1:A:148:GLU:N	1:A:148:GLU:CA	1:A:148:GLU:C	1:A:149:PHE:N	14	3.1
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	8	3.0
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	9	2.9
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	10	2.9
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	11	2.9
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	5	2.9
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	19	2.8
(1,224)	1:A:149:PHE:N	1:A:149:PHE:CA	1:A:149:PHE:C	1:A:150:PHE:N	7	2.8
(1,2)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	1:A:5:LEU:N	16	2.8
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	16	2.7
(1,16)	1:A:11:GLU:N	1:A:11:GLU:CA	1:A:11:GLU:C	1:A:12:ILE:N	8	2.7
(1,2)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	1:A:5:LEU:N	20	2.6
(1,186)	1:A:127:ASP:N	1:A:127:ASP:CA	1:A:127:ASP:C	1:A:128:VAL:N	17	2.6
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	3	2.6
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	11	2.6
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	19	2.6
(1,122)	1:A:83:HIS:N	1:A:83:HIS:CA	1:A:83:HIS:C	1:A:84:VAL:N	18	2.6
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	5	2.5
(1,213)	1:A:143:TRP:C	1:A:144:ASP:N	1:A:144:ASP:CA	1:A:144:ASP:C	7	2.5
(1,40)	1:A:35:ALA:N	1:A:35:ALA:CA	1:A:35:ALA:C	1:A:36:THR:N	12	2.4
(1,224)	1:A:149:PHE:N	1:A:149:PHE:CA	1:A:149:PHE:C	1:A:150:PHE:N	9	2.4
(1,16)	1:A:11:GLU:N	1:A:11:GLU:CA	1:A:11:GLU:C	1:A:12:ILE:N	20	2.4
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	10	2.3
(1,224)	1:A:149:PHE:N	1:A:149:PHE:CA	1:A:149:PHE:C	1:A:150:PHE:N	16	2.3
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	2	2.3
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	17	2.2
(1,37)	1:A:21:ALA:C	1:A:22:THR:N	1:A:22:THR:CA	1:A:22:THR:C	15	2.2
(1,200)	1:A:135:ASP:N	1:A:135:ASP:CA	1:A:135:ASP:C	1:A:136:TRP:N	15	2.2
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	10	2.2
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	13	2.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	15	2.2
(1,122)	1:A:83:HIS:N	1:A:83:HIS:CA	1:A:83:HIS:C	1:A:84:VAL:N	12	2.2
(1,160)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:LYS:N	15	2.1
(1,91)	1:A:61:GLY:C	1:A:62:MET:N	1:A:62:MET:CA	1:A:62:MET:C	6	2.0
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	7	2.0
(1,205)	1:A:137:LEU:C	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	15	2.0
(1,190)	1:A:129:LEU:N	1:A:129:LEU:CA	1:A:129:LEU:C	1:A:130:VAL:N	19	2.0
(1,186)	1:A:127:ASP:N	1:A:127:ASP:CA	1:A:127:ASP:C	1:A:128:VAL:N	6	2.0
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	18	2.0
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	5	1.9
(1,75)	1:A:53:ARG:C	1:A:54:ASN:N	1:A:54:ASN:CA	1:A:54:ASN:C	13	1.9
(1,225)	1:A:149:PHE:C	1:A:150:PHE:N	1:A:150:PHE:CA	1:A:150:PHE:C	19	1.9
(1,205)	1:A:137:LEU:C	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	13	1.9
(1,186)	1:A:127:ASP:N	1:A:127:ASP:CA	1:A:127:ASP:C	1:A:128:VAL:N	14	1.9
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	7	1.9
(1,16)	1:A:11:GLU:N	1:A:11:GLU:CA	1:A:11:GLU:C	1:A:12:ILE:N	11	1.9
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	20	1.8
(1,64)	1:A:47:VAL:N	1:A:47:VAL:CA	1:A:47:VAL:C	1:A:48:GLY:N	17	1.8
(1,40)	1:A:35:ALA:N	1:A:35:ALA:CA	1:A:35:ALA:C	1:A:36:THR:N	2	1.8
(1,40)	1:A:35:ALA:N	1:A:35:ALA:CA	1:A:35:ALA:C	1:A:36:THR:N	11	1.8
(1,38)	1:A:22:THR:N	1:A:22:THR:CA	1:A:22:THR:C	1:A:23:GLY:N	19	1.8
(1,225)	1:A:149:PHE:C	1:A:150:PHE:N	1:A:150:PHE:CA	1:A:150:PHE:C	12	1.8
(1,205)	1:A:137:LEU:C	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	5	1.8
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	12	1.8
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	17	1.8
(1,160)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:LYS:N	19	1.8
(1,16)	1:A:11:GLU:N	1:A:11:GLU:CA	1:A:11:GLU:C	1:A:12:ILE:N	19	1.8
(1,138)	1:A:98:LEU:N	1:A:98:LEU:CA	1:A:98:LEU:C	1:A:99:ILE:N	3	1.8
(1,77)	1:A:54:ASN:C	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	6	1.7
(1,225)	1:A:149:PHE:C	1:A:150:PHE:N	1:A:150:PHE:CA	1:A:150:PHE:C	2	1.7
(1,205)	1:A:137:LEU:C	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	17	1.7
(1,186)	1:A:127:ASP:N	1:A:127:ASP:CA	1:A:127:ASP:C	1:A:128:VAL:N	1	1.7
(1,186)	1:A:127:ASP:N	1:A:127:ASP:CA	1:A:127:ASP:C	1:A:128:VAL:N	7	1.7
(1,138)	1:A:98:LEU:N	1:A:98:LEU:CA	1:A:98:LEU:C	1:A:99:ILE:N	13	1.7
(1,10)	1:A:8:GLN:N	1:A:8:GLN:CA	1:A:8:GLN:C	1:A:9:SER:N	7	1.7
(1,91)	1:A:61:GLY:C	1:A:62:MET:N	1:A:62:MET:CA	1:A:62:MET:C	1	1.6
(1,91)	1:A:61:GLY:C	1:A:62:MET:N	1:A:62:MET:CA	1:A:62:MET:C	20	1.6
(1,83)	1:A:57:THR:C	1:A:58:ALA:N	1:A:58:ALA:CA	1:A:58:ALA:C	13	1.6
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	20	1.6
(1,40)	1:A:35:ALA:N	1:A:35:ALA:CA	1:A:35:ALA:C	1:A:36:THR:N	16	1.6
(1,225)	1:A:149:PHE:C	1:A:150:PHE:N	1:A:150:PHE:CA	1:A:150:PHE:C	3	1.6
(1,190)	1:A:129:LEU:N	1:A:129:LEU:CA	1:A:129:LEU:C	1:A:130:VAL:N	11	1.6
(1,186)	1:A:127:ASP:N	1:A:127:ASP:CA	1:A:127:ASP:C	1:A:128:VAL:N	3	1.6
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	4	1.6
(1,160)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:LYS:N	7	1.6
(1,110)	1:A:77:LEU:N	1:A:77:LEU:CA	1:A:77:LEU:C	1:A:78:SER:N	9	1.6
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	7	1.5
(1,64)	1:A:47:VAL:N	1:A:47:VAL:CA	1:A:47:VAL:C	1:A:48:GLY:N	9	1.5
(1,46)	1:A:38:ARG:N	1:A:38:ARG:CA	1:A:38:ARG:C	1:A:39:LYS:N	19	1.5
(1,29)	1:A:17:LEU:C	1:A:18:ARG:N	1:A:18:ARG:CA	1:A:18:ARG:C	17	1.5
(1,25)	1:A:15:ARG:C	1:A:16:TYR:N	1:A:16:TYR:CA	1:A:16:TYR:C	3	1.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,225)	1:A:149:PHE:C	1:A:150:PHE:N	1:A:150:PHE:CA	1:A:150:PHE:C	13	1.5
(1,190)	1:A:129:LEU:N	1:A:129:LEU:CA	1:A:129:LEU:C	1:A:130:VAL:N	4	1.5
(1,186)	1:A:127:ASP:N	1:A:127:ASP:CA	1:A:127:ASP:C	1:A:128:VAL:N	4	1.5
(1,186)	1:A:127:ASP:N	1:A:127:ASP:CA	1:A:127:ASP:C	1:A:128:VAL:N	5	1.5
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	1	1.5
(1,166)	1:A:116:SER:N	1:A:116:SER:CA	1:A:116:SER:C	1:A:117:SER:N	1	1.5
(1,160)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:LYS:N	4	1.5
(1,122)	1:A:83:HIS:N	1:A:83:HIS:CA	1:A:83:HIS:C	1:A:84:VAL:N	8	1.5
(1,122)	1:A:83:HIS:N	1:A:83:HIS:CA	1:A:83:HIS:C	1:A:84:VAL:N	10	1.5
(1,91)	1:A:61:GLY:C	1:A:62:MET:N	1:A:62:MET:CA	1:A:62:MET:C	2	1.4
(1,40)	1:A:35:ALA:N	1:A:35:ALA:CA	1:A:35:ALA:C	1:A:36:THR:N	4	1.4
(1,225)	1:A:149:PHE:C	1:A:150:PHE:N	1:A:150:PHE:CA	1:A:150:PHE:C	16	1.4
(1,224)	1:A:149:PHE:N	1:A:149:PHE:CA	1:A:149:PHE:C	1:A:150:PHE:N	3	1.4
(1,198)	1:A:134:ARG:N	1:A:134:ARG:CA	1:A:134:ARG:C	1:A:135:ASP:N	13	1.4
(1,195)	1:A:131:ARG:C	1:A:132:THR:N	1:A:132:THR:CA	1:A:132:THR:C	14	1.4
(1,186)	1:A:127:ASP:N	1:A:127:ASP:CA	1:A:127:ASP:C	1:A:128:VAL:N	11	1.4
(1,160)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:LYS:N	5	1.4
(1,160)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:LYS:N	9	1.4
(1,160)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:LYS:N	16	1.4
(1,160)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:LYS:N	18	1.4
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	14	1.3
(1,67)	1:A:49:ASP:C	1:A:50:GLY:N	1:A:50:GLY:CA	1:A:50:GLY:C	12	1.3
(1,62)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:VAL:N	12	1.3
(1,62)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:VAL:N	16	1.3
(1,60)	1:A:45:ARG:N	1:A:45:ARG:CA	1:A:45:ARG:C	1:A:46:ARG:N	4	1.3
(1,225)	1:A:149:PHE:C	1:A:150:PHE:N	1:A:150:PHE:CA	1:A:150:PHE:C	11	1.3
(1,205)	1:A:137:LEU:C	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	10	1.3
(1,202)	1:A:136:TRP:N	1:A:136:TRP:CA	1:A:136:TRP:C	1:A:137:LEU:N	5	1.3
(1,190)	1:A:129:LEU:N	1:A:129:LEU:CA	1:A:129:LEU:C	1:A:130:VAL:N	12	1.3
(1,186)	1:A:127:ASP:N	1:A:127:ASP:CA	1:A:127:ASP:C	1:A:128:VAL:N	8	1.3
(1,168)	1:A:117:SER:N	1:A:117:SER:CA	1:A:117:SER:C	1:A:118:ILE:N	14	1.3
(1,160)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:LYS:N	1	1.3
(1,138)	1:A:98:LEU:N	1:A:98:LEU:CA	1:A:98:LEU:C	1:A:99:ILE:N	1	1.3
(1,122)	1:A:83:HIS:N	1:A:83:HIS:CA	1:A:83:HIS:C	1:A:84:VAL:N	6	1.3
(1,10)	1:A:8:GLN:N	1:A:8:GLN:CA	1:A:8:GLN:C	1:A:9:SER:N	2	1.3
(1,69)	1:A:50:GLY:C	1:A:51:VAL:N	1:A:51:VAL:CA	1:A:51:VAL:C	20	1.2
(1,42)	1:A:36:THR:N	1:A:36:THR:CA	1:A:36:THR:C	1:A:37:SER:N	18	1.2
(1,225)	1:A:149:PHE:C	1:A:150:PHE:N	1:A:150:PHE:CA	1:A:150:PHE:C	5	1.2
(1,205)	1:A:137:LEU:C	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	1	1.2
(1,205)	1:A:137:LEU:C	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	8	1.2
(1,202)	1:A:136:TRP:N	1:A:136:TRP:CA	1:A:136:TRP:C	1:A:137:LEU:N	13	1.2
(1,2)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	1:A:5:LEU:N	19	1.2
(1,138)	1:A:98:LEU:N	1:A:98:LEU:CA	1:A:98:LEU:C	1:A:99:ILE:N	4	1.2
(1,122)	1:A:83:HIS:N	1:A:83:HIS:CA	1:A:83:HIS:C	1:A:84:VAL:N	15	1.2
(1,111)	1:A:77:LEU:C	1:A:78:SER:N	1:A:78:SER:CA	1:A:78:SER:C	1	1.2
(1,94)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ARG:N	18	1.1
(1,91)	1:A:61:GLY:C	1:A:62:MET:N	1:A:62:MET:CA	1:A:62:MET:C	19	1.1
(1,79)	1:A:55:HIS:C	1:A:56:GLU:N	1:A:56:GLU:CA	1:A:56:GLU:C	13	1.1
(1,78)	1:A:55:HIS:N	1:A:55:HIS:CA	1:A:55:HIS:C	1:A:56:GLU:N	13	1.1
(1,64)	1:A:47:VAL:N	1:A:47:VAL:CA	1:A:47:VAL:C	1:A:48:GLY:N	18	1.1
(1,62)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:VAL:N	7	1.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,59)	1:A:44:LEU:C	1:A:45:ARG:N	1:A:45:ARG:CA	1:A:45:ARG:C	9	1.1
(1,46)	1:A:38:ARG:N	1:A:38:ARG:CA	1:A:38:ARG:C	1:A:39:LYS:N	15	1.1
(1,40)	1:A:35:ALA:N	1:A:35:ALA:CA	1:A:35:ALA:C	1:A:36:THR:N	14	1.1
(1,40)	1:A:35:ALA:N	1:A:35:ALA:CA	1:A:35:ALA:C	1:A:36:THR:N	18	1.1
(1,40)	1:A:35:ALA:N	1:A:35:ALA:CA	1:A:35:ALA:C	1:A:36:THR:N	19	1.1
(1,37)	1:A:21:ALA:C	1:A:22:THR:N	1:A:22:THR:CA	1:A:22:THR:C	10	1.1
(1,25)	1:A:15:ARG:C	1:A:16:TYR:N	1:A:16:TYR:CA	1:A:16:TYR:C	17	1.1
(1,224)	1:A:149:PHE:N	1:A:149:PHE:CA	1:A:149:PHE:C	1:A:150:PHE:N	2	1.1
(1,224)	1:A:149:PHE:N	1:A:149:PHE:CA	1:A:149:PHE:C	1:A:150:PHE:N	14	1.1
(1,205)	1:A:137:LEU:C	1:A:138:VAL:N	1:A:138:VAL:CA	1:A:138:VAL:C	14	1.1
(1,2)	1:A:4:GLU:N	1:A:4:GLU:CA	1:A:4:GLU:C	1:A:5:LEU:N	3	1.1
(1,192)	1:A:130:VAL:N	1:A:130:VAL:CA	1:A:130:VAL:C	1:A:131:ARG:N	1	1.1
(1,190)	1:A:129:LEU:N	1:A:129:LEU:CA	1:A:129:LEU:C	1:A:130:VAL:N	2	1.1
(1,190)	1:A:129:LEU:N	1:A:129:LEU:CA	1:A:129:LEU:C	1:A:130:VAL:N	9	1.1
(1,190)	1:A:129:LEU:N	1:A:129:LEU:CA	1:A:129:LEU:C	1:A:130:VAL:N	20	1.1
(1,186)	1:A:127:ASP:N	1:A:127:ASP:CA	1:A:127:ASP:C	1:A:128:VAL:N	9	1.1
(1,182)	1:A:125:ILE:N	1:A:125:ILE:CA	1:A:125:ILE:C	1:A:126:THR:N	4	1.1
(1,160)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:LYS:N	3	1.1
(1,16)	1:A:11:GLU:N	1:A:11:GLU:CA	1:A:11:GLU:C	1:A:12:ILE:N	17	1.1
(1,138)	1:A:98:LEU:N	1:A:98:LEU:CA	1:A:98:LEU:C	1:A:99:ILE:N	5	1.1
(1,138)	1:A:98:LEU:N	1:A:98:LEU:CA	1:A:98:LEU:C	1:A:99:ILE:N	15	1.1
(1,138)	1:A:98:LEU:N	1:A:98:LEU:CA	1:A:98:LEU:C	1:A:99:ILE:N	20	1.1
(1,122)	1:A:83:HIS:N	1:A:83:HIS:CA	1:A:83:HIS:C	1:A:84:VAL:N	1	1.1
(1,122)	1:A:83:HIS:N	1:A:83:HIS:CA	1:A:83:HIS:C	1:A:84:VAL:N	9	1.1