



wwPDB NMR Structure Validation Summary Report

Jun 6, 2023 – 01:17 AM EDT

PDB ID : 2MB9
BMRB ID : 19392
Title : Human Bcl10 CARD
Authors : Zheng, C.; Bracken, C.; Wu, H.
Deposited on : 2013-07-26

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

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

A user guide is available at

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

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

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

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

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

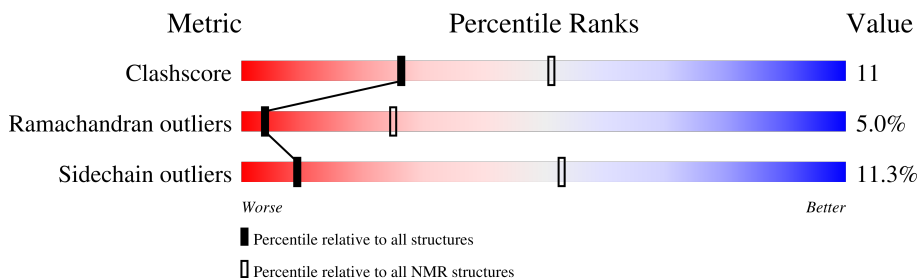
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	118	 62% 25% .. 10%

2 Ensemble composition and analysis i

This entry contains 10 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:12-A:115 (104)	2.23	2

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 3 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 5, 7
2	3, 9
3	4, 6
Single-model clusters	8; 10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1822 atoms, of which 936 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called B-cell lymphoma/leukemia 10.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	106	1822	552	936	165	167	2	0

There are 4 discrepancies between the modelled and reference sequences:

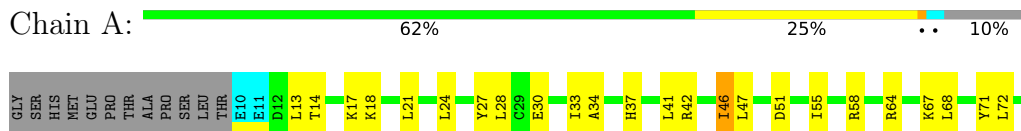
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP O95999
A	-1	SER	-	expression tag	UNP O95999
A	0	HIS	-	expression tag	UNP O95999
A	53	ARG	GLU	engineered mutation	UNP O95999

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

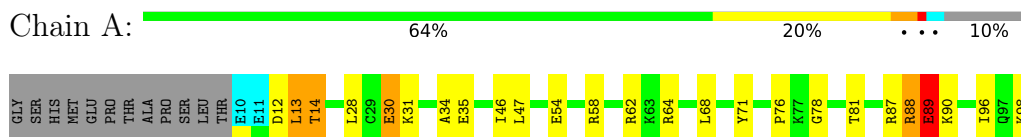
- Molecule 1: B-cell lymphoma/leukemia 10



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 2. Colouring as in section 4.1 above.

- Molecule 1: B-cell lymphoma/leukemia 10



5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 10 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
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	1359
Number of shifts mapped to atoms	1251
Number of unparsed shifts	0
Number of shifts with mapping errors	108
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

6 Model quality i

6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.87±0.04	0±0/875 (0.0± 0.0%)	0.98±0.04	1±2/1166 (0.1± 0.2%)
All	All	0.87	0/8750 (0.0%)	0.98	12/11660 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.9±0.7
All	All	0	9

There are no bond-length outliers.

5 of 11 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	14	THR	CA-CB-CG2	-15.91	90.12	112.40	2	1
1	A	34	ALA	N-CA-CB	-9.74	96.46	110.10	1	1
1	A	14	THR	CA-C-N	8.71	136.35	117.20	2	1
1	A	34	ALA	CB-CA-C	-8.11	97.93	110.10	1	1
1	A	71	TYR	CB-CG-CD1	7.61	125.57	121.00	3	2

There are no chirality outliers.

5 of 8 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	36	ARG	Peptide,Sidechain	2
1	A	37	HIS	Peptide	1
1	A	107	ARG	Sidechain	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	64	ARG	Sidechain	1
1	A	49	ARG	Sidechain	1

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	868	924	921	20±6
All	All	8680	9240	9210	199

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 11.

5 of 148 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ILE:HB	1:A:47:LEU:HD22	0.74	1.57	3	2
1:A:13:LEU:HD23	1:A:104:LEU:HA	0.72	1.60	2	2
1:A:47:LEU:HD21	1:A:72:LEU:HD11	0.69	1.64	3	1
1:A:13:LEU:HD11	1:A:107:ARG:CZ	0.66	2.21	5	1
1:A:17:LYS:O	1:A:21:LEU:HG	0.65	1.91	5	5

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	103/118 (87%)	85±6 (83±5%)	12±4 (12±4%)	5±2 (5±2%)	4	25
All	All	1030/1180 (87%)	853 (83%)	125 (12%)	52 (5%)	4	25

5 of 24 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	76	PRO	7
1	A	89	GLU	5
1	A	90	LYS	4
1	A	58	ARG	3
1	A	59	THR	3

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	98/110 (89%)	87±3 (89±3%)	11±3 (11±3%)	9 53
All	All	980/1100 (89%)	869 (89%)	111 (11%)	9 53

5 of 50 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	47	LEU	7
1	A	115	LYS	6
1	A	30	GLU	5
1	A	50	GLU	4
1	A	89	GLU	4

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 79% for the well-defined parts and 79% 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	1359
Number of shifts mapped to atoms	1251
Number of unparsed shifts	0
Number of shifts with mapping errors	108
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. First 5 (of 108) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	0	HIS	C	174.666	.	.
1	A	0	HIS	CA	56.088	.	.
1	A	0	HIS	CB	29.966	.	.
1	A	0	HIS	HA	4.652	.	.
1	A	0	HIS	HB2	3.185	.	.
1	A	0	HIS	HB3	3.113	.	.
1	A	1	MET	C	175.646	.	.
1	A	1	MET	CA	55.201	.	.
1	A	1	MET	CB	33.069	.	.
1	A	1	MET	CG	31.995	.	.
1	A	1	MET	H	8.307	.	.
1	A	1	MET	HA	4.437	.	.
1	A	1	MET	HB2	1.905	.	.
1	A	1	MET	HB3	2.014	.	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	HG2	2.43	.	.
1	A	1	MET	HG3	2.478	.	.
1	A	1	MET	N	122.021	.	.
1	A	2	GLU	C	174.62	.	.
1	A	2	GLU	CA	54.377	.	.
1	A	2	GLU	CB	29.731	.	.
1	A	2	GLU	CG	36.178	.	.
1	A	2	GLU	H	8.395	.	.
1	A	2	GLU	HA	4.57	.	.
1	A	2	GLU	HB2	1.883	.	.
1	A	2	GLU	HB3	2.034	.	.
1	A	2	GLU	HG2	2.436	.	.
1	A	2	GLU	HG3	2.287	.	.
1	A	2	GLU	N	123.797	.	.
1	A	3	PRO	C	177.015	.	.
1	A	3	PRO	CA	63.241	.	.
1	A	3	PRO	CB	32.172	.	.
1	A	3	PRO	CD	50.718	.	.
1	A	3	PRO	CG	27.418	.	.
1	A	3	PRO	HA	4.466	.	.
1	A	3	PRO	HB2	2.289	.	.
1	A	3	PRO	HB3	1.923	.	.
1	A	3	PRO	HD2	3.792	.	.
1	A	3	PRO	HD3	3.726	.	.
1	A	3	PRO	HG2	2.129	.	.
1	A	3	PRO	HG3	2.017	.	.
1	A	4	THR	C	173.995	.	.
1	A	4	THR	CA	61.765	.	.
1	A	4	THR	CB	69.933	.	.
1	A	4	THR	CG2	21.692	.	.
1	A	4	THR	H	8.162	.	.
1	A	4	THR	HA	4.263	.	.
1	A	4	THR	HB	4.154	.	.
1	A	4	THR	N	114.442	.	.
1	A	4	THR	HG21	1.199	.	.
1	A	4	THR	HG22	1.199	.	.
1	A	4	THR	HG23	1.199	.	.
1	A	5	ALA	C	175.299	.	.
1	A	5	ALA	CA	50.553	.	.
1	A	5	ALA	CB	18.453	.	.
1	A	5	ALA	H	8.26	.	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	ALA	HA	4.605	.	.
1	A	5	ALA	N	127.909	.	.
1	A	5	ALA	HB1	1.357	.	.
1	A	5	ALA	HB2	1.357	.	.
1	A	5	ALA	HB3	1.357	.	.
1	A	6	PRO	C	176.161	.	.
1	A	6	PRO	CA	63.09	.	.
1	A	6	PRO	CB	32.322	.	.
1	A	6	PRO	CD	50.452	.	.
1	A	6	PRO	CG	27.419	.	.
1	A	6	PRO	HA	4.457	.	.
1	A	6	PRO	HB2	1.876	.	.
1	A	6	PRO	HB3	2.281	.	.
1	A	6	PRO	HD2	3.795	.	.
1	A	6	PRO	HD3	3.631	.	.
1	A	6	PRO	HG3	1.996	.	.
1	A	7	SER	C	173.813	.	.
1	A	7	SER	CA	57.676	.	.
1	A	7	SER	CB	64.673	.	.
1	A	7	SER	H	8.249	.	.
1	A	7	SER	HA	4.497	.	.
1	A	7	SER	HB2	3.603	.	.
1	A	7	SER	HB3	3.808	.	.
1	A	7	SER	N	115.227	.	.
1	A	8	LEU	C	177.893	.	.
1	A	8	LEU	CA	54.606	.	.
1	A	8	LEU	CB	42.854	.	.
1	A	8	LEU	CD1	24.08	.	.
1	A	8	LEU	CD2	26.304	.	.
1	A	8	LEU	CG	29.169	.	.
1	A	8	LEU	H	8.22	.	.
1	A	8	LEU	HA	4.656	.	.
1	A	8	LEU	HB2	1.771	.	.
1	A	8	LEU	HB3	1.659	.	.
1	A	8	LEU	HG	1.144	.	.
1	A	8	LEU	N	122.306	.	.
1	A	8	LEU	HD11	0.828	.	.
1	A	8	LEU	HD12	0.828	.	.
1	A	8	LEU	HD13	0.828	.	.
1	A	8	LEU	HD21	0.887	.	.
1	A	8	LEU	HD22	0.887	.	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	LEU	HD23	0.887	.	.
1	A	9	THR	C	175.386	.	.
1	A	9	THR	CA	61.076	.	.
1	A	9	THR	CB	71.33	.	.
1	A	9	THR	CG2	22.29	.	.
1	A	9	THR	H	9.056	.	.
1	A	9	THR	HA	4.449	.	.
1	A	9	THR	HB	4.648	.	.
1	A	9	THR	N	114.593	.	.
1	A	9	THR	HG21	1.343	.	.
1	A	9	THR	HG22	1.343	.	.
1	A	9	THR	HG23	1.343	.	.

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	115	-0.57 ± 0.18	Should be checked
$^{13}\text{C}_\beta$	113	0.17 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	115	-0.49 ± 0.17	None needed (< 0.5 ppm)
^{15}N	109	0.63 ± 0.25	Should be applied

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 79%, i.e. 1234 atoms were assigned a chemical shift out of a possible 1567. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	512/520 (98%)	206/209 (99%)	206/208 (99%)	100/103 (97%)
Sidechain	708/985 (72%)	489/631 (77%)	212/301 (70%)	7/53 (13%)
Aromatic	14/62 (23%)	14/30 (47%)	0/26 (0%)	0/6 (0%)
Overall	1234/1567 (79%)	709/870 (81%)	418/535 (78%)	107/162 (66%)

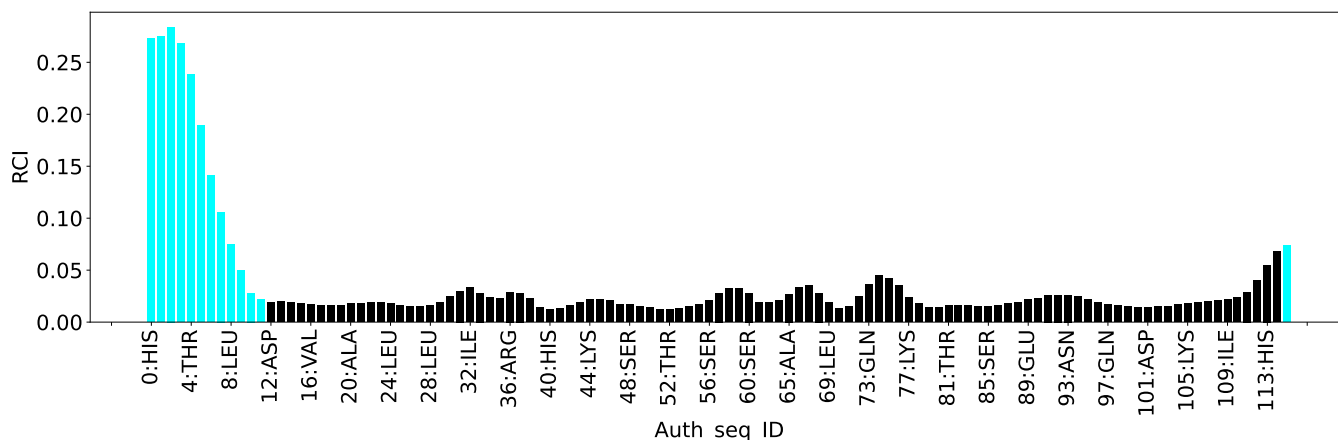
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1291
Intra-residue ($ i-j =0$)	681
Sequential ($ i-j =1$)	296
Medium range ($ i-j >1$ and $ i-j <5$)	150
Long range ($ i-j \geq 5$)	164
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	203
Number of unmapped restraints	0
Number of restraints per residue	12.7
Number of long range restraints per residue ¹	1.4

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	39.7	0.2
0.2-0.5 (Medium)	39.8	0.5
>0.5 (Large)	103.8	5.93

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)	32.1	9.9
10.0-20.0 (Medium)	2.7	18.8
>20.0 (Large)	0.2	28.4

9 Distance violation analysis

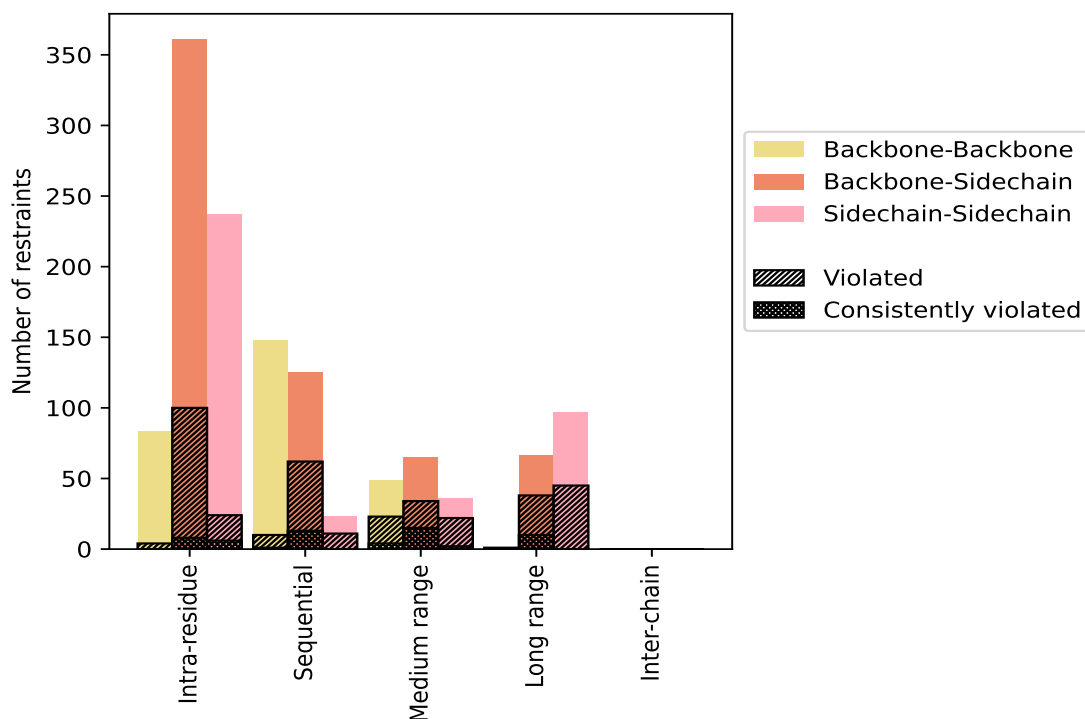
9.1 Summary of distance violations

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	681	52.7	128	18.8	9.9	14	2.1	1.1
Backbone-Backbone	83	6.4	4	4.8	0.3	0	0.0	0.0
Backbone-Sidechain	361	28.0	100	27.7	7.7	8	2.2	0.6
Sidechain-Sidechain	237	18.4	24	10.1	1.9	6	2.5	0.5
Sequential ($i-j =1$)	296	22.9	83	28.0	6.4	14	4.7	1.1
Backbone-Backbone	148	11.5	10	6.8	0.8	1	0.7	0.1
Backbone-Sidechain	125	9.7	62	49.6	4.8	13	10.4	1.0
Sidechain-Sidechain	23	1.8	11	47.8	0.9	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	150	11.6	79	52.7	6.1	21	14.0	1.6
Backbone-Backbone	49	3.8	23	46.9	1.8	4	8.2	0.3
Backbone-Sidechain	65	5.0	34	52.3	2.6	15	23.1	1.2
Sidechain-Sidechain	36	2.8	22	61.1	1.7	2	5.6	0.2
Long range ($i-j \geq 5$)	164	12.7	84	51.2	6.5	10	6.1	0.8
Backbone-Backbone	1	0.1	1	100.0	0.1	0	0.0	0.0
Backbone-Sidechain	66	5.1	38	57.6	2.9	10	15.2	0.8
Sidechain-Sidechain	97	7.5	45	46.4	3.5	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1291	100.0	374	29.0	29.0	59	4.6	4.6
Backbone-Backbone	281	21.8	38	13.5	2.9	5	1.8	0.4
Backbone-Sidechain	617	47.8	234	37.9	18.1	46	7.5	3.6
Sidechain-Sidechain	393	30.4	102	26.0	7.9	8	2.0	0.6

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

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



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

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

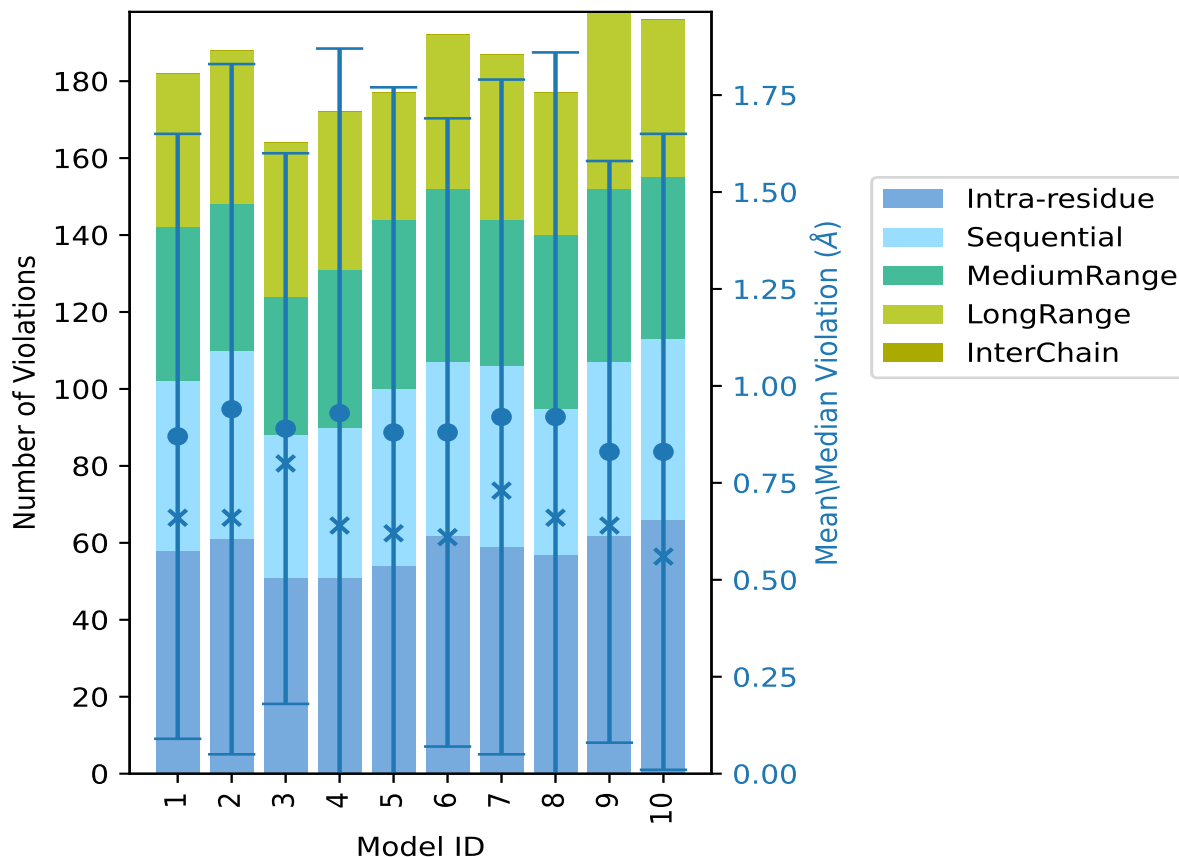
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵					
1	58	44	40	40	0	182	0.87	4.14	0.78	0.66
2	61	49	38	40	0	188	0.94	4.59	0.89	0.66
3	51	37	36	40	0	164	0.89	3.73	0.71	0.8
4	51	39	41	41	0	172	0.93	5.93	0.94	0.64
5	54	46	44	33	0	177	0.88	5.08	0.89	0.62
6	62	45	45	40	0	192	0.88	3.52	0.81	0.61
7	59	47	38	43	0	187	0.92	4.74	0.87	0.73
8	57	38	45	37	0	177	0.92	4.94	0.94	0.66
9	62	45	45	46	0	198	0.83	3.32	0.75	0.64
10	66	47	42	41	0	196	0.83	4.98	0.82	0.56

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 917(IR:553, SQ:213, MR:71, LR:80, 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	%
33	18	14	21	0	86	1	10.0
15	8	18	11	0	52	2	20.0
13	5	3	8	0	29	3	30.0
10	5	7	3	0	25	4	40.0

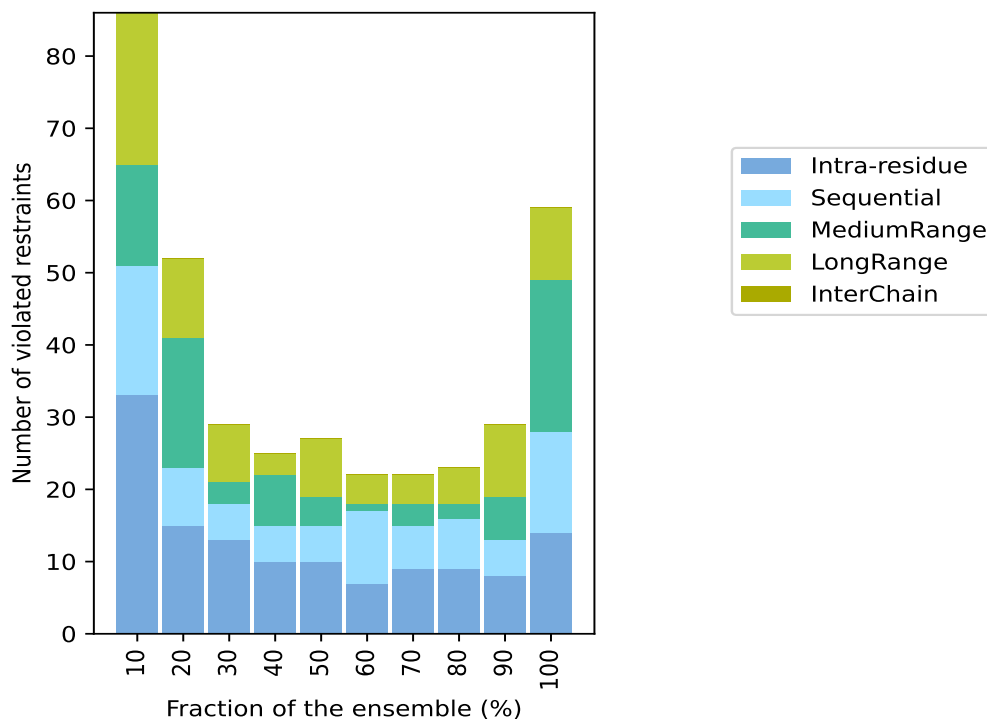
Continued on next page...

Continued from previous page...

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
10	5	4	8	0	27	5	50.0
7	10	1	4	0	22	6	60.0
9	6	3	4	0	22	7	70.0
9	7	2	5	0	23	8	80.0
8	5	6	10	0	29	9	90.0
14	14	21	10	0	59	10	100.0

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

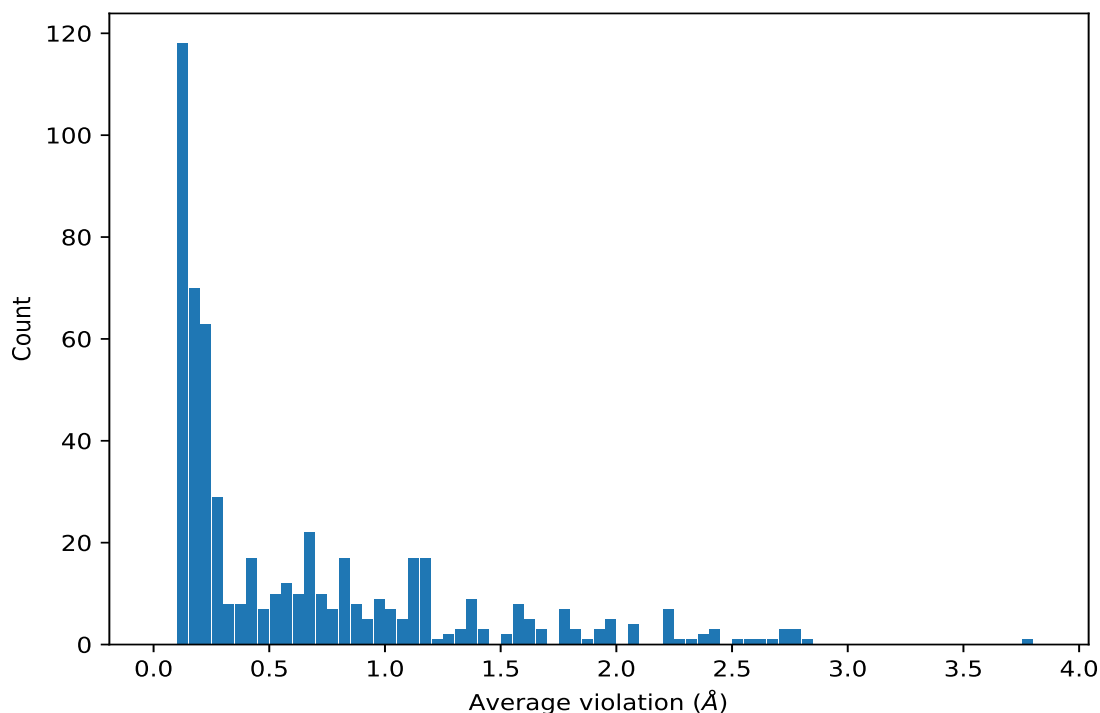
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation 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.

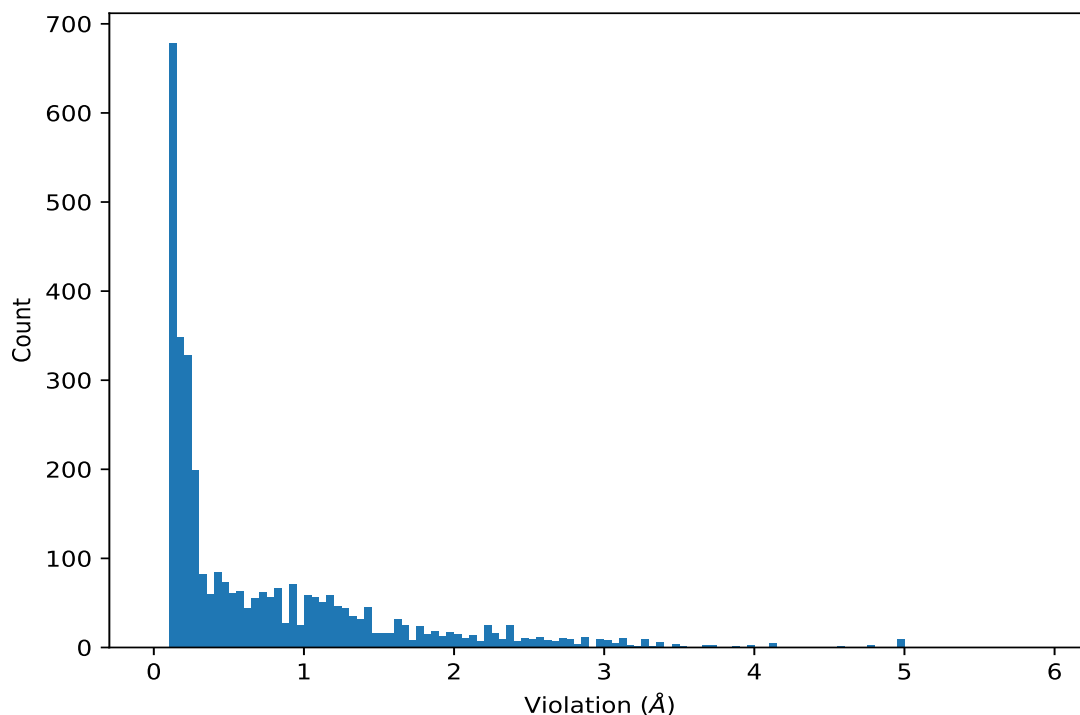
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,347)	1:A:64:ARG:H	1:A:35:GLU:HG3	10	3.79	1.27	3.54
(1,210)	1:A:74:GLU:H	1:A:70:ASP:HA	10	2.81	0.94	2.7
(1,321)	1:A:17:LYS:H	1:A:106:LEU:HD11	10	2.74	0.62	3.05
(1,321)	1:A:17:LYS:H	1:A:106:LEU:HD12	10	2.74	0.62	3.05
(1,321)	1:A:17:LYS:H	1:A:106:LEU:HD13	10	2.74	0.62	3.05
(1,160)	1:A:70:ASP:H	1:A:71:TYR:HB2	10	2.69	0.44	2.78
(1,861)	1:A:54:GLU:H	1:A:51:ASP:HB3	10	2.64	0.4	2.76
(1,1167)	1:A:53:ARG:H	1:A:55:ILE:HG12	10	2.52	1.04	2.24
(1,997)	1:A:106:LEU:H	1:A:104:LEU:HB2	10	2.44	0.22	2.46
(1,312)	1:A:107:ARG:H	1:A:110:LYS:HB2	10	2.43	0.19	2.41
(1,574)	1:A:67:LYS:H	1:A:68:LEU:HB2	10	2.42	0.36	2.24
(1,755)	1:A:56:SER:H	1:A:64:ARG:HG3	10	2.38	1.23	2.5

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

The following table provides the 10 worst performing restraints, sorted by the violation 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)
(1,347)	1:A:64:ARG:H	1:A:35:GLU:HG3	4	5.93
(1,347)	1:A:64:ARG:H	1:A:35:GLU:HG3	5	5.08
(1,1082)	1:A:52:THR:HG21	1:A:46:ILE:HD11	10	4.98
(1,1082)	1:A:52:THR:HG21	1:A:46:ILE:HD12	10	4.98
(1,1082)	1:A:52:THR:HG21	1:A:46:ILE:HD13	10	4.98
(1,1082)	1:A:52:THR:HG22	1:A:46:ILE:HD11	10	4.98
(1,1082)	1:A:52:THR:HG22	1:A:46:ILE:HD12	10	4.98
(1,1082)	1:A:52:THR:HG22	1:A:46:ILE:HD13	10	4.98
(1,1082)	1:A:52:THR:HG23	1:A:46:ILE:HD11	10	4.98
(1,1082)	1:A:52:THR:HG23	1:A:46:ILE:HD12	10	4.98
(1,1082)	1:A:52:THR:HG23	1:A:46:ILE:HD13	10	4.98

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:A:64:ARG:H	1:A:35:GLU:HG3	8	4.94
(1,886)	1:A:96:ILE:HD11	1:A:89:GLU:HB2	5	4.78
(1,886)	1:A:96:ILE:HD12	1:A:89:GLU:HB2	5	4.78
(1,886)	1:A:96:ILE:HD13	1:A:89:GLU:HB2	5	4.78
(1,1167)	1:A:53:ARG:H	1:A:55:ILE:HG12	7	4.74
(1,347)	1:A:64:ARG:H	1:A:35:GLU:HG3	2	4.59
(1,1156)	1:A:75:ASN:H	1:A:18:LYS:HE3	7	4.55
(1,938)	1:A:102:GLU:HB3	1:A:106:LEU:HG	8	4.52
(1,952)	1:A:82:LEU:H	1:A:84:GLU:HB2	8	4.31

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

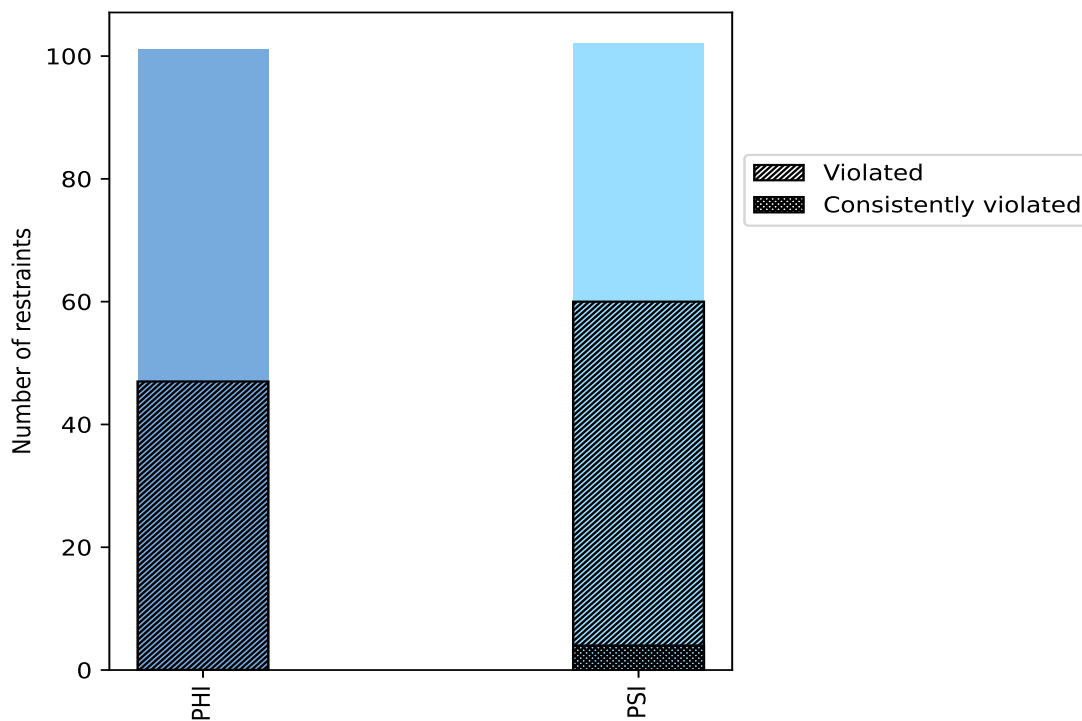
10.1 Summary of dihedral-angle violations [i](#)

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	101	49.8	47	46.5	23.2	0	0.0	0.0
PSI	102	50.2	60	58.8	29.6	4	3.9	2.0
Total	203	100.0	107	52.7	52.7	4	2.0	2.0

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

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



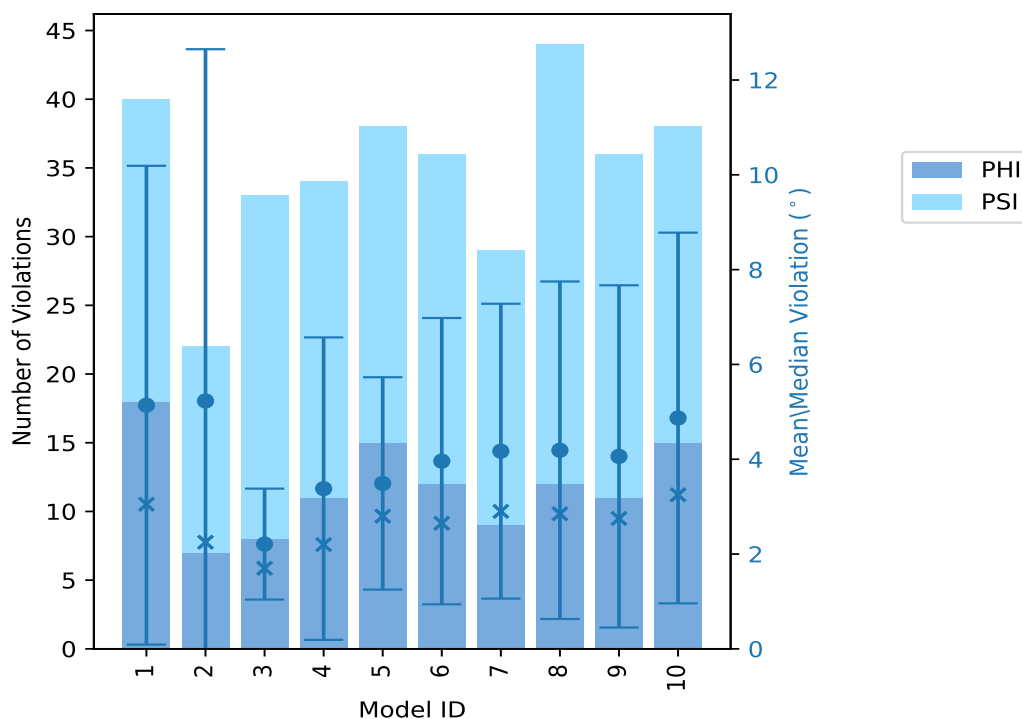
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	18	22	40	5.14	18.8	5.05	3.05
2	7	15	22	5.23	28.4	7.42	2.25
3	8	25	33	2.21	5.4	1.17	1.7
4	11	23	34	3.38	14.9	3.19	2.2
5	15	23	38	3.49	9.6	2.24	2.8
6	12	24	36	3.96	12.1	3.02	2.65
7	9	20	29	4.17	12.2	3.11	2.9
8	12	32	44	4.19	16.5	3.56	2.85
9	11	25	36	4.06	16.4	3.61	2.75
10	15	23	38	4.87	14.2	3.91	3.25

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

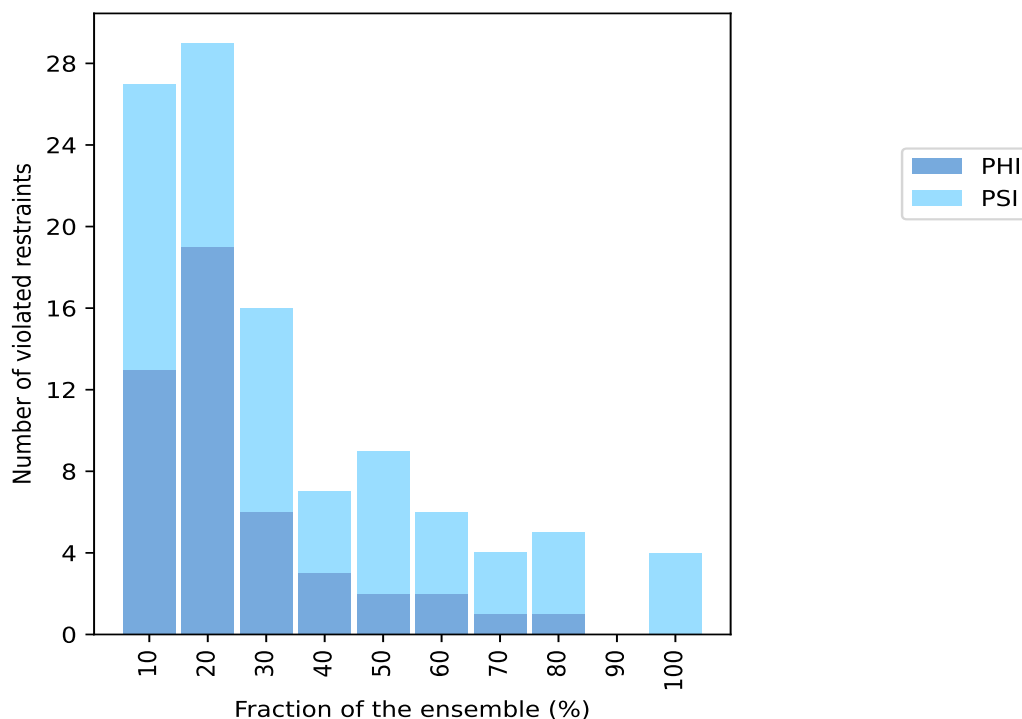
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
13	14	27	1	10.0
19	10	29	2	20.0
6	10	16	3	30.0
3	4	7	4	40.0
2	7	9	5	50.0
2	4	6	6	60.0
1	3	4	7	70.0
1	4	5	8	80.0
0	0	0	9	90.0
0	4	4	10	100.0

¹ Number of models with violations

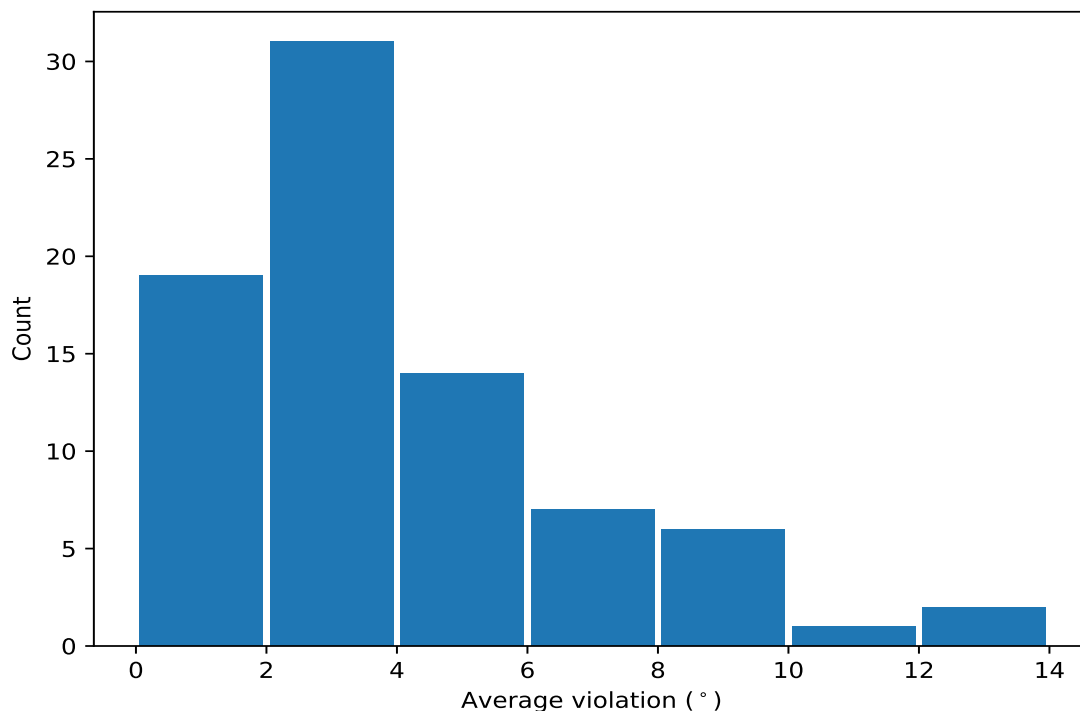
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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 violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

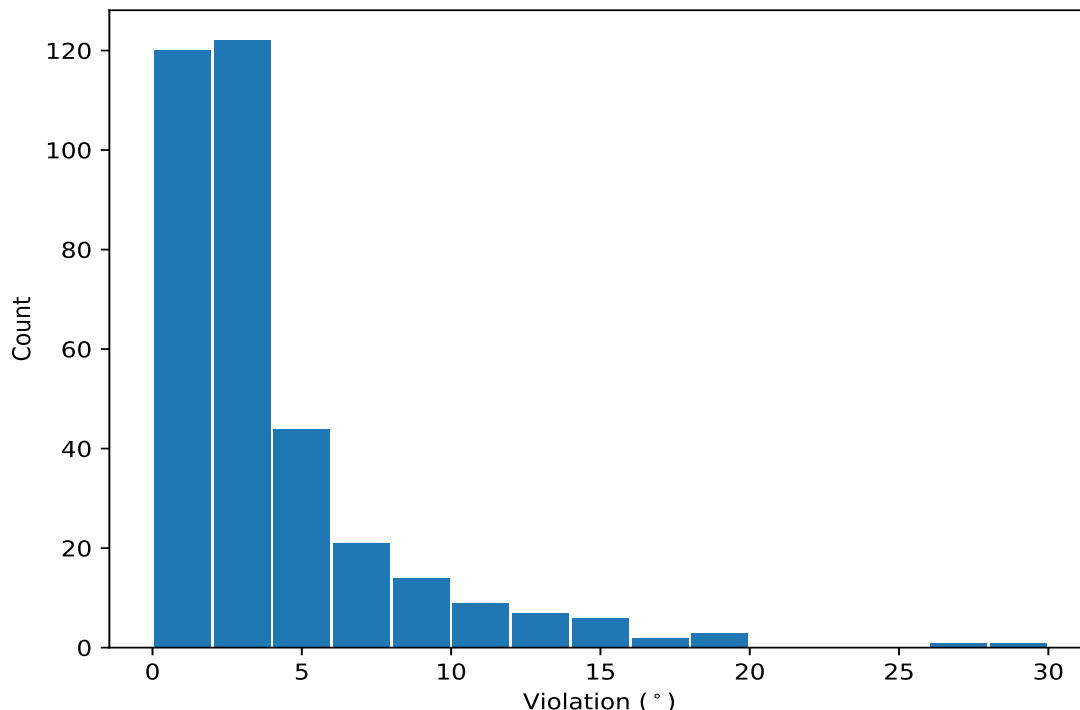
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,47)	1:A:33:ILE:N	1:A:33:ILE:CA	1:A:33:ILE:C	1:A:34:ALA:N	10	7.73	4.65	6.05
(1,129)	1:A:75:ASN:N	1:A:75:ASN:CA	1:A:75:ASN:C	1:A:76:PRO:N	10	5.97	4.0	5.1
(1,13)	1:A:16:VAL:N	1:A:16:VAL:CA	1:A:16:VAL:C	1:A:17:LYS:N	10	4.32	1.38	4.2
(1,69)	1:A:44:LYS:N	1:A:44:LYS:CA	1:A:44:LYS:C	1:A:45:LYS:N	10	3.32	1.55	3.1
(1,157)	1:A:89:GLU:N	1:A:89:GLU:CA	1:A:89:GLU:C	1:A:90:LYS:N	8	6.2	1.79	5.95
(1,53)	1:A:36:ARG:N	1:A:36:ARG:CA	1:A:36:ARG:C	1:A:37:HIS:N	8	5.42	2.99	5.15
(1,9)	1:A:14:THR:N	1:A:14:THR:CA	1:A:14:THR:C	1:A:15:GLU:N	8	5.34	7.88	2.4
(1,48)	1:A:33:ILE:C	1:A:34:ALA:N	1:A:34:ALA:CA	1:A:34:ALA:C	8	5.28	4.64	3.4
(1,123)	1:A:72:LEU:N	1:A:72:LEU:CA	1:A:72:LEU:C	1:A:73:GLN:N	8	3.18	2.91	1.9
(1,94)	1:A:57:CYS:C	1:A:58:ARG:N	1:A:58:ARG:CA	1:A:58:ARG:C	7	4.86	3.44	2.8

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

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

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

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



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

The following table provides the list of violations for the 10 worst performing restraints, sorted by the violation 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 (°)
(1,8)	1:A:13:LEU:C	1:A:14:THR:N	1:A:14:THR:CA	1:A:14:THR:C	2	28.4
(1,9)	1:A:14:THR:N	1:A:14:THR:CA	1:A:14:THR:C	1:A:15:GLU:N	2	26.1
(1,47)	1:A:33:ILE:N	1:A:33:ILE:CA	1:A:33:ILE:C	1:A:34:ALA:N	1	18.8
(1,55)	1:A:37:HIS:N	1:A:37:HIS:CA	1:A:37:HIS:C	1:A:38:PHE:N	1	18.6
(1,56)	1:A:37:HIS:C	1:A:38:PHE:N	1:A:38:PHE:CA	1:A:38:PHE:C	1	18.0
(1,125)	1:A:73:GLN:N	1:A:73:GLN:CA	1:A:73:GLN:C	1:A:74:GLU:N	8	16.5
(1,132)	1:A:76:PRO:C	1:A:77:LYS:N	1:A:77:LYS:CA	1:A:77:LYS:C	9	16.4
(1,131)	1:A:76:PRO:N	1:A:76:PRO:CA	1:A:76:PRO:C	1:A:77:LYS:N	9	15.9
(1,77)	1:A:49:ARG:N	1:A:49:ARG:CA	1:A:49:ARG:C	1:A:50:GLU:N	4	14.9
(1,54)	1:A:36:ARG:C	1:A:37:HIS:N	1:A:37:HIS:CA	1:A:37:HIS:C	1	14.9