



wwPDB NMR Structure Validation Summary Report ⓘ

Nov 28, 2023 – 04:05 PM EST

PDB ID : 2LCA
BMRB ID : 17575
Title : Solution structure of the C domain of RV0899 from mycobacterium tuberculosis
Authors : Marassi, F.; Yao, Y.
Deposited on : 2011-04-26

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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
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) : 2.36

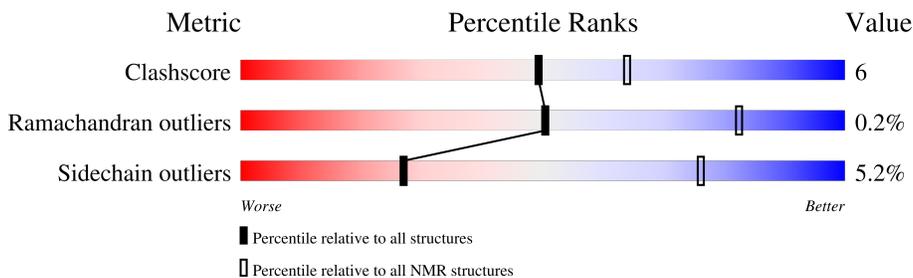
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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	137	64% 8% 23% .

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:209-A:224, A:238-A:262, A:269-A:326 (99)	0.50	11

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1720 atoms, of which 793 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein Rv0899/MT0922.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	131	1720	574	793	171	180	2	0

There are 6 discrepancies between the modelled and reference sequences:

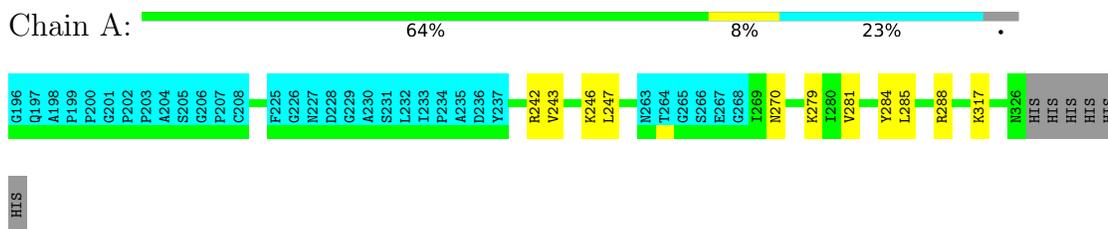
Chain	Residue	Modelled	Actual	Comment	Reference
A	327	HIS	-	expression tag	UNP P65593
A	328	HIS	-	expression tag	UNP P65593
A	329	HIS	-	expression tag	UNP P65593
A	330	HIS	-	expression tag	UNP P65593
A	331	HIS	-	expression tag	UNP P65593
A	332	HIS	-	expression tag	UNP P65593

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.

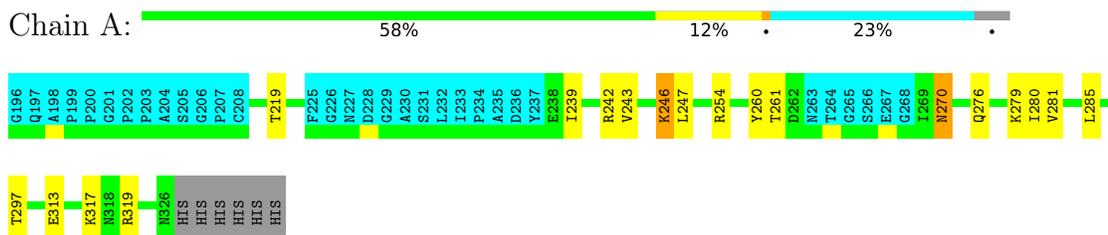
- Molecule 1: Uncharacterized protein Rv0899/MT0922



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

The representative model is number 11. Colouring as in section 4.1 above.

- Molecule 1: Uncharacterized protein Rv0899/MT0922



5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
X-PLOR NIH	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	1165
Number of shifts mapped to atoms	1068
Number of unparsed shifts	0
Number of shifts with mapping errors	97
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

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	718	645	745	9±3
All	All	14360	12900	14900	178

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 6.

5 of 50 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:218:VAL:HG12	1:A:239:ILE:HG23	0.63	1.70	9	3
1:A:281:VAL:O	1:A:285:LEU:HG	0.63	1.93	5	18
1:A:305:PRO:HA	1:A:318:ASN:OD1	0.63	1.94	3	9
1:A:218:VAL:HG11	1:A:242:ARG:HB3	0.58	1.72	9	3
1:A:284:TYR:O	1:A:288:ARG:HG2	0.57	1.99	7	9

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	98/137 (72%)	94±1 (96±1%)	4±1 (4±1%)	0±0 (0±0%)	50 82
All	All	1960/2740 (72%)	1887 (96%)	70 (4%)	3 (0%)	50 82

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	303	VAL	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	75/102 (74%)	71±1 (95±2%)	4±1 (5±2%)	27 76
All	All	1500/2040 (74%)	1422 (95%)	78 (5%)	27 76

5 of 16 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	246	LYS	20
1	A	242	ARG	19
1	A	270	ASN	9
1	A	254	ARG	6
1	A	317	LYS	6

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

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 71% 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

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	1165
Number of shifts mapped to atoms	1068
Number of unparsed shifts	0
Number of shifts with mapping errors	97
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 97) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	205	SER	HB3	4.491	.	2
1	A	208	CYS	HB3	3.197	.	2
1	A	210	ASP	HB3	2.88	.	2
1	A	211	LEU	HB3	1.726	.	2
1	A	212	GLN	HB3	2.23	.	2
1	A	212	GLN	HG3	2.48	.	2
1	A	213	SER	HB3	3.927	.	2
1	A	215	ILE	HG13	1.659	.	2
1	A	216	ASN	HB3	3.006	.	2
1	A	222	PRO	HB3	2.21	.	2
1	A	222	PRO	HG3	1.966	.	2
1	A	222	PRO	HD3	3.7	.	2
1	A	223	ILE	HG13	1.49	.	2
1	A	225	PHE	HB3	2.935	.	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	234	PRO	HB3	2.308	.	2
1	A	238	GLU	HB3	2.16	.	2
1	A	238	GLU	HG3	2.34	.	2
1	A	239	ILE	HG13	1.67	.	2
1	A	240	LEU	HB3	2.154	.	2
1	A	241	ASN	HB3	3.34	.	2
1	A	242	ARG	HB3	2.12	.	2
1	A	242	ARG	HG3	2.03	.	2
1	A	242	ARG	HD3	3.267	.	2
1	A	245	ASP	HB3	2.8	.	2
1	A	246	LYS	HB3	2.054	.	2
1	A	246	LYS	HG3	1.677	.	2
1	A	246	LYS	HD3	1.68	.	2
1	A	246	LYS	HE3	2.957	.	2
1	A	247	LEU	HB3	1.837	.	2
1	A	248	LYS	HB3	1.79	.	2
1	A	248	LYS	HG3	1.605	.	2
1	A	250	CYS	HB3	3.228	.	2
1	A	251	PRO	HB3	2.31	.	2
1	A	251	PRO	HG3	2.086	.	2
1	A	251	PRO	HD3	3.735	.	2
1	A	252	ASP	HB3	2.78	.	2
1	A	254	ARG	HB3	1.841	.	2
1	A	254	ARG	HG3	1.509	.	2
1	A	254	ARG	HD3	2.9	.	2
1	A	257	ILE	HG13	1.413	.	2
1	A	258	ASN	HB3	2.726	.	2
1	A	260	TYR	HB3	3.564	.	2
1	A	262	ASP	HB3	3.136	.	2
1	A	263	ASN	HB3	3.195	.	2
1	A	269	ILE	HG13	1.493	.	2
1	A	270	ASN	HB3	2.84	.	2
1	A	271	ILE	HG13	1.787	.	2
1	A	272	PRO	HB3	2.303	.	2
1	A	272	PRO	HG3	2.264	.	2
1	A	272	PRO	HD3	3.52	.	2
1	A	273	LEU	HB3	1.749	.	2
1	A	274	SER	HB3	3.785	.	2
1	A	276	GLN	HB3	2.282	.	2
1	A	276	GLN	HG3	2.499	.	2
1	A	277	ARG	HB3	1.567	.	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	277	ARG	HG3	1.327	.	2
1	A	277	ARG	HD3	2.68	.	2
1	A	279	LYS	HB3	2.06	.	2
1	A	279	LYS	HG3	1.506	.	2
1	A	279	LYS	HD3	2.06	.	2
1	A	280	ILE	HG13	1.9	.	2
1	A	283	ASP	HB3	2.854	.	2
1	A	284	TYR	HB3	3.306	.	2
1	A	285	LEU	HB3	2.187	.	2
1	A	288	ARG	HB3	2.106	.	2
1	A	288	ARG	HG3	1.48	.	2
1	A	288	ARG	HD3	2.893	.	2
1	A	293	ASP	HB3	2.854	.	2
1	A	294	HIS	HB3	3.992	.	2
1	A	295	ILE	HG13	1.635	.	2
1	A	300	LEU	HB3	1.461	.	2
1	A	302	SER	HB3	3.936	.	2
1	A	304	ASN	HB3	3.007	.	2
1	A	305	PRO	HB3	2.333	.	2
1	A	305	PRO	HG3	1.942	.	2
1	A	305	PRO	HD3	3.671	.	2
1	A	306	ILE	HG13	1.139	.	2
1	A	309	ASN	HB3	3.157	.	2
1	A	312	PRO	HB3	2.402	.	2
1	A	312	PRO	HD3	4.025	.	2
1	A	313	GLU	HB3	2.016	.	2
1	A	313	GLU	HG3	2.405	.	2
1	A	315	ARG	HB3	1.917	.	2
1	A	317	LYS	HB3	1.841	.	2
1	A	317	LYS	HG3	1.569	.	2
1	A	317	LYS	HD3	1.57	.	2
1	A	318	ASN	HB3	2.532	.	2
1	A	319	ARG	HB3	2.336	.	2
1	A	319	ARG	HG3	2.188	.	2
1	A	319	ARG	HD3	3.375	.	2
1	A	320	ARG	HB3	1.981	.	2
1	A	320	ARG	HG3	1.756	.	2
1	A	320	ARG	HD3	3.252	.	2
1	A	322	GLU	HB3	2.157	.	2
1	A	322	GLU	HG3	2.308	.	2
1	A	323	ILE	HG13	1.659	.	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	326	ASN	HB3	2.69	.	2

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
$^{13}\text{C}_\alpha$	112	-0.53 ± 0.18	Should be checked
$^{13}\text{C}_\beta$	100	0.29 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	100	0.75 ± 0.66	None needed (imprecise)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 1063 atoms were assigned a chemical shift out of a possible 1298. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	384/493 (78%)	196/201 (98%)	98/198 (49%)	90/94 (96%)
Sidechain	665/780 (85%)	460/512 (90%)	195/233 (84%)	10/35 (29%)
Aromatic	14/25 (56%)	7/12 (58%)	7/12 (58%)	0/1 (0%)
Overall	1063/1298 (82%)	663/725 (91%)	300/443 (68%)	100/130 (77%)

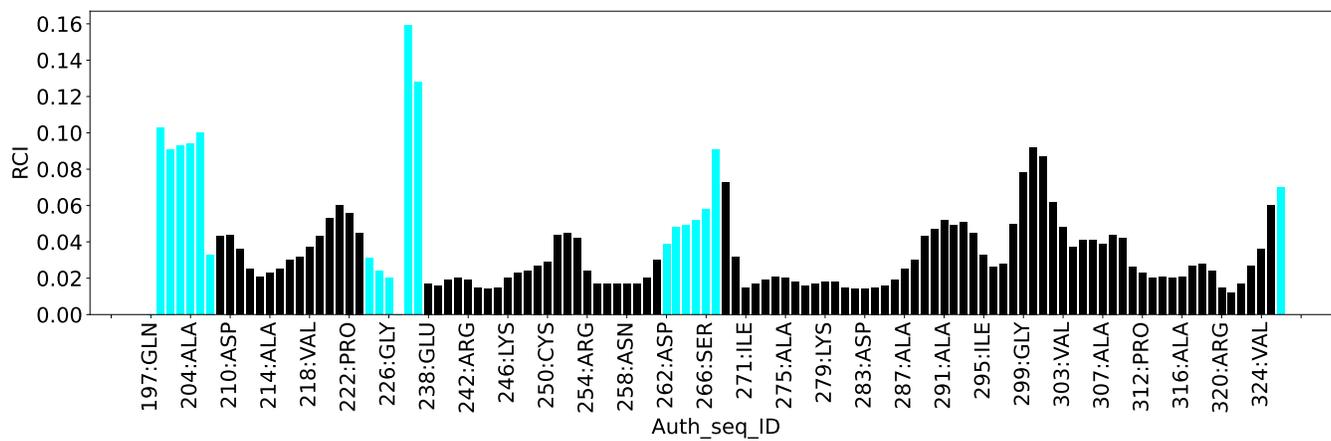
7.1.4 Statistically unusual chemical shifts [i](#)

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	1897
Intra-residue ($ i-j =0$)	511
Sequential ($ i-j =1$)	468
Medium range ($ i-j >1$ and $ i-j <5$)	400
Long range ($ i-j \geq 5$)	518
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	167
Number of unmapped restraints	319
Number of restraints per residue	15.1
Number of long range restraints per residue ¹	3.8

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)	41.3	0.2
0.2-0.5 (Medium)	29.1	0.5
>0.5 (Large)	37.4	4.26

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)	3.2	7.18
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis i

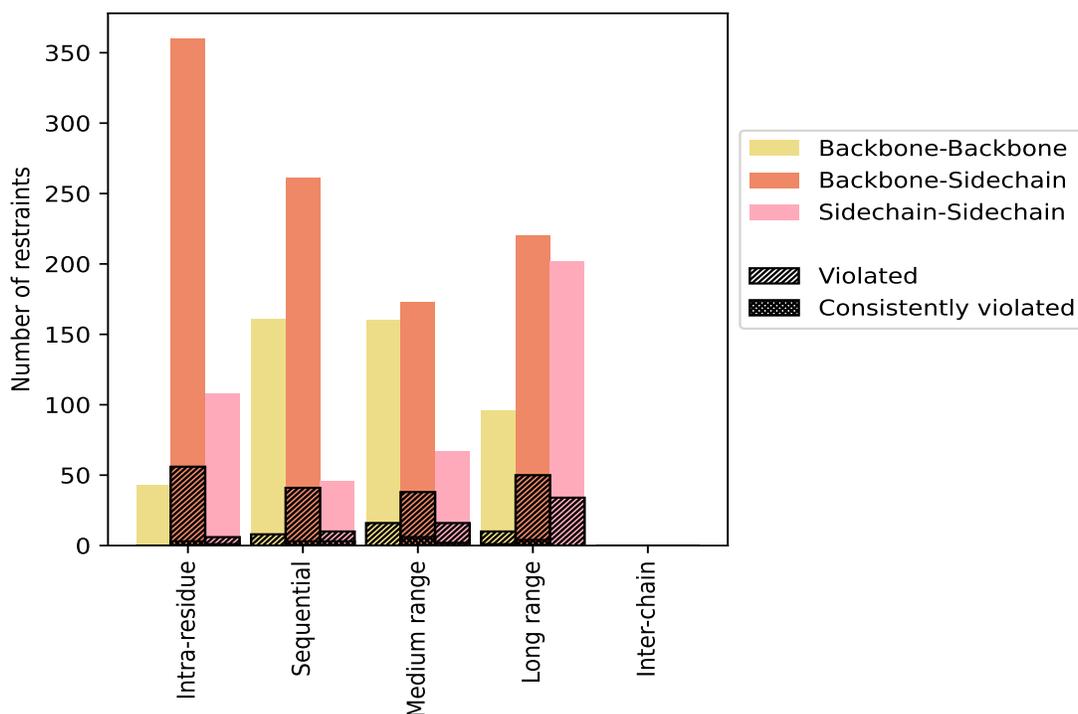
9.1 Summary of distance violations i

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	511	26.9	62	12.1	3.3	4	0.8	0.2
Backbone-Backbone	43	2.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	360	19.0	56	15.6	3.0	3	0.8	0.2
Sidechain-Sidechain	108	5.7	6	5.6	0.3	1	0.9	0.1
Sequential ($i-j =1$)	468	24.7	59	12.6	3.1	6	1.3	0.3
Backbone-Backbone	161	8.5	8	5.0	0.4	0	0.0	0.0
Backbone-Sidechain	261	13.8	41	15.7	2.2	3	1.1	0.2
Sidechain-Sidechain	46	2.4	10	21.7	0.5	3	6.5	0.2
Medium range ($i-j >1$ & $i-j <5$)	400	21.1	70	17.5	3.7	8	2.0	0.4
Backbone-Backbone	160	8.4	16	10.0	0.8	0	0.0	0.0
Backbone-Sidechain	173	9.1	38	22.0	2.0	6	3.5	0.3
Sidechain-Sidechain	67	3.5	16	23.9	0.8	2	3.0	0.1
Long range ($i-j \geq 5$)	518	27.3	94	18.1	5.0	5	1.0	0.3
Backbone-Backbone	96	5.1	10	10.4	0.5	1	1.0	0.1
Backbone-Sidechain	220	11.6	50	22.7	2.6	4	1.8	0.2
Sidechain-Sidechain	202	10.6	34	16.8	1.8	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	1897	100.0	285	15.0	15.0	23	1.2	1.2
Backbone-Backbone	460	24.2	34	7.4	1.8	1	0.2	0.1
Backbone-Sidechain	1014	53.5	185	18.2	9.8	16	1.6	0.8
Sidechain-Sidechain	423	22.3	66	15.6	3.5	6	1.4	0.3

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	28	26	34	29	0	117	0.56	4.23	0.61	0.32
2	15	25	35	35	0	110	0.53	3.51	0.66	0.24
3	27	23	34	35	0	119	0.56	4.03	0.59	0.26
4	28	22	27	37	0	114	0.53	3.64	0.59	0.25
5	18	25	31	39	0	113	0.5	3.65	0.57	0.25
6	21	25	34	40	0	120	0.48	2.88	0.51	0.26
7	11	18	27	36	0	92	0.47	3.76	0.58	0.23
8	24	25	31	36	0	116	0.56	4.01	0.62	0.25
9	23	27	30	33	0	113	0.54	3.45	0.58	0.31
10	18	26	31	31	0	106	0.5	2.69	0.52	0.26
11	25	26	31	29	0	111	0.56	4.26	0.62	0.32

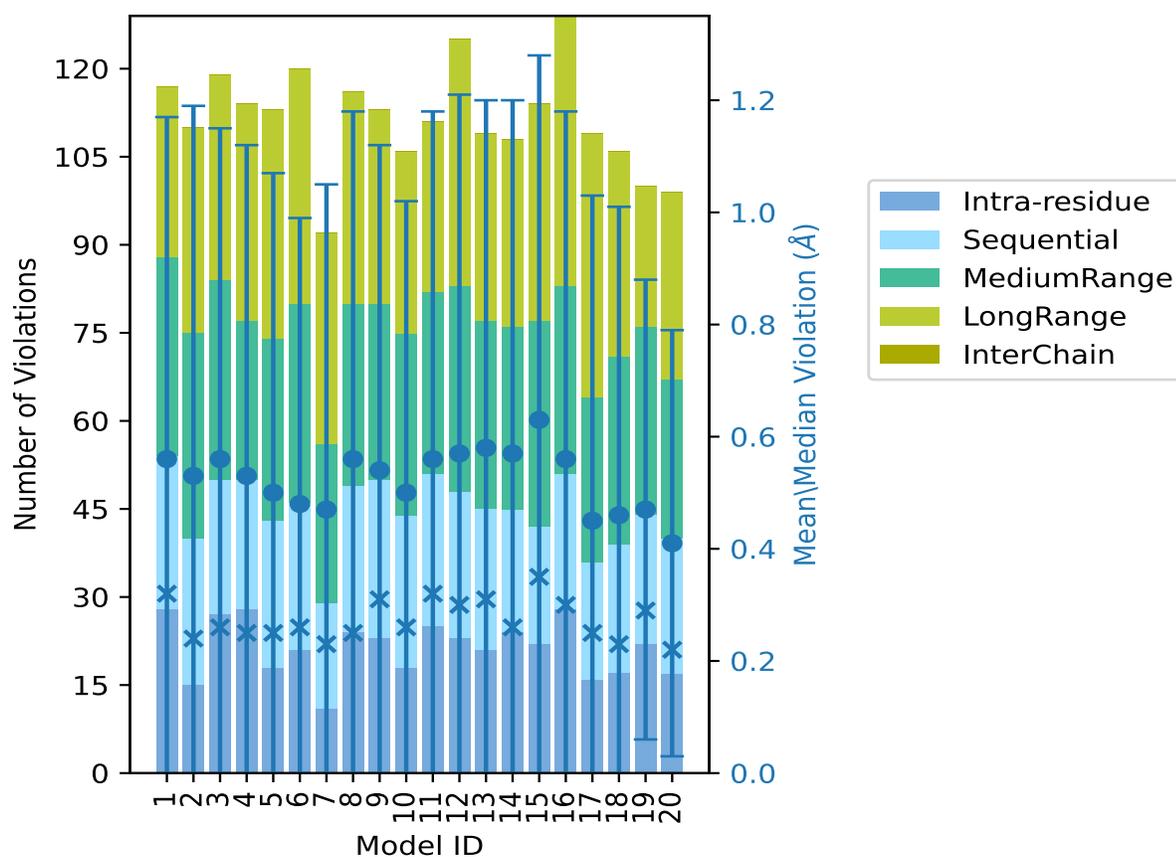
Continued on next page...

Continued from previous page...

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					
12	23	25	35	42	0	125	0.57	4.08	0.64	0.3
13	21	24	32	32	0	109	0.58	3.3	0.62	0.31
14	24	21	31	32	0	108	0.57	4.19	0.63	0.26
15	22	20	35	37	0	114	0.63	3.78	0.65	0.35
16	28	23	32	46	0	129	0.56	4.09	0.62	0.3
17	16	20	28	45	0	109	0.45	4.23	0.58	0.25
18	17	22	32	35	0	106	0.46	3.65	0.55	0.23
19	22	22	32	24	0	100	0.47	1.94	0.41	0.29
20	17	23	27	32	0	99	0.41	1.68	0.38	0.22

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

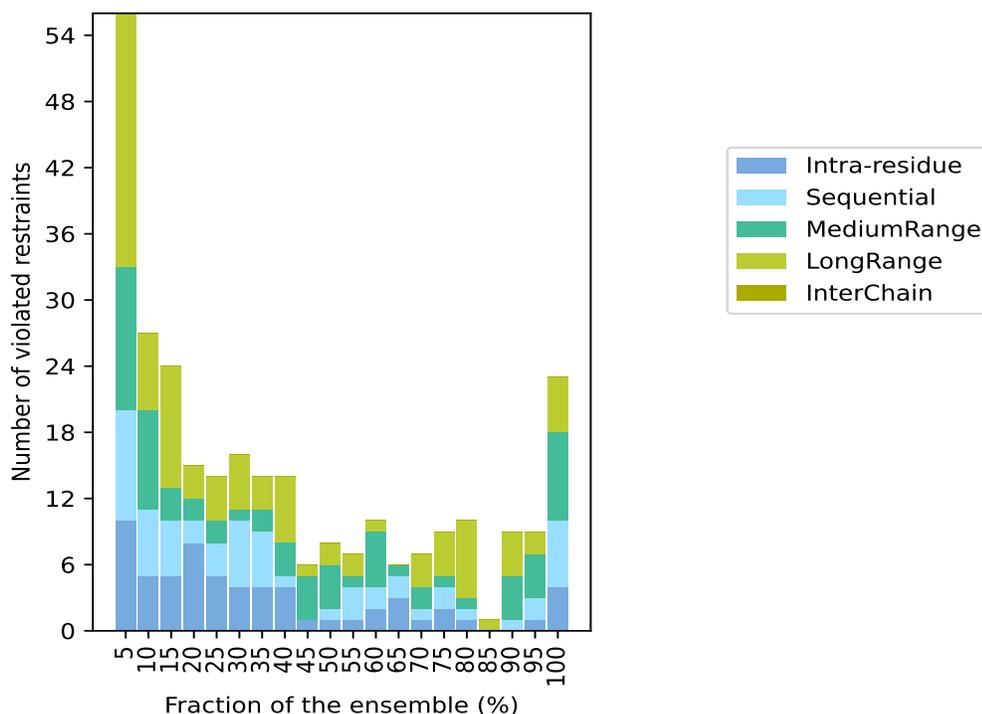
9.3 Distance violation statistics for the ensemble

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, 1612(IR:449, SQ:409, MR:330, LR:424, 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	%
10	10	13	23	0	56	1	5.0
5	6	9	7	0	27	2	10.0
5	5	3	11	0	24	3	15.0
8	2	2	3	0	15	4	20.0
5	3	2	4	0	14	5	25.0
4	6	1	5	0	16	6	30.0
4	5	2	3	0	14	7	35.0
4	1	3	6	0	14	8	40.0
1	0	4	1	0	6	9	45.0
1	1	4	2	0	8	10	50.0
1	3	1	2	0	7	11	55.0
2	2	5	1	0	10	12	60.0
3	2	1	0	0	6	13	65.0
1	1	2	3	0	7	14	70.0
2	2	1	4	0	9	15	75.0
1	1	1	7	0	10	16	80.0
0	0	0	1	0	1	17	85.0
0	1	4	4	0	9	18	90.0
1	2	4	2	0	9	19	95.0
4	6	8	5	0	23	20	100.0

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

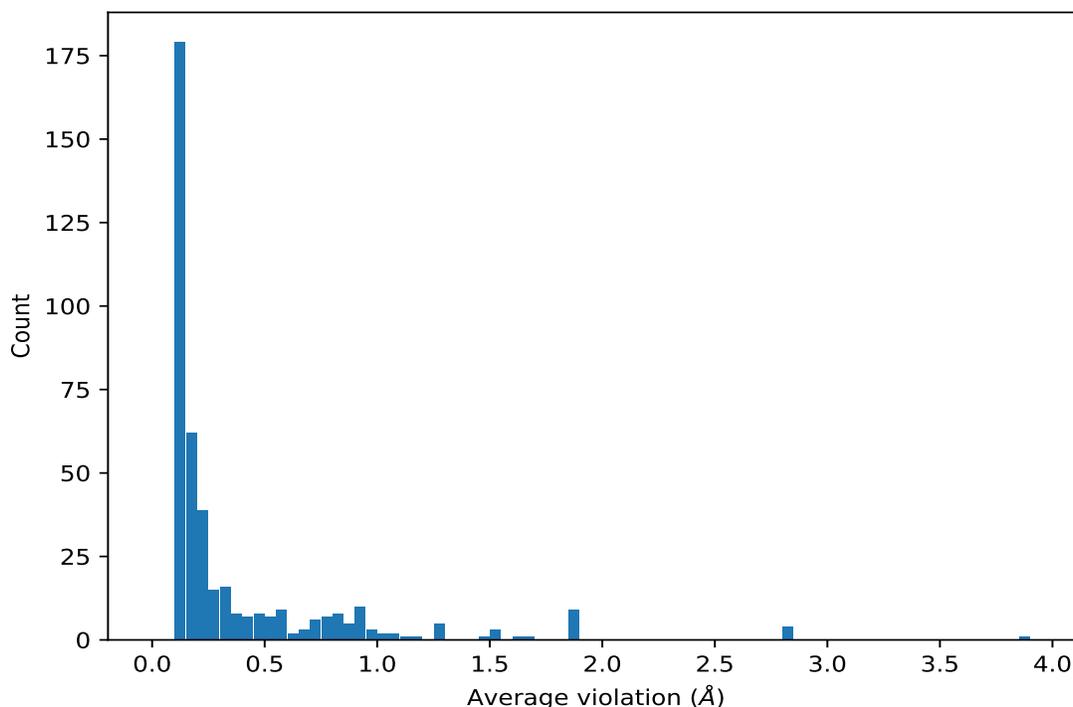
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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.

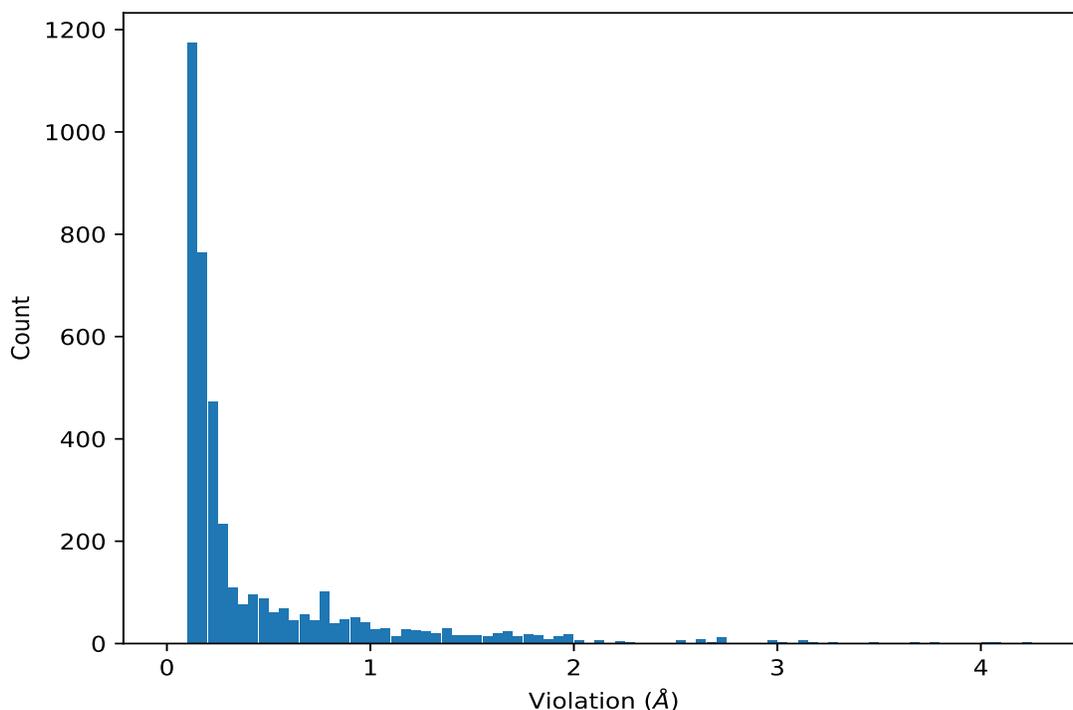
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1740)	1:254:A:ARG:H	1:294:A:HIS:HB2	20	1.29	0.35	1.33
(1,1602)	1:210:A:ASP:HB2	1:213:A:SER:HA	20	1.15	0.18	1.17
(1,1791)	1:273:A:LEU:HG	1:274:A:SER:HB2	20	1.08	0.41	1.32
(1,1671)	1:238:A:GLU:HB2	1:242:A:ARG:H	20	0.93	0.06	0.94
(1,1868)	1:306:A:ILE:H	1:320:A:ARG:HD2	20	0.92	0.45	0.92
(1,1821)	1:279:A:LYS:HE2	1:283:A:ASP:H	20	0.91	0.63	1.14
(1,1707)	1:245:A:ASP:H	1:248:A:LYS:HD2	20	0.86	0.63	0.45
(1,1738)	1:252:A:ASP:HB2	1:253:A:ALA:HB1	20	0.82	0.06	0.8
(1,1738)	1:252:A:ASP:HB2	1:253:A:ALA:HB2	20	0.82	0.06	0.8
(1,1738)	1:252:A:ASP:HB2	1:253:A:ALA:HB3	20	0.82	0.06	0.8
(1,1730)	1:248:A:LYS:H	1:248:A:LYS:HD2	20	0.74	0.22	0.86
(1,1784)	1:269:A:ILE:HG12	1:272:A:PRO:HD2	20	0.73	0.32	0.78

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)
(1,1366)	1:225:A:PHE:HE2	1:321:A:VAL:H	11	4.26
(1,1366)	1:225:A:PHE:HE2	1:321:A:VAL:H	1	4.23
(1,1366)	1:225:A:PHE:HE2	1:321:A:VAL:H	17	4.23
(1,1366)	1:225:A:PHE:HE2	1:321:A:VAL:H	14	4.19
(1,1366)	1:225:A:PHE:HE2	1:321:A:VAL:H	16	4.09
(1,1366)	1:225:A:PHE:HE2	1:321:A:VAL:H	12	4.08
(1,1366)	1:225:A:PHE:HE2	1:321:A:VAL:H	3	4.03
(1,1366)	1:225:A:PHE:HE2	1:321:A:VAL:H	8	4.01
(1,1366)	1:225:A:PHE:HE2	1:321:A:VAL:H	15	3.78
(1,1366)	1:225:A:PHE:HE2	1:321:A:VAL:H	7	3.76

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

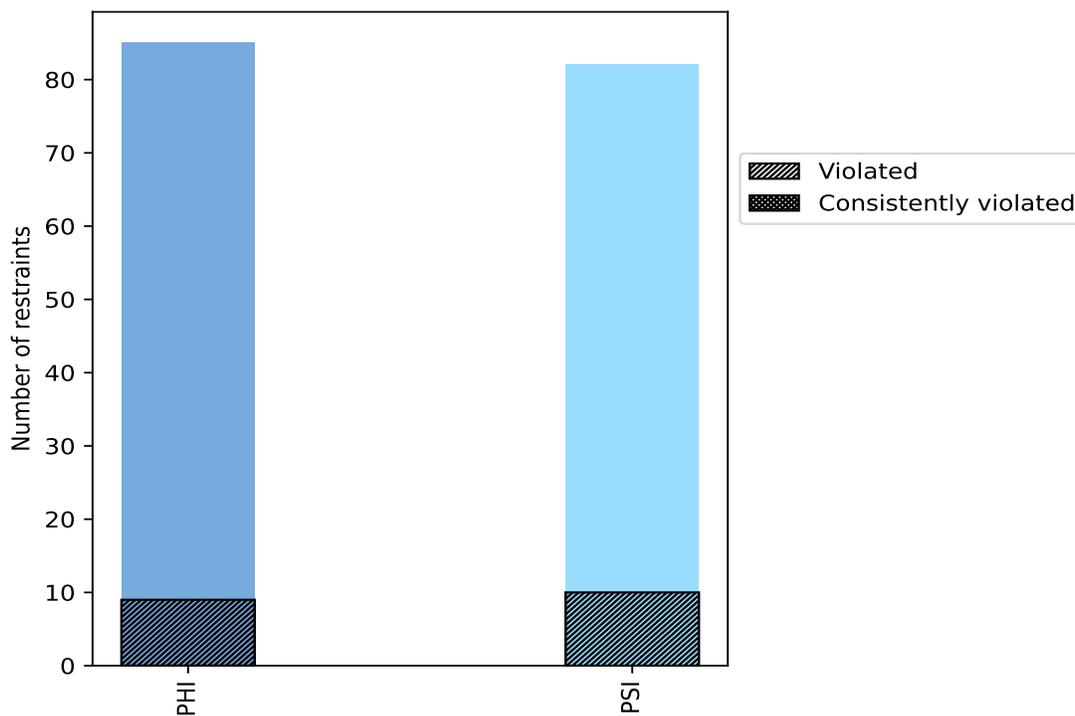
10.1 Summary of dihedral-angle violations [i](#)

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	85	50.9	9	10.6	5.4	0	0.0	0.0
PSI	82	49.1	10	12.2	6.0	0	0.0	0.0
Total	167	100.0	19	11.4	11.4	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](#)



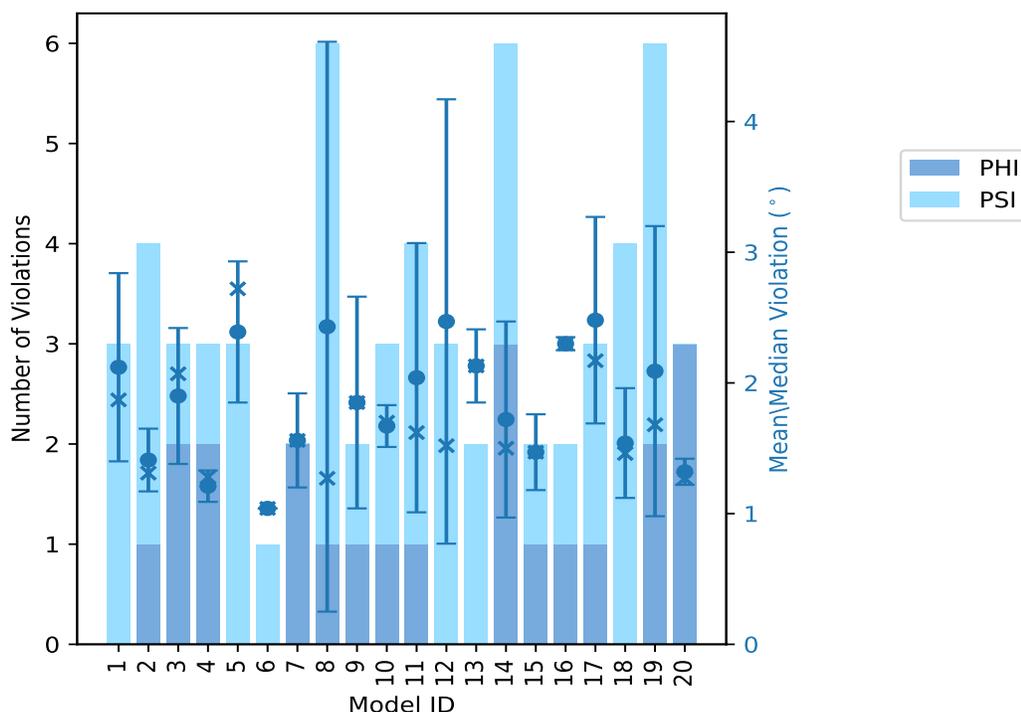
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PHI	PSI	Total				
1	0	3	3	2.12	3.11	0.72	1.87
2	1	3	4	1.41	1.82	0.24	1.31
3	2	1	3	1.9	2.44	0.52	2.07
4	2	1	3	1.21	1.31	0.12	1.28
5	0	3	3	2.39	2.81	0.54	2.72
6	0	1	1	1.04	1.04	0.0	1.04
7	2	0	2	1.56	1.92	0.36	1.56
8	1	5	6	2.43	7.18	2.18	1.27
9	1	1	2	1.85	2.66	0.81	1.85
10	1	2	3	1.67	1.85	0.16	1.7
11	1	3	4	2.04	3.74	1.03	1.62
12	0	3	3	2.47	4.86	1.7	1.52
13	0	2	2	2.13	2.42	0.28	2.13
14	3	3	6	1.72	3.34	0.75	1.5
15	1	1	2	1.47	1.76	0.29	1.47
16	1	1	2	2.3	2.35	0.05	2.3
17	1	2	3	2.48	3.57	0.79	2.17
18	0	4	4	1.54	2.16	0.42	1.46
19	2	4	6	2.09	4.53	1.11	1.68
20	3	0	3	1.32	1.46	0.1	1.27

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	%
5	2	7	1	5.0
1	1	2	2	10.0
0	1	1	3	15.0
2	1	3	4	20.0
0	3	3	5	25.0
0	0	0	6	30.0
1	0	1	7	35.0
0	1	1	8	40.0
0	1	1	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

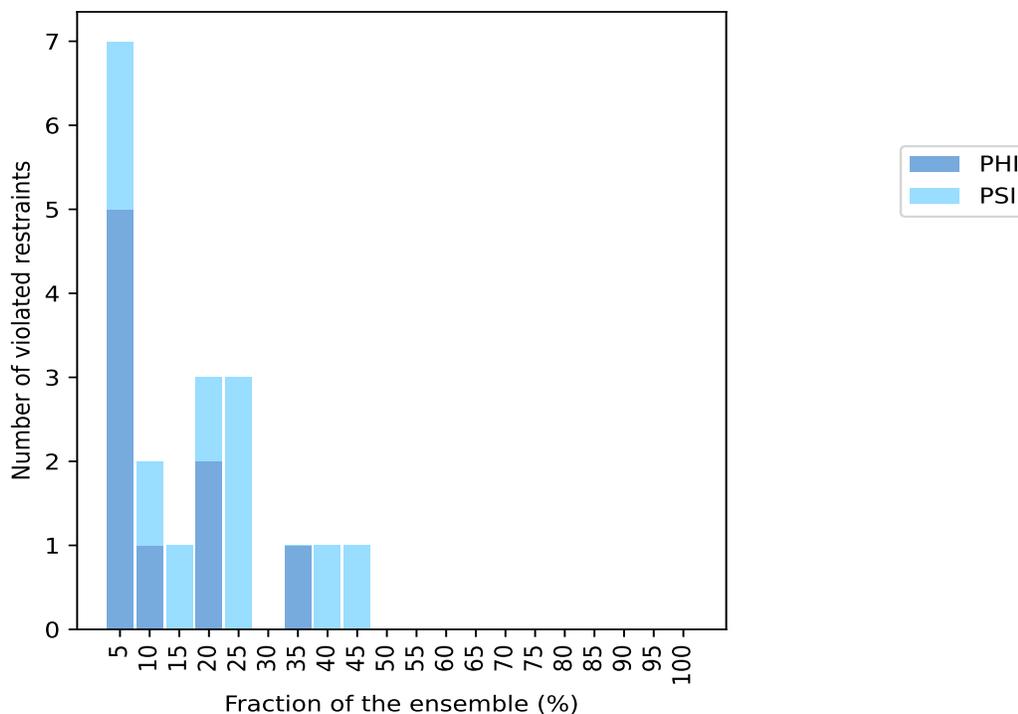
Continued on next page...

Continued from previous page...

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	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
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	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](#)

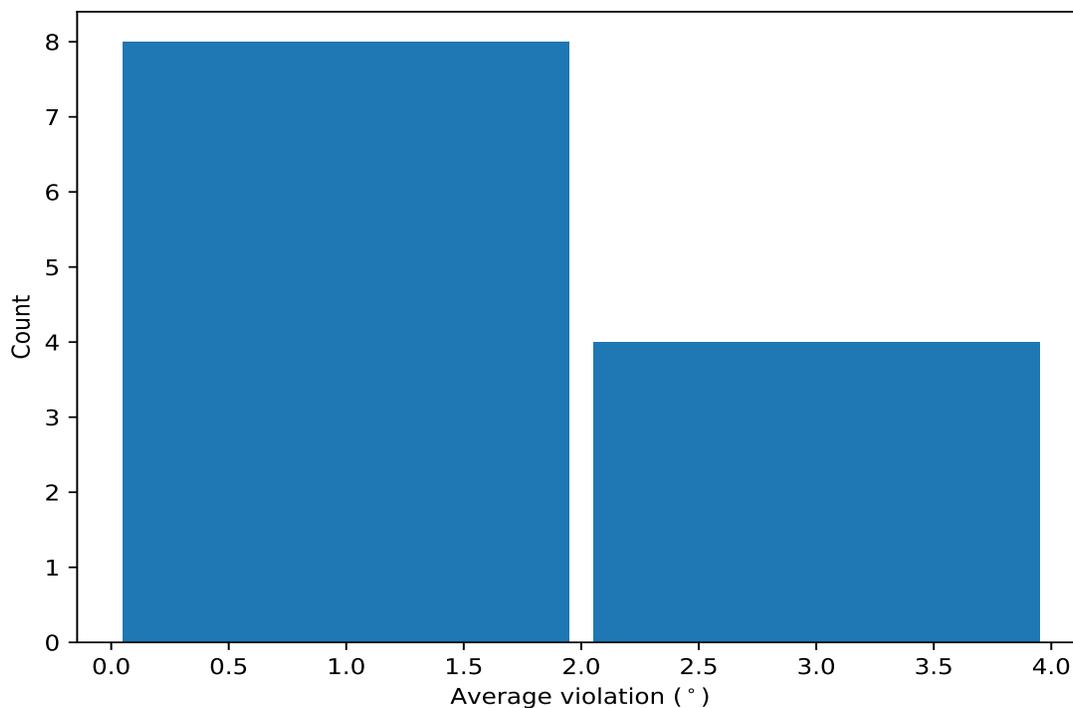


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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 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.

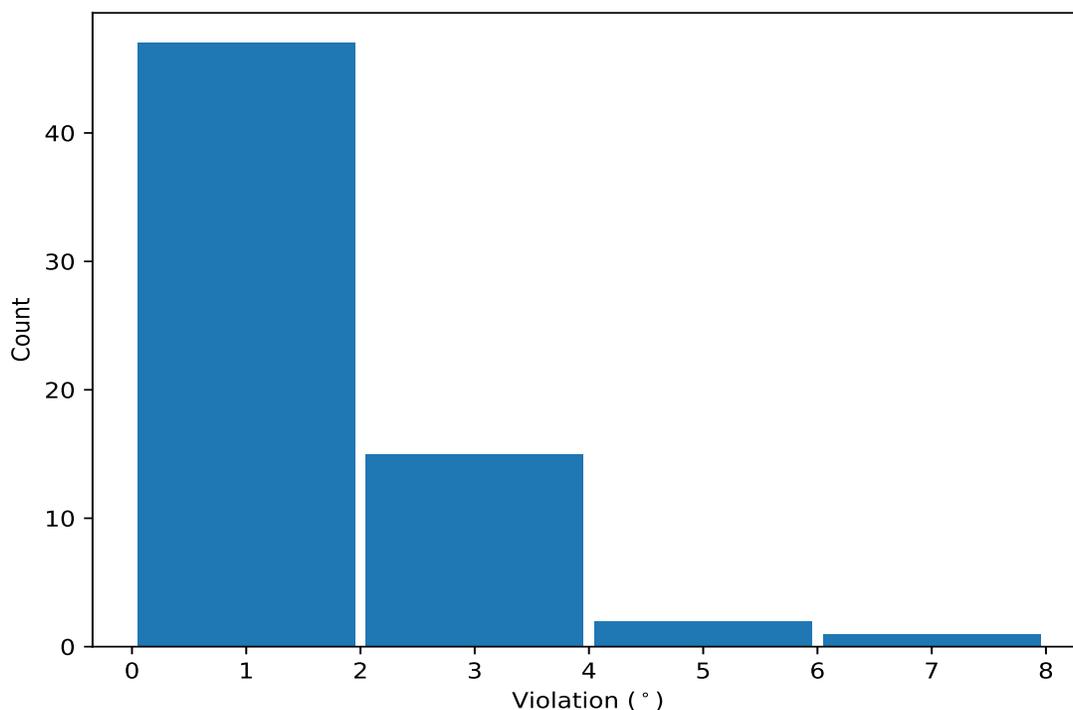
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,34)	1:238:A:GLU:N	1:238:A:GLU:CA	1:238:A:GLU:C	1:239:A:ILE:N	9	2.25	0.83	1.87
(1,4)	1:208:A:CYS:N	1:208:A:CYS:CA	1:208:A:CYS:C	1:209:A:ALA:N	8	2.79	1.23	2.49
(1,157)	1:319:A:ARG:C	1:320:A:ARG:N	1:320:A:ARG:CA	1:320:A:ARG:C	7	1.29	0.18	1.27
(1,30)	1:225:A:PHE:N	1:225:A:PHE:CA	1:225:A:PHE:C	1:226:A:GLY:N	5	2.95	2.25	1.7
(1,28)	1:224:A:ALA:N	1:224:A:ALA:CA	1:224:A:ALA:C	1:225:A:PHE:N	5	1.67	0.53	1.46
(1,136)	1:309:A:ASN:N	1:309:A:ASN:CA	1:309:A:ASN:C	1:310:A:ALA:N	5	1.22	0.17	1.18
(1,79)	1:268:A:GLY:C	1:269:A:ILE:N	1:269:A:ILE:CA	1:269:A:ILE:C	4	1.92	0.16	1.88
(1,80)	1:269:A:ILE:N	1:269:A:ILE:CA	1:269:A:ILE:C	1:270:A:ASN:N	4	1.28	0.23	1.23
(1,135)	1:308:A:SER:C	1:309:A:ASN:N	1:309:A:ASN:CA	1:309:A:ASN:C	4	1.24	0.17	1.24
(1,32)	1:234:A:PRO:N	1:234:A:PRO:CA	1:234:A:PRO:C	1:235:A:ALA:N	3	1.75	0.65	1.39

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 (°)
(1,30)	1:225:A:PHE:N	1:225:A:PHE:CA	1:225:A:PHE:C	1:226:A:GLY:N	8	7.18
(1,4)	1:208:A:CYS:N	1:208:A:CYS:CA	1:208:A:CYS:C	1:209:A:ALA:N	12	4.86
(1,4)	1:208:A:CYS:N	1:208:A:CYS:CA	1:208:A:CYS:C	1:209:A:ALA:N	19	4.53
(1,34)	1:238:A:GLU:N	1:238:A:GLU:CA	1:238:A:GLU:C	1:239:A:ILE:N	11	3.74
(1,34)	1:238:A:GLU:N	1:238:A:GLU:CA	1:238:A:GLU:C	1:239:A:ILE:N	17	3.57
(1,30)	1:225:A:PHE:N	1:225:A:PHE:CA	1:225:A:PHE:C	1:226:A:GLY:N	14	3.34
(1,4)	1:208:A:CYS:N	1:208:A:CYS:CA	1:208:A:CYS:C	1:209:A:ALA:N	1	3.11
(1,2)	1:204:A:ALA:N	1:204:A:ALA:CA	1:204:A:ALA:C	1:205:A:SER:N	5	2.81
(1,4)	1:208:A:CYS:N	1:208:A:CYS:CA	1:208:A:CYS:C	1:209:A:ALA:N	5	2.72
(1,32)	1:234:A:PRO:N	1:234:A:PRO:CA	1:234:A:PRO:C	1:235:A:ALA:N	9	2.66