



wwPDB NMR Structure Validation Summary Report ⓘ

Oct 28, 2025 – 09:22 am GMT

PDB ID : 9HW9 / pdb_00009hw9
BMRB ID : 52205
Title : Structural characterization of the type 3 fimbrial subunit MrkA from *Klebsiella pneumoniae* by solution NMR spectroscopy
Authors : Monaci, V.; Cantini, F.
Deposited on : 2025-01-03

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

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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 : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

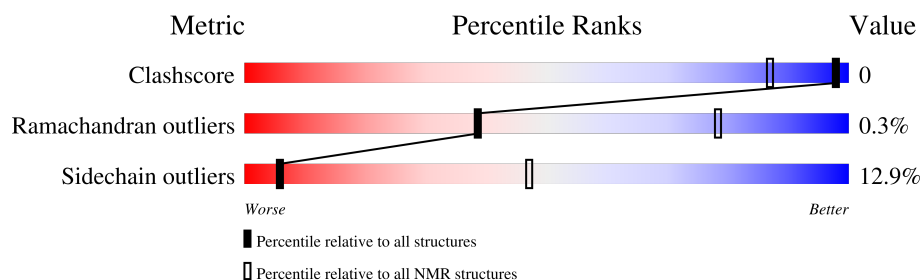
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR


The overall completeness of chemical shifts assignment is 94%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	201	

2 Ensemble composition and analysis

This entry contains 20 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: *target function*.

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:16-A:60, A:73-A:174, A:185-A:198 (161)	0.65	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 9 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2828 atoms, of which 1376 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Fimbrial subunit type 3.

Mol	Chain	Residues	Atoms						Trace
1	A	201	Total	C	H	N	O	S	0
			2828	892	1376	256	301	3	

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P12267
A	2	GLY	-	expression tag	UNP P12267
A	3	SER	-	expression tag	UNP P12267
A	4	HIS	-	expression tag	UNP P12267
A	5	HIS	-	expression tag	UNP P12267
A	6	HIS	-	expression tag	UNP P12267
A	7	HIS	-	expression tag	UNP P12267
A	8	HIS	-	expression tag	UNP P12267
A	9	HIS	-	expression tag	UNP P12267
A	10	HIS	-	expression tag	UNP P12267
A	11	HIS	-	expression tag	UNP P12267
A	12	HIS	-	expression tag	UNP P12267
A	13	HIS	-	expression tag	UNP P12267
A	14	GLY	-	expression tag	UNP P12267
A	59	ASN	ASP	conflict	UNP P12267
A	89	SER	ALA	conflict	UNP P12267
A	101	SER	ALA	conflict	UNP P12267
A	133	LYS	ALA	conflict	UNP P12267
A	140	ALA	GLN	conflict	UNP P12267
A	155	ALA	THR	conflict	UNP P12267
A	176	GLY	-	expression tag	UNP P12267
A	177	GLY	-	expression tag	UNP P12267
A	178	GLY	-	expression tag	UNP P12267
A	179	GLY	-	expression tag	UNP P12267
A	180	GLY	-	expression tag	UNP P12267
A	181	GLY	-	expression tag	UNP P12267
A	182	ALA	-	expression tag	UNP P12267
A	183	ASP	-	expression tag	UNP P12267
A	184	THR	-	expression tag	UNP P12267
A	185	THR	-	expression tag	UNP P12267
A	186	VAL	-	expression tag	UNP P12267

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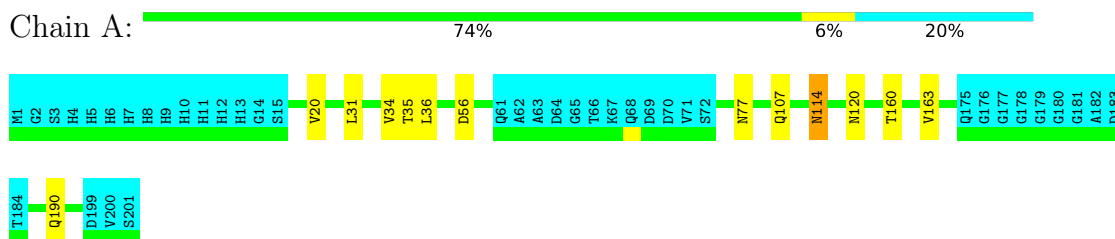
Chain	Residue	Modelled	Actual	Comment	Reference
A	187	GLY	-	expression tag	UNP P12267
A	188	GLY	-	expression tag	UNP P12267
A	189	GLY	-	expression tag	UNP P12267
A	190	GLN	-	expression tag	UNP P12267
A	191	VAL	-	expression tag	UNP P12267
A	192	ASN	-	expression tag	UNP P12267
A	193	PHE	-	expression tag	UNP P12267
A	194	PHE	-	expression tag	UNP P12267
A	195	GLY	-	expression tag	UNP P12267
A	196	LYS	-	expression tag	UNP P12267
A	197	VAL	-	expression tag	UNP P12267
A	198	THR	-	expression tag	UNP P12267
A	199	ASP	-	expression tag	UNP P12267
A	200	VAL	-	expression tag	UNP P12267
A	201	SER	-	expression tag	UNP P12267

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.

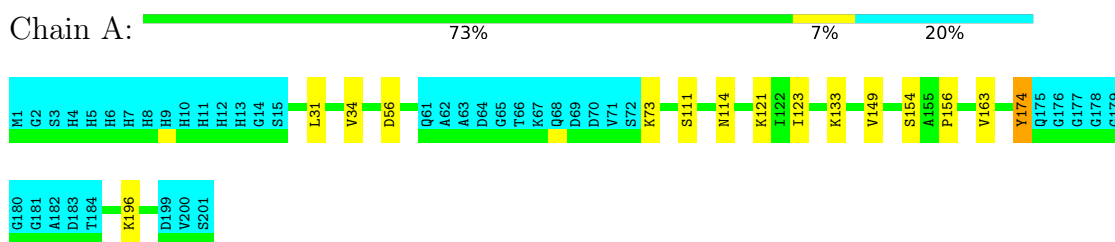
- Molecule 1: Fimbrial subunit type 3



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: Fimbrial subunit type 3



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure calculation	3
Amber	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	2090
Number of shifts mapped to atoms	2090
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

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	0.85±0.01	0±0/1185 (0.0± 0.0%)	1.47±0.03	4±2/1622 (0.2± 0.1%)
All	All	0.85	0/23700 (0.0%)	1.47	74/32440 (0.2%)

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	1.1±0.8
All	All	0	21

There are no bond-length outliers.

5 of 36 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	114	ASN	CA-CB-CG	8.76	121.36	112.60	16	4
1	A	97	ASN	CA-CB-CG	7.59	120.19	112.60	8	1
1	A	56	ASP	CA-CB-CG	6.86	119.46	112.60	8	8
1	A	107	GLN	OE1-CD-NE2	-6.70	115.90	122.60	15	10
1	A	113	ASP	CA-C-N	6.61	134.17	121.54	19	6

There are no chirality outliers.

5 of 15 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	94	TYR	Sidechain	3
1	A	114	ASN	Peptide	3
1	A	50	PRO	Peptide	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	148	TYR	Sidechain	2
1	A	151	TYR	Peptide	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	1165	1144	1144	1±1
All	All	23300	22880	22880	20

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 0.

5 of 11 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:H	1:A:36:LEU:HD22	0.53	1.64	11	5
1:A:103:ALA:HB1	1:A:106:ILE:HD13	0.51	1.83	3	4
1:A:106:ILE:HD12	1:A:106:ILE:N	0.48	2.23	1	2
1:A:106:ILE:HD13	1:A:159:VAL:HG23	0.47	1.86	4	1
1:A:169:THR:HG22	1:A:190:GLN:OE1	0.47	2.08	5	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	161/201 (80%)	153±2 (95±1%)	7±2 (5±1%)	1±0 (0±0%)	38	78
All	All	3220/4020 (80%)	3061 (95%)	148 (5%)	11 (0%)	38	78

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occur-

rence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	114	ASN	4
1	A	49	LYS	3
1	A	120	ASN	3
1	A	140	ALA	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	124/152 (82%)	108±2 (87±2%)	16±2 (13±2%)	6	47
All	All	2480/3040 (82%)	2161 (87%)	319 (13%)	6	47

5 of 57 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	31	LEU	19
1	A	34	VAL	18
1	A	114	ASN	18
1	A	163	VAL	15
1	A	190	GLN	15

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 oligosaccharides 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 94% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	2090
Number of shifts mapped to atoms	2090
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	187	0.21 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	162	0.07 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	169	0.34 ± 0.10	None needed (< 0.5 ppm)
^{15}N	179	0.57 ± 0.32	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 1854 atoms were assigned a chemical shift out of a possible 1972. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	793/812 (98%)	332/334 (99%)	307/322 (95%)	154/156 (99%)
Sidechain	963/1027 (94%)	658/676 (97%)	286/321 (89%)	19/30 (63%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	98/133 (74%)	54/62 (87%)	43/70 (61%)	1/1 (100%)
Overall	1854/1972 (94%)	1044/1072 (97%)	636/713 (89%)	174/187 (93%)

7.1.4 Statistically unusual chemical shifts [i](#)

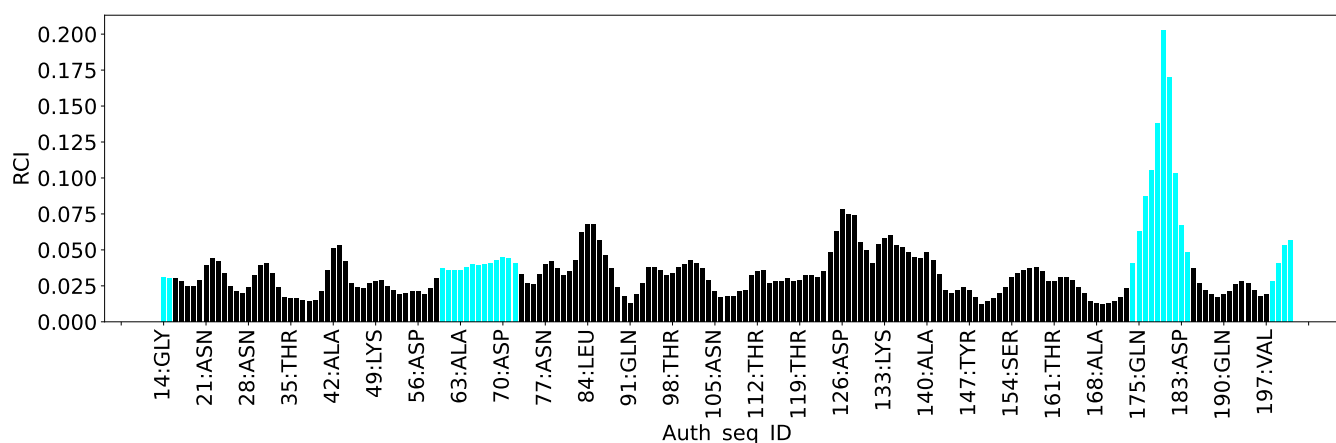
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	46	THR	HG1	5.46	0.08 – 2.19	20.5
1	A	131	LYS	HE2	4.34	1.95 – 3.88	7.4
1	A	131	LYS	HE3	4.34	1.92 – 3.89	7.3
1	A	78	TRP	HE1	6.36	6.88 – 13.28	-5.8
1	A	91	GLN	HA	2.14	2.17 – 6.35	-5.1
1	A	170	TYR	HB3	0.91	0.93 – 4.76	-5.1

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	2248
Intra-residue ($ i-j =0$)	434
Sequential ($ i-j =1$)	683
Medium range ($ i-j >1$ and $ i-j <5$)	257
Long range ($ i-j \geq 5$)	874
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	269
Number of unmapped restraints	0
Number of restraints per residue	12.5
Number of long range restraints per residue ¹	4.3

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)	1.0	0.19
0.2-0.5 (Medium)	None	None
>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)	13.5	9.96
10.0-20.0 (Medium)	0.6	13.93
>20.0 (Large)	None	None

9 Distance violation analysis

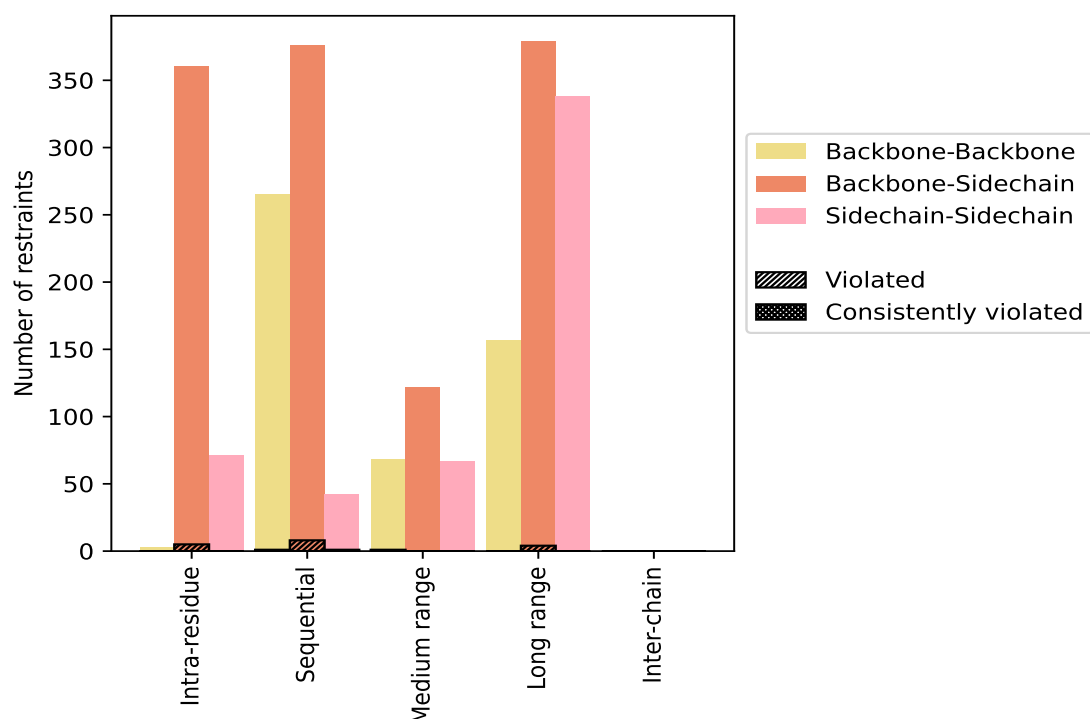
9.1 Summary of distance violations

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 ($i-j =0$)	434	19.3	5	1.2	0.2	0	0.0	0.0
Backbone-Backbone	3	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	360	16.0	5	1.4	0.2	0	0.0	0.0
Sidechain-Sidechain	71	3.2	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	683	30.4	10	1.5	0.4	0	0.0	0.0
Backbone-Backbone	265	11.8	1	0.4	0.0	0	0.0	0.0
Backbone-Sidechain	376	16.7	8	2.1	0.4	0	0.0	0.0
Sidechain-Sidechain	42	1.9	1	2.4	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	257	11.4	1	0.4	0.0	0	0.0	0.0
Backbone-Backbone	68	3.0	1	1.5	0.0	0	0.0	0.0
Backbone-Sidechain	122	5.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	67	3.0	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	874	38.9	4	0.5	0.2	0	0.0	0.0
Backbone-Backbone	157	7.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	379	16.9	4	1.1	0.2	0	0.0	0.0
Sidechain-Sidechain	338	15.0	0	0.0	0.0	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	2248	100.0	20	0.9	0.9	0	0.0	0.0
Backbone-Backbone	493	21.9	2	0.4	0.1	0	0.0	0.0
Backbone-Sidechain	1237	55.0	17	1.4	0.8	0	0.0	0.0
Sidechain-Sidechain	518	23.0	1	0.2	0.0	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	0	0	0	1	0	1	0.1	0.1	0.0	0.1
2	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	2	0	0	0	0	2	0.13	0.15	0.02	0.13
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	1	0	0	0	1	0.19	0.19	0.0	0.19
6	1	0	0	0	0	1	0.1	0.1	0.0	0.1
7	2	1	0	0	0	3	0.13	0.15	0.02	0.12
8	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	1	1	0	1	0	3	0.11	0.11	0.0	0.11
10	1	1	0	0	0	2	0.12	0.12	0.0	0.12

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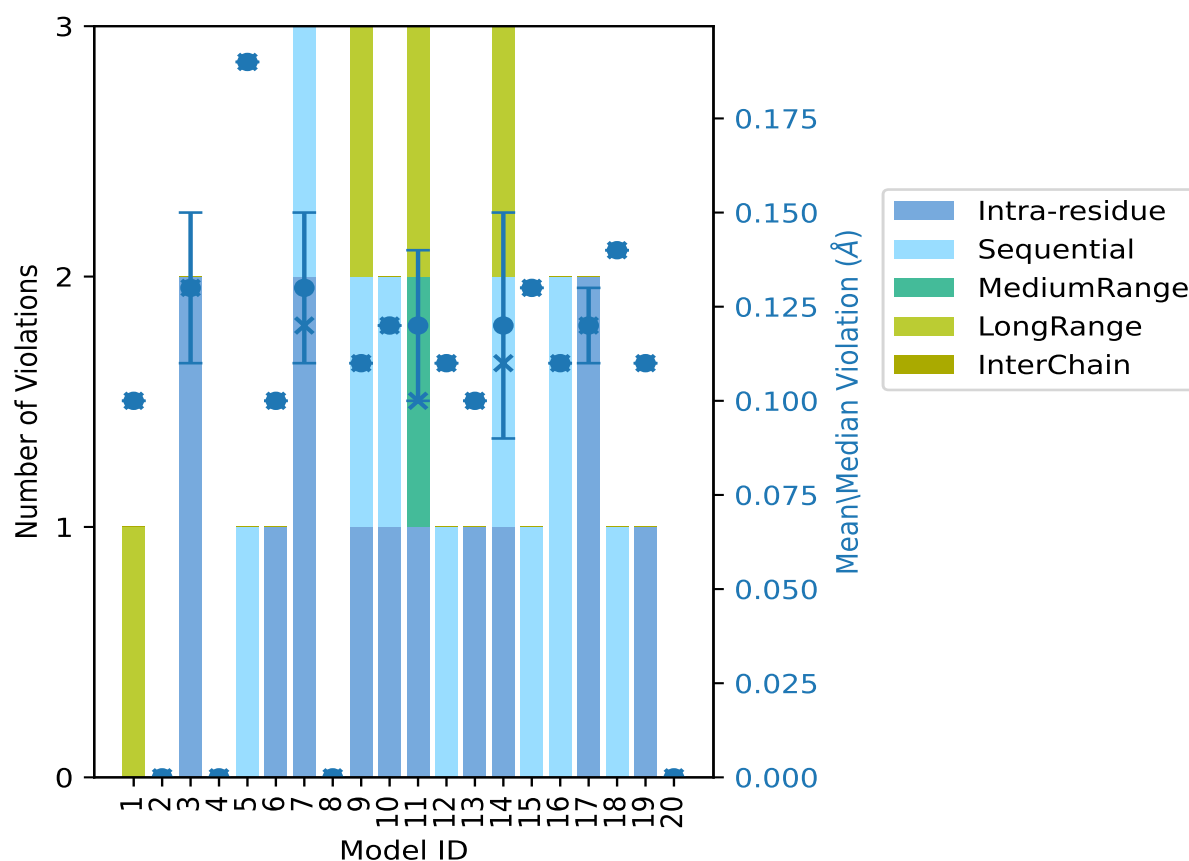
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	0	1	1	0	3	0.12	0.15	0.02	0.1
12	0	1	0	0	0	1	0.11	0.11	0.0	0.11
13	1	0	0	0	0	1	0.1	0.1	0.0	0.1
14	1	1	0	1	0	3	0.12	0.16	0.03	0.11
15	0	1	0	0	0	1	0.13	0.13	0.0	0.13
16	0	2	0	0	0	2	0.11	0.11	0.0	0.11
17	2	0	0	0	0	2	0.12	0.13	0.01	0.12
18	0	1	0	0	0	1	0.14	0.14	0.0	0.14
19	1	0	0	0	0	1	0.11	0.11	0.0	0.11
20	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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 ⓘ



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

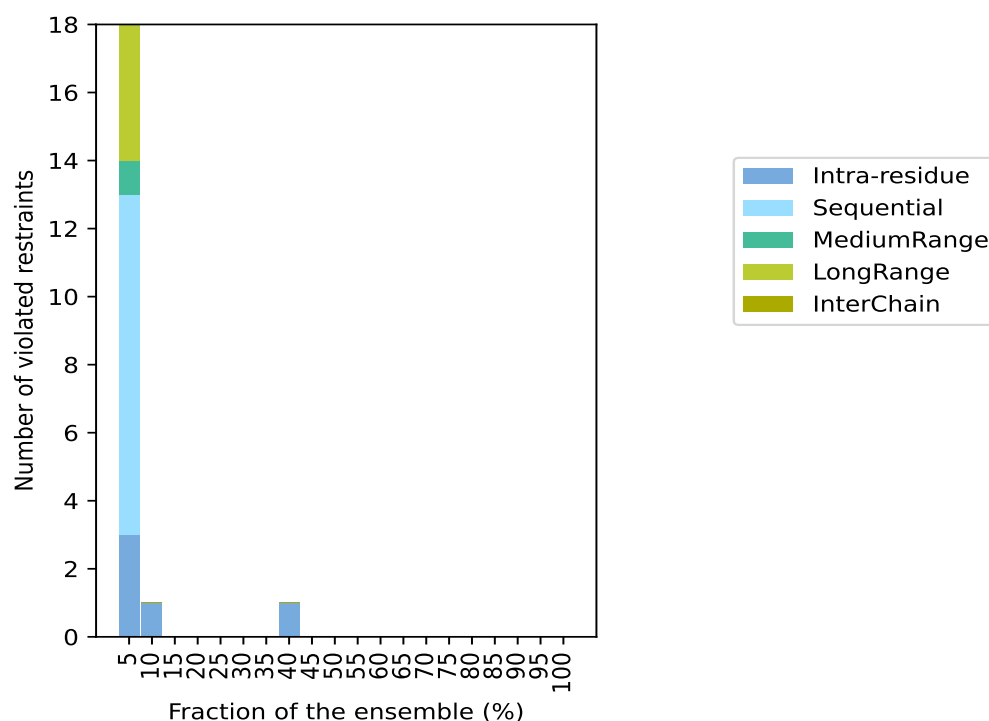
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2228(IR:429, SQ:673, MR:256, LR:870, IC:0) restraints are 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	%
3	10	1	4	0	18	1	5.0
1	0	0	0	0	1	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
1	0	0	0	0	1	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

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

⁵Inter-chain restraints, ⁶ Number of models with violations

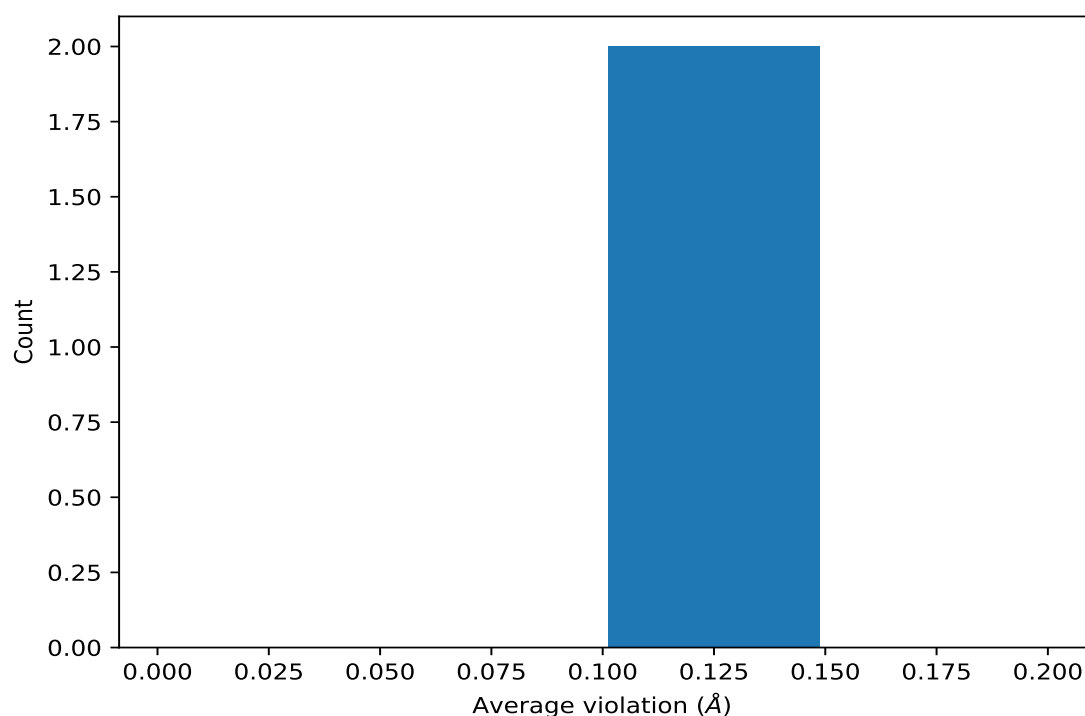
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 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.

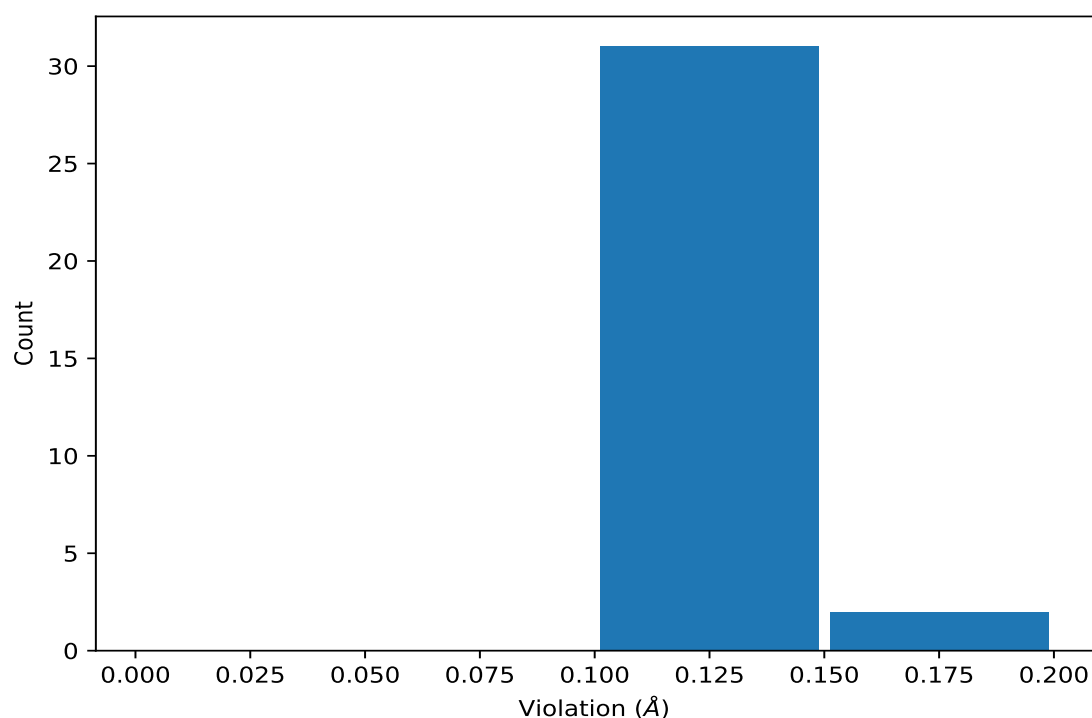
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,778)	1:68:A:GLN:HA	1:68:A:GLN:HE21	8	0.11	0.01	0.11
(1,372)	1:37:A:THR:H	1:37:A:THR:HB	2	0.15	0.0	0.15

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)
(1,834)	1:73:A:LYS:HB2	1:74:A:LEU:H	5	0.19
(1,8)	1:14:A:GLY:HA3	1:15:A:SER:H	14	0.16
(1,1642)	1:131:A:LYS:H	1:131:A:LYS:HD2	3	0.15
(1,1642)	1:131:A:LYS:H	1:131:A:LYS:HD3	3	0.15
(1,372)	1:37:A:THR:H	1:37:A:THR:HB	7	0.15
(1,372)	1:37:A:THR:H	1:37:A:THR:HB	11	0.15
(1,2245)	1:200:A:VAL:HB	1:201:A:SER:H	18	0.14
(1,1657)	1:133:A:LYS:H	1:133:A:LYS:HB3	17	0.13
(1,782)	1:68:A:GLN:HB2	1:69:A:ASP:HB2	15	0.13
(1,1850)	1:154:A:SER:HB2	1:155:A:ALA:H	10	0.12
(1,778)	1:68:A:GLN:HA	1:68:A:GLN:HE21	7	0.12

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

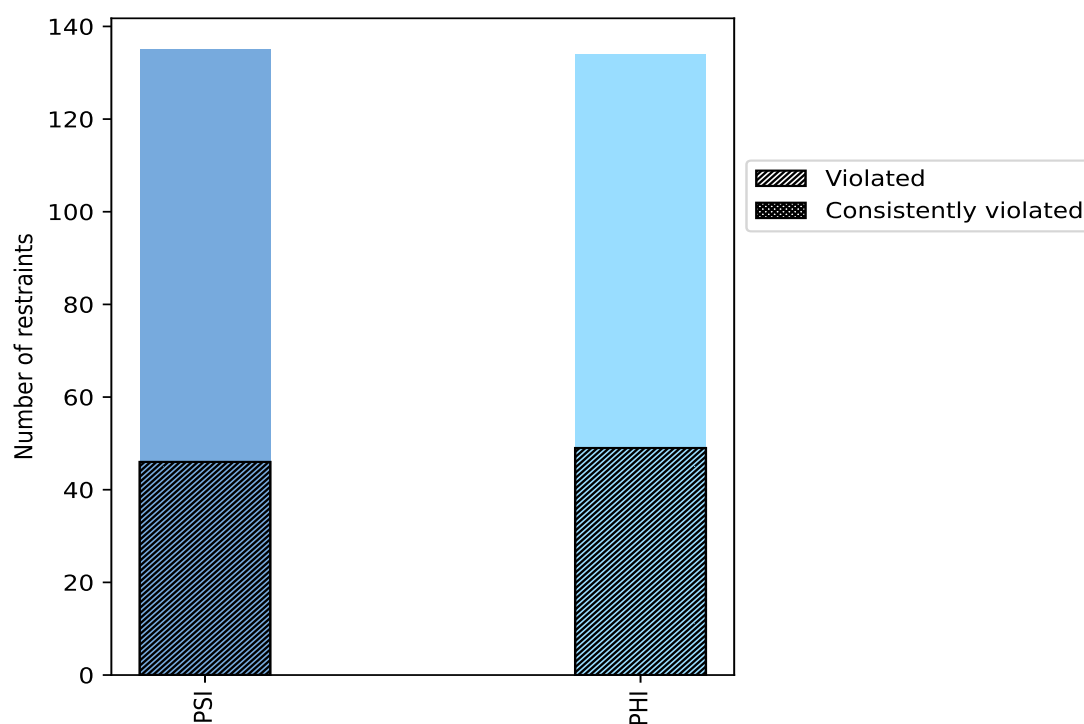
10.1 Summary of dihedral-angle violations [i](#)

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	135	50.2	46	34.1	17.1	0	0.0	0.0
PHI	134	49.8	49	36.6	18.2	0	0.0	0.0
Total	269	100.0	95	35.3	35.3	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](#)



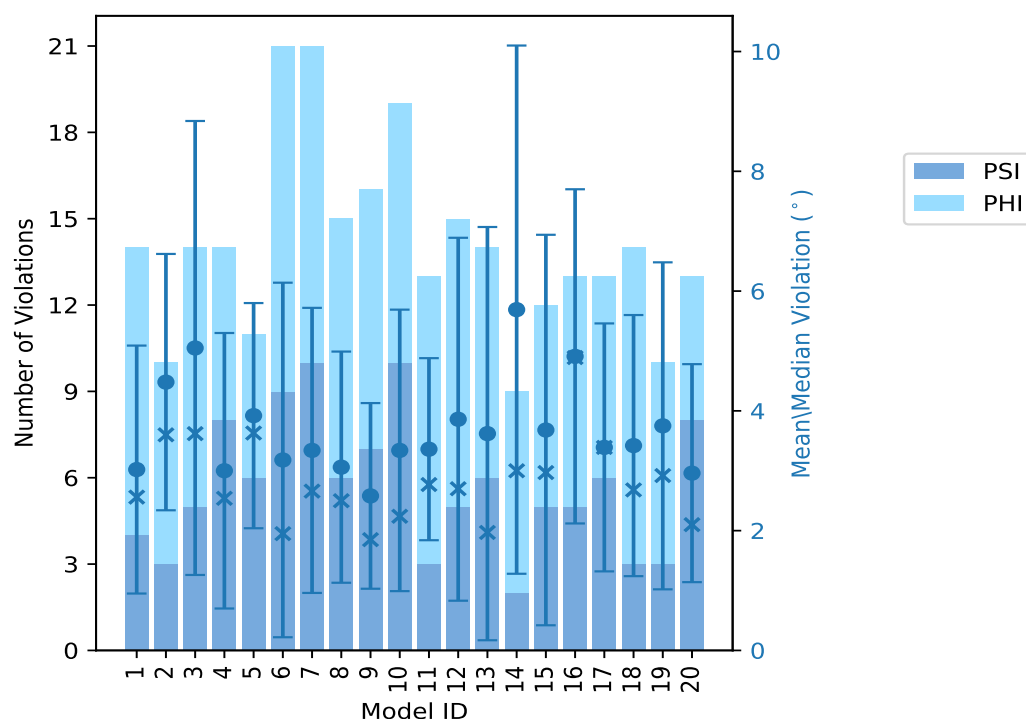
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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	4	10	14	3.02	8.55	2.07	2.56
2	3	7	10	4.48	10.04	2.14	3.6
3	5	9	14	5.05	13.3	3.79	3.62
4	8	6	14	3.0	9.88	2.3	2.54
5	6	5	11	3.92	7.29	1.88	3.63
6	9	12	21	3.18	13.91	2.96	1.95
7	10	11	21	3.34	9.32	2.38	2.66
8	6	9	15	3.06	7.63	1.93	2.5
9	7	9	16	2.58	7.13	1.55	1.85
10	10	9	19	3.34	9.19	2.35	2.24
11	3	10	13	3.36	5.96	1.52	2.77
12	5	10	15	3.86	12.57	3.03	2.7
13	6	8	14	3.62	13.45	3.45	1.97
14	2	7	9	5.69	13.93	4.41	3.0
15	5	7	12	3.68	13.76	3.26	2.97
16	5	8	13	4.91	9.96	2.79	4.89
17	6	7	13	3.39	8.85	2.07	3.39
18	3	11	14	3.42	8.86	2.18	2.68
19	3	7	10	3.75	11.42	2.73	2.92
20	8	5	13	2.96	7.76	1.82	2.1

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	%
22	14	36	1	5.0
7	12	19	2	10.0
5	8	13	3	15.0
6	4	10	4	20.0
3	4	7	5	25.0
0	0	0	6	30.0
0	1	1	7	35.0
3	1	4	8	40.0
0	1	1	9	45.0
0	1	1	10	50.0
0	2	2	11	55.0

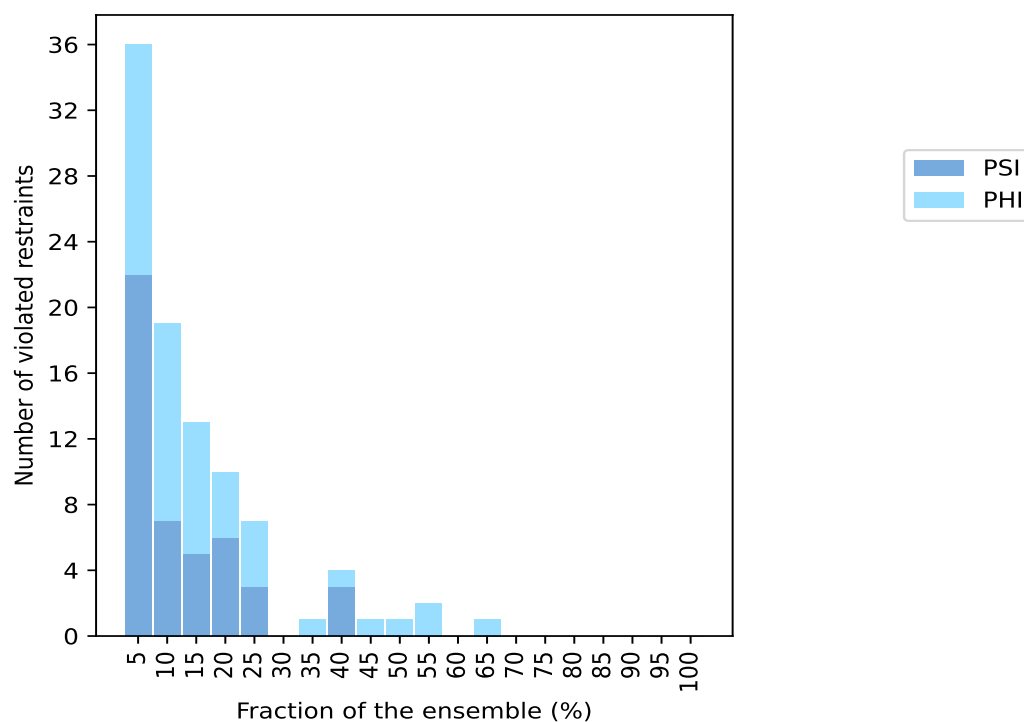
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	12	60.0
0	1	1	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

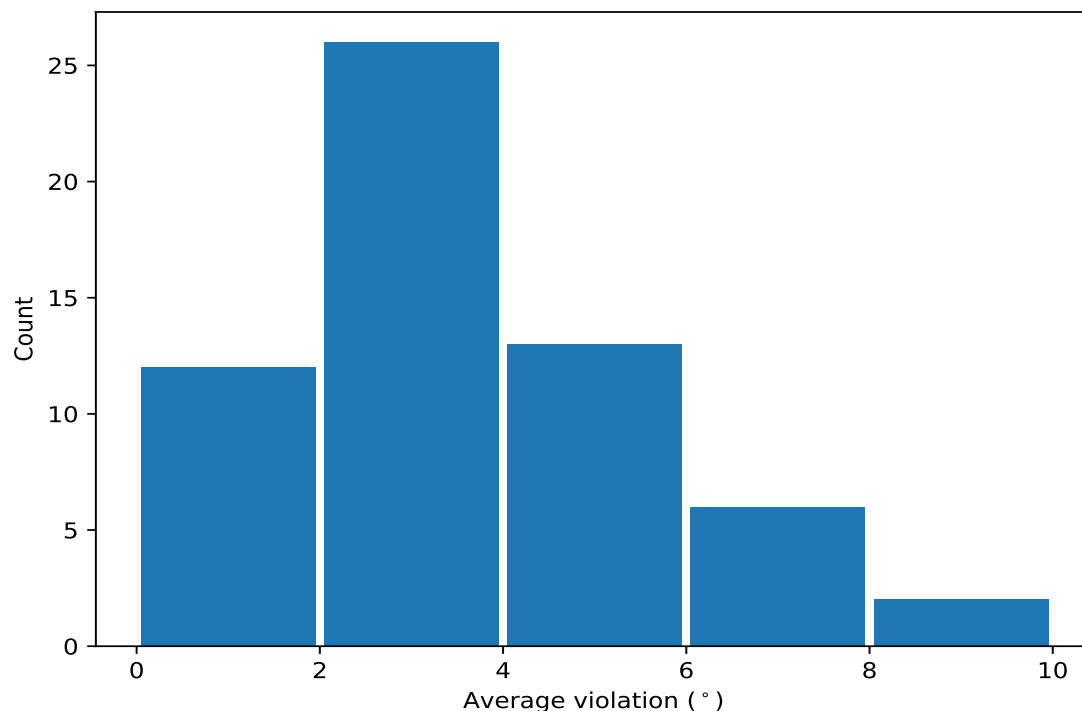


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints [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.

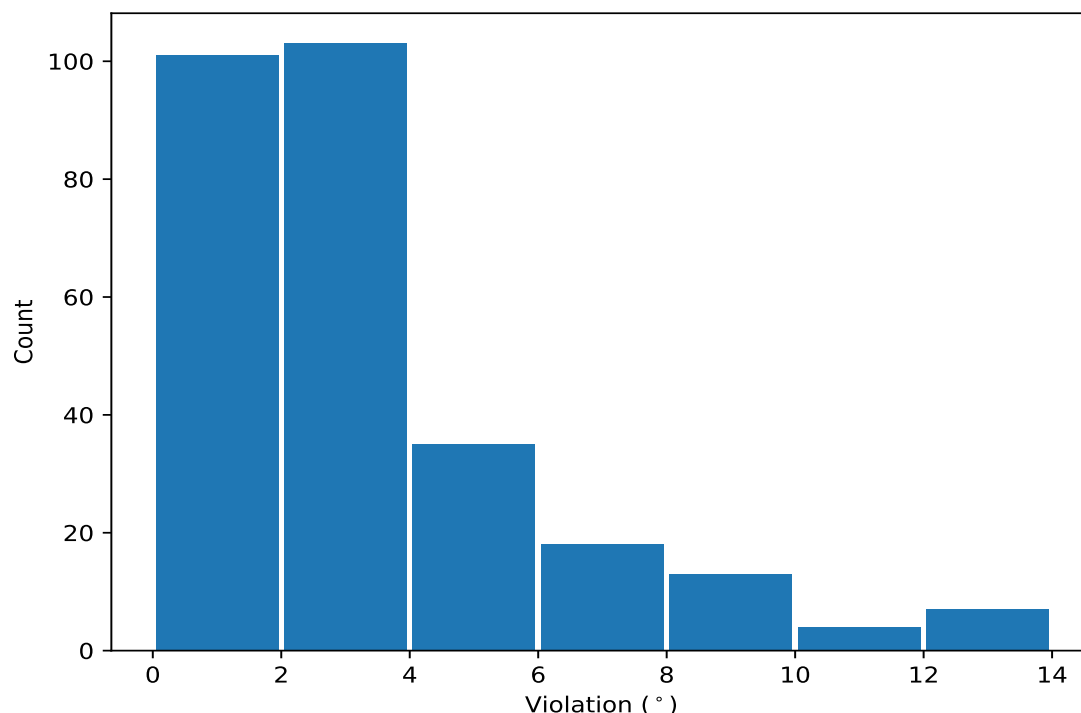
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,9)	1:18:A:VAL:C	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	13	2.6	0.83	2.7
(1,95)	1:73:A:LYS:C	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:C	11	3.13	1.32	3.15
(1,244)	1:190:A:GLN:C	1:191:A:VAL:N	1:191:A:VAL:CA	1:191:A:VAL:C	11	2.21	0.78	1.93
(1,47)	1:42:A:ALA:C	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	10	3.47	1.84	3.24
(1,88)	1:65:A:GLY:C	1:66:A:THR:N	1:66:A:THR:CA	1:66:A:THR:C	9	3.2	1.85	2.56
(1,174)	1:132:A:ALA:C	1:133:A:LYS:N	1:133:A:LYS:CA	1:133:A:LYS:C	8	7.64	4.29	5.68
(1,208)	1:155:A:ALA:N	1:155:A:ALA:CA	1:155:A:ALA:C	1:156:A:PRO:N	8	4.33	2.97	3.18
(1,94)	1:73:A:LYS:N	1:73:A:LYS:CA	1:73:A:LYS:C	1:74:A:LEU:N	8	3.13	1.35	3.01
(1,91)	1:71:A:VAL:N	1:71:A:VAL:CA	1:71:A:VAL:C	1:72:A:SER:N	8	2.79	0.97	2.76
(1,141)	1:107:A:GLN:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	7	7.42	3.4	9.19

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 (°)
(1,172)	1:131:A:LYS:C	1:132:A:ALA:N	1:132:A:ALA:CA	1:132:A:ALA:C	14	13.93
(1,235)	1:182:A:ALA:N	1:182:A:ALA:CA	1:182:A:ALA:C	1:183:A:ASP:N	6	13.91
(1,262)	1:68:A:GLN:C	1:69:A:ASP:N	1:69:A:ASP:CA	1:69:A:ASP:C	15	13.76
(1,174)	1:132:A:ALA:C	1:133:A:LYS:N	1:133:A:LYS:CA	1:133:A:LYS:C	13	13.45
(1,174)	1:132:A:ALA:C	1:133:A:LYS:N	1:133:A:LYS:CA	1:133:A:LYS:C	3	13.3
(1,233)	1:172:A:ILE:C	1:173:A:THR:N	1:173:A:THR:CA	1:173:A:THR:C	12	12.57
(1,174)	1:132:A:ALA:C	1:133:A:LYS:N	1:133:A:LYS:CA	1:133:A:LYS:C	14	12.35
(1,180)	1:136:A:ALA:C	1:137:A:SER:N	1:137:A:SER:CA	1:137:A:SER:C	3	11.76
(1,141)	1:107:A:GLN:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	19	11.42
(1,141)	1:107:A:GLN:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	3	10.09