



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2MY8
BMRB ID : 16884
Title : NMR Structure of RRM-3 domain of ETR-3
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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 : 4.02b-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

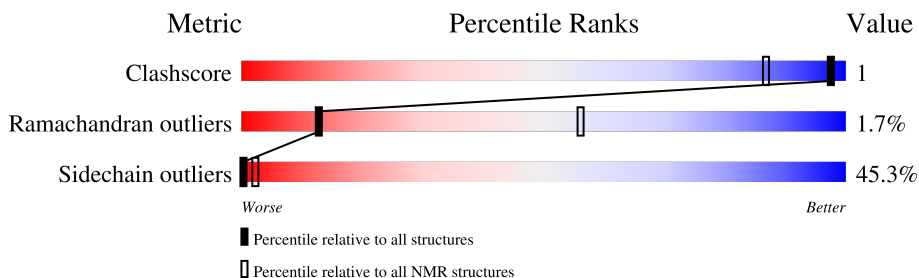
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	97	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 19 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:398-A:437, A:449-A:479 (71)	0.28	19

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 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1531 atoms, of which 764 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CUGBP Elav-like family member 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	97	1531	490	764	131	140	6	0

There are 4 discrepancies between the modelled and reference sequences:

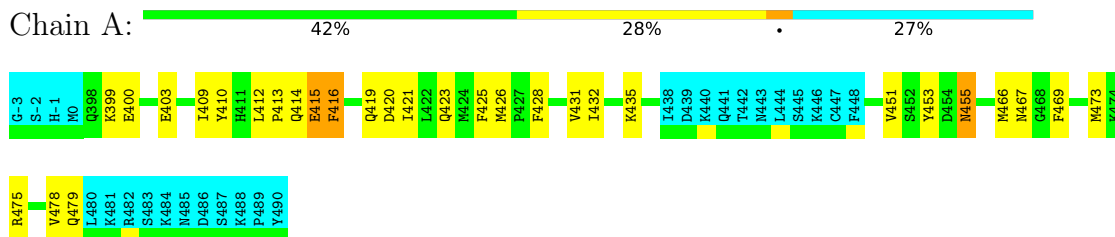
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP O95319
A	-2	SER	-	expression tag	UNP O95319
A	-1	HIS	-	expression tag	UNP O95319
A	0	MET	-	expression tag	UNP O95319

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.

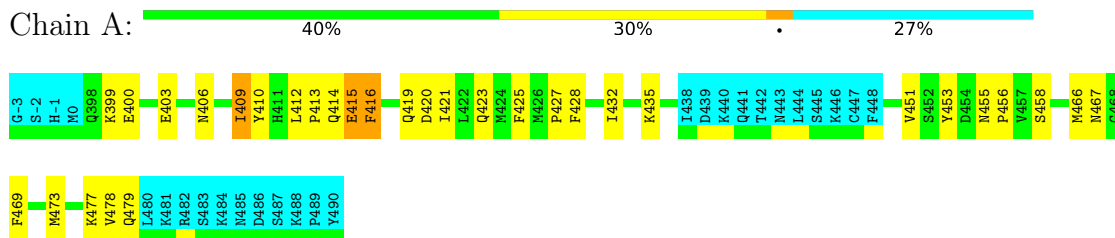
- Molecule 1: CUGBP Elav-like family member 2



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

The representative model is number 19. Colouring as in section 4.1 above.

- Molecule 1: CUGBP Elav-like family member 2



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing, molecular dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
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	1082
Number of shifts mapped to atoms	1082
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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	1.53±0.02	1±0/570 (0.1± 0.1%)	1.40±0.03	5±1/768 (0.7± 0.2%)
All	All	1.53	13/11400 (0.1%)	1.41	109/15360 (0.7%)

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	2.0±0.0
All	All	0	40

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	455	ASN	C-N	5.67	1.45	1.34	13	13

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	410	TYR	CB-CG-CD1	9.75	126.85	121.00	3	18
1	A	416	PHE	CB-CG-CD2	-9.23	114.34	120.80	11	20
1	A	416	PHE	CB-CG-CD1	8.88	127.02	120.80	18	20
1	A	410	TYR	CB-CG-CD2	-8.38	115.97	121.00	4	14
1	A	453	TYR	CB-CG-CD1	8.10	125.86	121.00	8	16

There are no chirality outliers.

All 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	413	PRO	Peptide	20
1	A	415	GLU	Peptide	20

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	556	546	545	1±1
All	All	11120	10920	10900	12

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 1.

5 of 7 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:425:PHE:CZ	1:A:466:MET:HG3	0.50	2.42	17	2
1:A:425:PHE:CZ	1:A:466:MET:HG2	0.49	2.43	13	5
1:A:466:MET:CE	1:A:476:LEU:HG	0.43	2.43	20	1
1:A:466:MET:HE2	1:A:478:VAL:HG23	0.42	1.92	20	1
1:A:459:ALA:O	1:A:463:ILE:HD13	0.41	2.16	1	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	71/97 (73%)	61±2 (86±2%)	9±2 (13±3%)	1±1 (2±1%)	13	56
All	All	1420/1940 (73%)	1216 (86%)	180 (13%)	24 (2%)	13	56

All 5 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	427	PRO	10
1	A	456	PRO	8
1	A	416	PHE	3
1	A	399	LYS	2
1	A	411	HIS	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	58/83 (70%)	32±1 (55±3%)	26±1 (45±3%)	0 2
All	All	1160/1660 (70%)	635 (55%)	525 (45%)	0 2

5 of 45 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	399	LYS	20
1	A	412	LEU	20
1	A	416	PHE	20
1	A	419	GLN	20
1	A	420	ASP	20

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 82% 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 [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	1082
Number of shifts mapped to atoms	1082
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	36

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
$^{13}\text{C}_\alpha$	97	5.57 ± 0.09	Should be applied
$^{13}\text{C}_\beta$	89	5.37 ± 0.10	Should be applied
$^{13}\text{C}'$	97	5.71 ± 0.10	Should be applied
^{15}N	92	0.16 ± 0.51	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 84%, i.e. 812 atoms were assigned a chemical shift out of a possible 967. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	354/354 (100%)	145/145 (100%)	142/142 (100%)	67/67 (100%)
Sidechain	420/517 (81%)	277/337 (82%)	131/161 (81%)	12/19 (63%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	38/96 (40%)	19/47 (40%)	19/47 (40%)	0/2 (0%)
Overall	812/967 (84%)	441/529 (83%)	292/350 (83%)	79/88 (90%)

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	444	LEU	CG	19.40	21.37 – 32.19	-6.8
1	A	402	PRO	CD	43.40	45.11 – 55.58	-6.6
1	A	480	LEU	CG	19.70	21.37 – 32.19	-6.5
1	A	435	LYS	CE	36.30	37.57 – 46.21	-6.5
1	A	412	LEU	CG	19.80	21.37 – 32.19	-6.5
1	A	481	LYS	CE	36.40	37.57 – 46.21	-6.3
1	A	398	GLN	CG	27.00	28.36 – 39.21	-6.3
1	A	399	LYS	CE	36.50	37.57 – 46.21	-6.2
1	A	440	LYS	CE	36.50	37.57 – 46.21	-6.2
1	A	477	LYS	CE	36.50	37.57 – 46.21	-6.2
1	A	484	LYS	CE	36.50	37.57 – 46.21	-6.2
1	A	476	LEU	CG	20.40	21.37 – 32.19	-5.9
1	A	474	LYS	CE	36.80	37.57 – 46.21	-5.9
1	A	417	GLY	CA	37.80	38.93 – 51.79	-5.9
1	A	413	PRO	CD	44.20	45.11 – 55.58	-5.9
1	A	482	ARG	CD	37.80	38.57 – 47.75	-5.8
1	A	416	PHE	CD1	124.30	125.33 – 137.83	-5.8
1	A	475	ARG	CD	37.90	38.57 – 47.75	-5.7
1	A	427	PRO	CB	25.40	26.06 – 37.61	-5.6
1	A	460	GLN	CG	27.80	28.36 – 39.21	-5.5
1	A	402	PRO	C	168.80	169.47 – 184.06	-5.5
1	A	464	GLN	CG	27.90	28.36 – 39.21	-5.4
1	A	470	GLN	CG	27.90	28.36 – 39.21	-5.4
1	A	402	PRO	CG	21.30	21.69 – 32.72	-5.3
1	A	407	LEU	CG	21.00	21.37 – 32.19	-5.3
1	A	401	GLY	CA	38.50	38.93 – 51.79	-5.3
1	A	484	LYS	CG	19.00	19.35 – 30.45	-5.3
1	A	489	PRO	CD	44.80	45.11 – 55.58	-5.3
1	A	489	PRO	CG	21.40	21.69 – 32.72	-5.3
1	A	419	GLN	CG	28.10	28.36 – 39.21	-5.2
1	A	399	LYS	CG	19.10	19.35 – 30.45	-5.2
1	A	433	SER	C	165.90	166.15 – 183.14	-5.2

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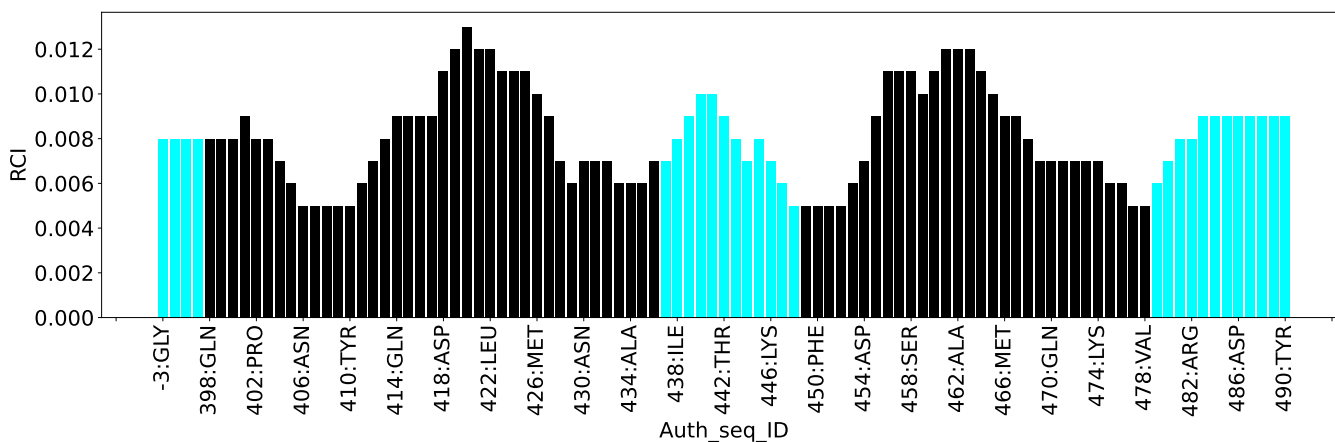
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	440	LYS	CD	23.40	23.50 – 34.42	-5.1
1	A	474	LYS	CD	23.40	23.50 – 34.42	-5.1
1	A	489	PRO	CB	26.00	26.06 – 37.61	-5.0
1	A	456	PRO	CD	45.10	45.11 – 55.58	-5.0

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	2438
Intra-residue ($ i-j =0$)	373
Sequential ($ i-j =1$)	722
Medium range ($ i-j >1$ and $ i-j <5$)	472
Long range ($ i-j \geq 5$)	871
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	142
Number of unmapped restraints	0
Number of restraints per residue	26.6
Number of long range restraints per residue ¹	9.0

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)	261.8	0.2
0.2-0.5 (Medium)	516.6	0.5
>0.5 (Large)	419.8	3.61

8.2.2 Average number of dihedral-angle violations per model

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)	37.7	10.0
10.0-20.0 (Medium)	7.8	19.8
>20.0 (Large)	2.6	25.9

9 Distance violation analysis i

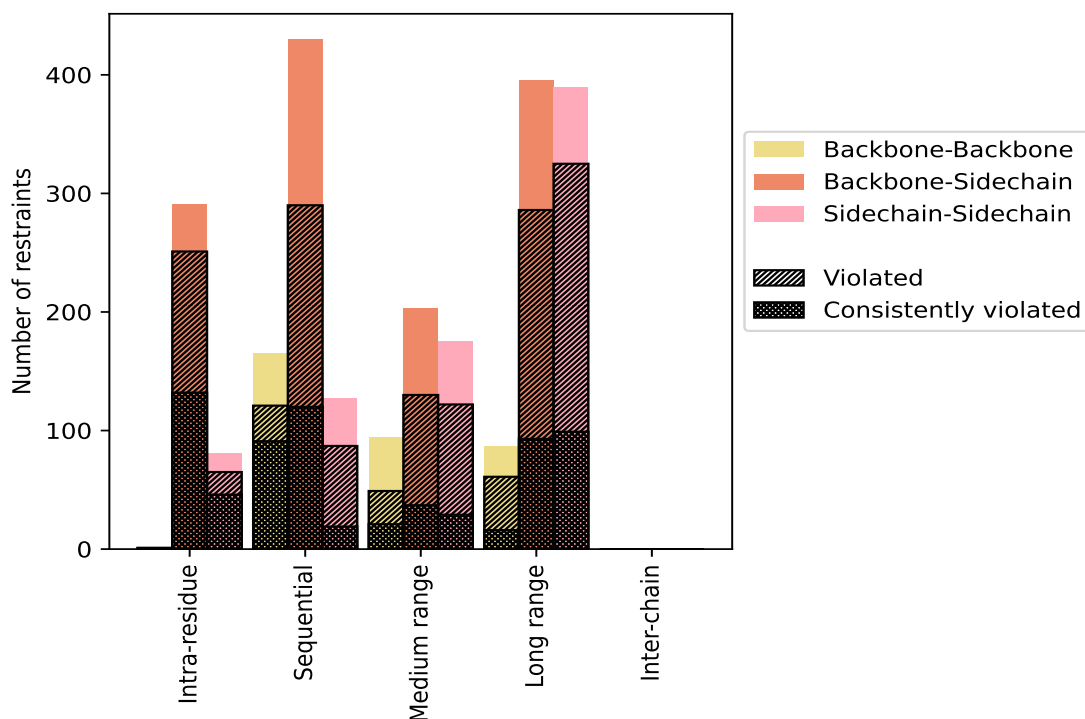
9.1 Summary of distance violations i

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 ($i-j =0$)	373	15.3	317	85.0	13.0	179	48.0	7.3
Backbone-Backbone	1	0.0	1	100.0	0.0	1	100.0	0.0
Backbone-Sidechain	291	11.9	251	86.3	10.3	132	45.4	5.4
Sidechain-Sidechain	81	3.3	65	80.2	2.7	46	56.8	1.9
Sequential ($i-j =1$)	722	29.6	498	69.0	20.4	230	31.9	9.4
Backbone-Backbone	165	6.8	121	73.3	5.0	91	55.2	3.7
Backbone-Sidechain	430	17.6	290	67.4	11.9	120	27.9	4.9
Sidechain-Sidechain	127	5.2	87	68.5	3.6	19	15.0	0.8
Medium range ($i-j >1$ & $i-j <5$)	472	19.4	301	63.8	12.3	87	18.4	3.6
Backbone-Backbone	94	3.9	49	52.1	2.0	21	22.3	0.9
Backbone-Sidechain	203	8.3	130	64.0	5.3	37	18.2	1.5
Sidechain-Sidechain	175	7.2	122	69.7	5.0	29	16.6	1.2
Long range ($i-j \geq 5$)	871	35.7	672	77.2	27.6	208	23.9	8.5
Backbone-Backbone	87	3.6	61	70.1	2.5	16	18.4	0.7
Backbone-Sidechain	395	16.2	286	72.4	11.7	93	23.5	3.8
Sidechain-Sidechain	389	16.0	325	83.5	13.3	99	25.4	4.1
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	2438	100.0	1788	73.3	73.3	704	28.9	28.9
Backbone-Backbone	347	14.2	232	66.9	9.5	129	37.2	5.3
Backbone-Sidechain	1319	54.1	957	72.6	39.3	382	29.0	15.7
Sidechain-Sidechain	772	31.7	599	77.6	24.6	193	25.0	7.9

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	247	358	165	430	0	1200	0.6	3.41	0.55	0.36
2	243	363	170	435	0	1211	0.59	3.1	0.54	0.36
3	254	350	170	416	0	1190	0.61	3.52	0.56	0.37
4	252	358	177	430	0	1217	0.58	3.12	0.54	0.35
5	242	349	173	420	0	1184	0.6	3.11	0.54	0.36
6	244	356	175	421	0	1196	0.6	2.84	0.53	0.37
7	245	348	175	426	0	1194	0.6	3.0	0.54	0.36
8	240	348	181	429	0	1198	0.59	3.54	0.54	0.37
9	245	362	168	427	0	1202	0.59	3.09	0.54	0.36
10	246	350	169	431	0	1196	0.61	3.2	0.55	0.37
11	252	358	172	421	0	1203	0.6	3.23	0.55	0.35

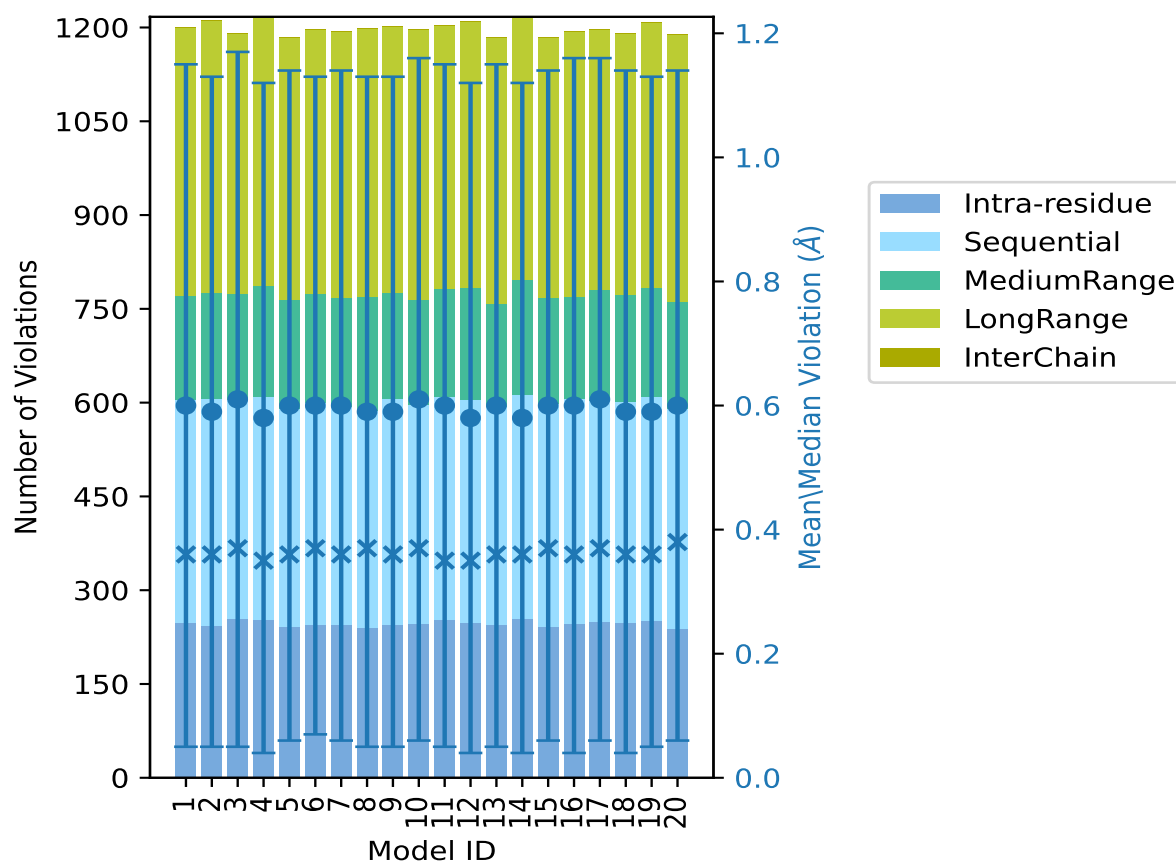
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
12	247	358	178	427	0	1210	0.58	3.19	0.54	0.35
13	245	348	165	426	0	1184	0.6	2.92	0.55	0.36
14	255	357	185	420	0	1217	0.58	3.15	0.54	0.36
15	242	357	168	417	0	1184	0.6	3.43	0.54	0.37
16	247	359	164	424	0	1194	0.6	3.53	0.56	0.36
17	249	354	178	415	0	1196	0.61	3.36	0.55	0.37
18	248	353	172	418	0	1191	0.59	3.12	0.55	0.36
19	251	358	175	424	0	1208	0.59	3.39	0.54	0.36
20	239	351	172	426	0	1188	0.6	3.61	0.54	0.38

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

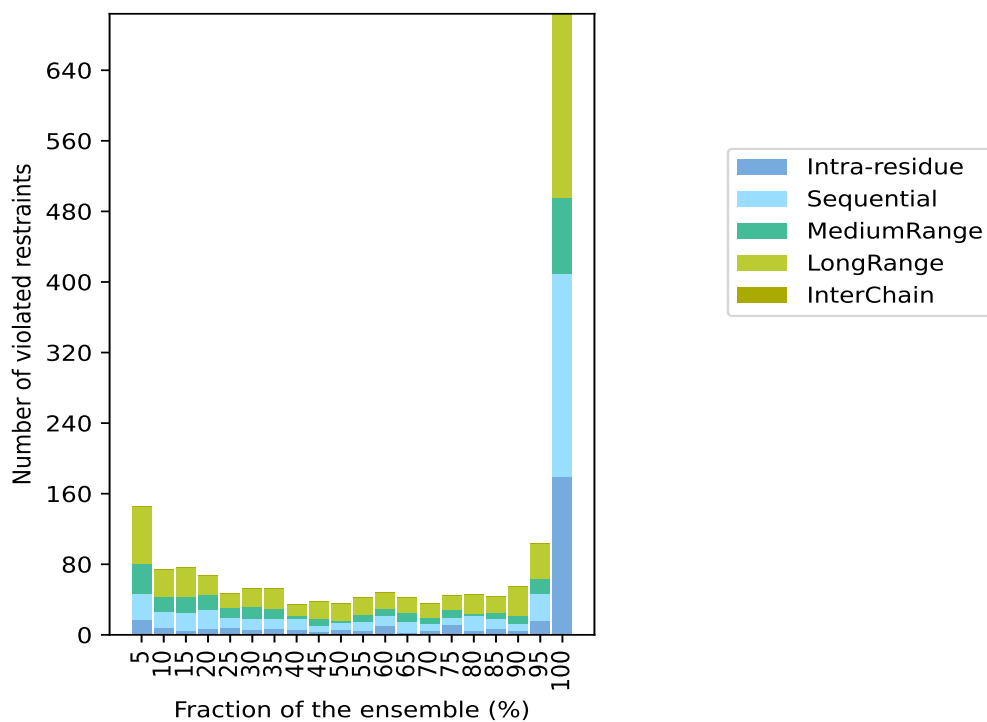
9.3 Distance violation statistics for the ensemble

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, 650(IR:56, SQ:224, MR:171, LR:199, 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	%
17	29	35	64	0	145	1	5.0
8	18	17	31	0	74	2	10.0
5	20	18	33	0	76	3	15.0
7	22	16	22	0	67	4	20.0
8	11	12	16	0	47	5	25.0
6	12	14	21	0	53	6	30.0
7	11	12	23	0	53	7	35.0
6	12	4	12	0	34	8	40.0
4	6	8	20	0	38	9	45.0
5	9	2	20	0	36	10	50.0
4	11	8	19	0	42	11	55.0
10	12	7	19	0	48	12	60.0
2	13	10	17	0	42	13	65.0
5	8	7	16	0	36	14	70.0
11	9	8	17	0	45	15	75.0
5	16	3	22	0	46	16	80.0
7	11	7	18	0	43	17	85.0
5	8	8	34	0	55	18	90.0
16	30	18	40	0	104	19	95.0
179	230	87	208	0	704	20	100.0

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

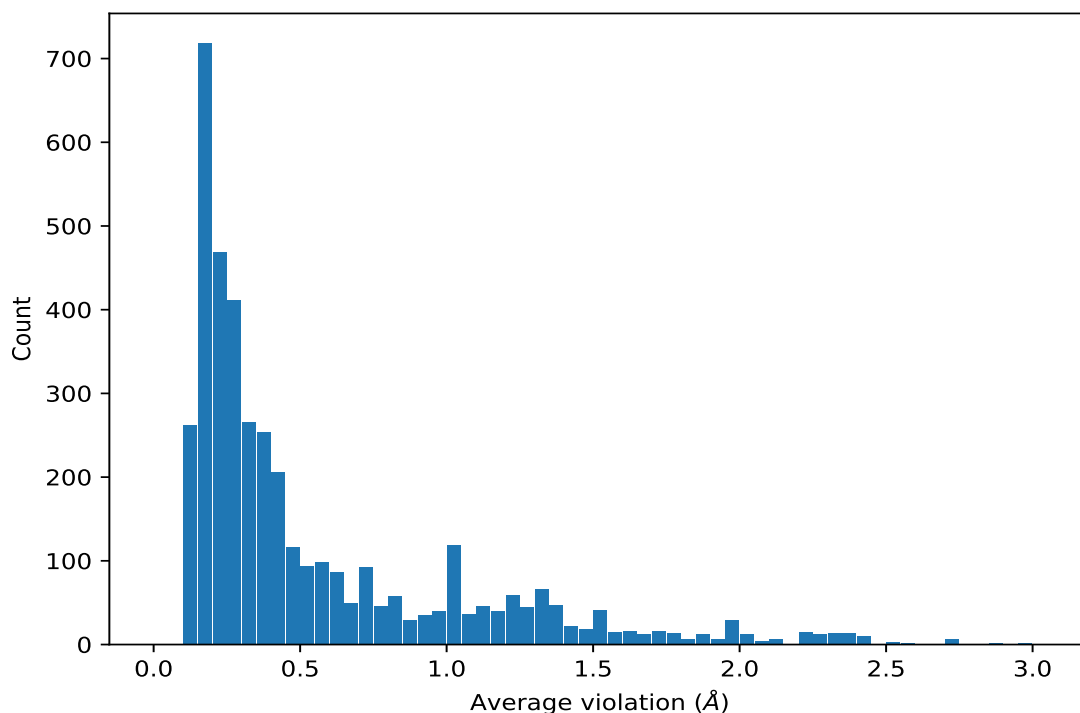
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD2	20	2.96	0.54	3.2
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD3	20	2.96	0.54	3.2
(1,1292)	1:A:408:PHE:HD1	1:A:450:PHE:HA	20	2.86	0.11	2.87
(1,1292)	1:A:408:PHE:HD2	1:A:450:PHE:HA	20	2.86	0.11	2.87
(1,450)	1:A:439:ASP:HB2	1:A:444:LEU:HD11	20	2.74	0.11	2.74
(1,450)	1:A:439:ASP:HB2	1:A:444:LEU:HD12	20	2.74	0.11	2.74
(1,450)	1:A:439:ASP:HB2	1:A:444:LEU:HD13	20	2.74	0.11	2.74
(1,450)	1:A:439:ASP:HB2	1:A:444:LEU:HD21	20	2.74	0.11	2.74
(1,450)	1:A:439:ASP:HB2	1:A:444:LEU:HD22	20	2.74	0.11	2.74
(1,450)	1:A:439:ASP:HB2	1:A:444:LEU:HD23	20	2.74	0.11	2.74
(1,1114)	1:A:414:GLN:H	1:A:414:GLN:HG3	20	2.66	0.03	2.66
(1,744)	1:A:412:LEU:HG	1:A:416:PHE:HB2	20	2.64	0.07	2.64
(1,2283)	1:A:423:GLN:HB2	1:A:423:GLN:HE21	20	2.59	0.56	3.08
(1,2283)	1:A:423:GLN:HB3	1:A:423:GLN:HE21	20	2.59	0.56	3.08
(1,1107)	1:A:420:ASP:HA	1:A:423:GLN:HE21	20	2.52	0.49	2.72
(1,166)	1:A:449:GLY:HA2	1:A:450:PHE:HD1	20	2.5	0.2	2.44

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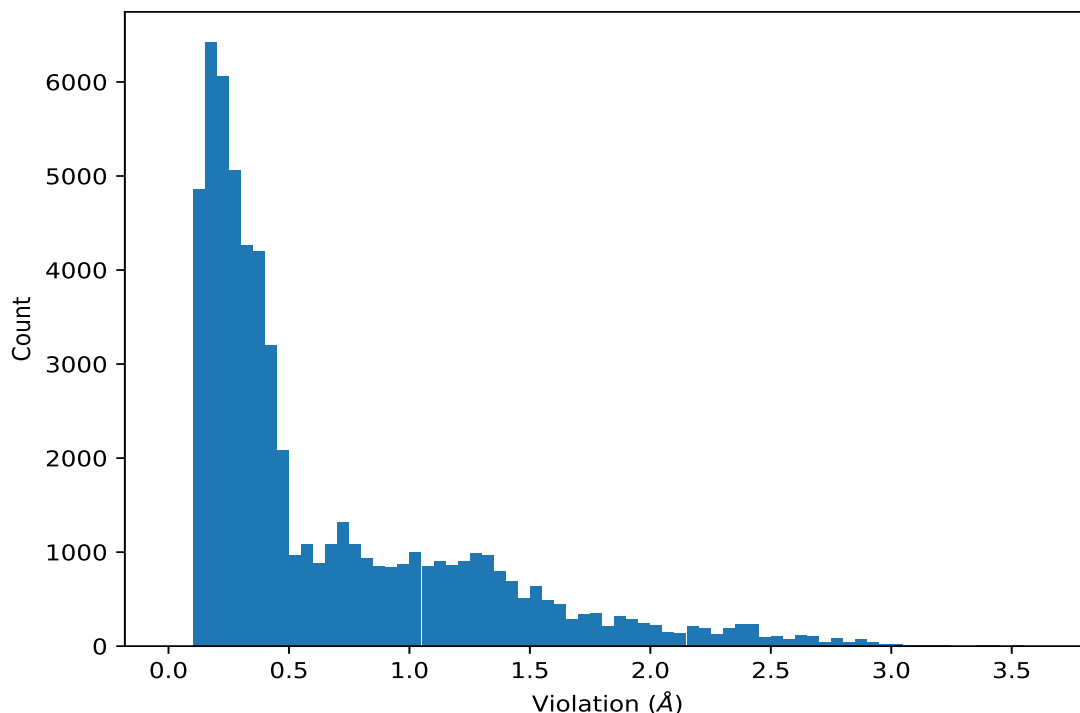
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,166)	1:A:449:GLY:HA2	1:A:450:PHE:HD2	20	2.5	0.2	2.44
(1,460)	1:A:398:GLN:HA	1:A:433:SER:HB3	20	2.48	0.21	2.45
(1,1880)	1:A:412:LEU:HD11	1:A:416:PHE:H	20	2.44	0.09	2.42

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)
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD2	20	3.61
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD3	20	3.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD2	8	3.54
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD3	8	3.54
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD2	16	3.53
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD3	16	3.53
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD2	3	3.52
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD3	3	3.52
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD2	15	3.43
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD3	15	3.43
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD2	1	3.41
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD3	1	3.41
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD2	19	3.39
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD3	19	3.39
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD2	17	3.36
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD3	17	3.36
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD2	11	3.23
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD3	11	3.23
(1,2158)	1:A:415:GLU:H	1:A:474:LYS:HD2	10	3.2

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

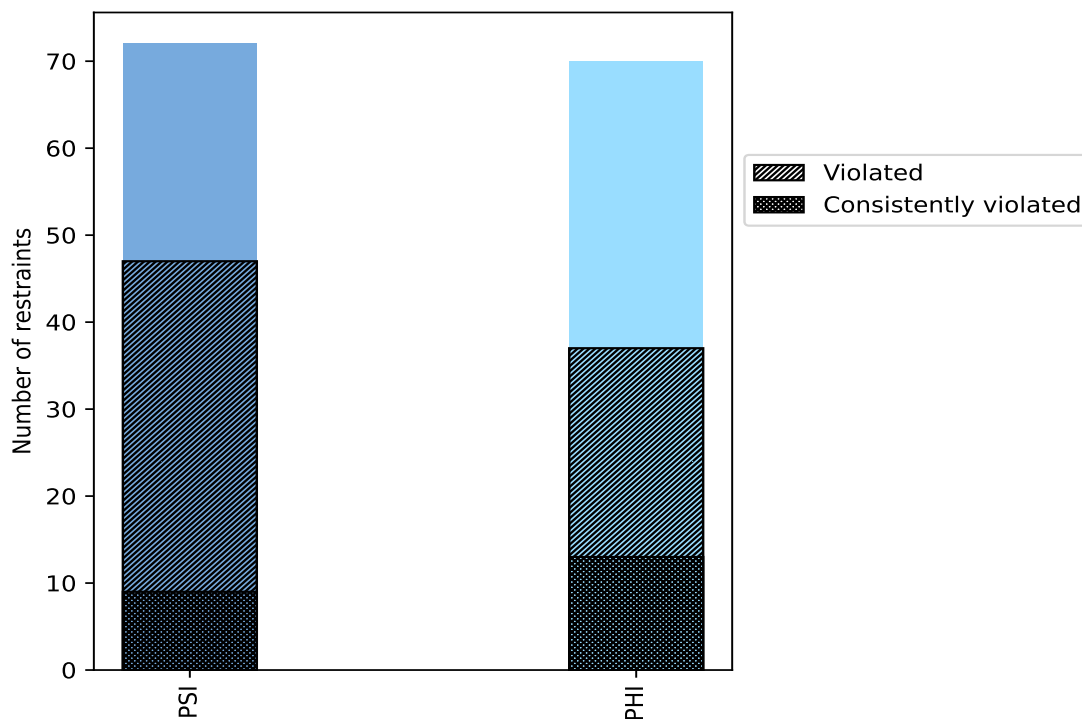
10.1 Summary of dihedral-angle violations [i](#)

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	72	50.7	47	65.3	33.1	9	12.5	6.3
PHI	70	49.3	37	52.9	26.1	13	18.6	9.2
Total	142	100.0	84	59.2	59.2	22	15.5	15.5

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

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



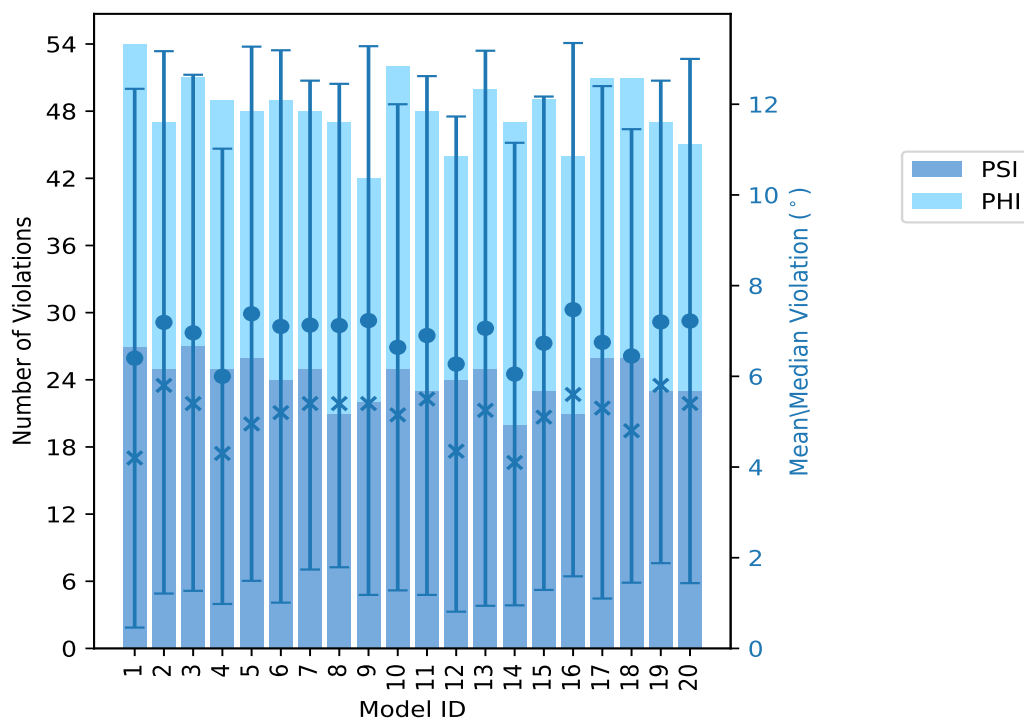
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	27	27	54	6.4	24.9	5.94	4.2
2	25	22	47	7.19	23.7	5.98	5.8
3	27	24	51	6.96	23.4	5.69	5.4
4	25	24	49	6.0	22.5	5.02	4.3
5	26	22	48	7.38	23.9	5.89	4.95
6	24	25	49	7.1	24.5	6.09	5.2
7	25	23	48	7.13	23.7	5.39	5.4
8	21	26	47	7.12	23.2	5.33	5.4
9	22	20	42	7.23	25.9	6.05	5.4
10	25	27	52	6.64	24.9	5.36	5.15
11	23	25	48	6.9	23.7	5.72	5.5
12	24	20	44	6.27	21.5	5.46	4.35
13	25	25	50	7.06	24.3	6.12	5.25
14	20	27	47	6.05	22.0	5.1	4.1
15	23	26	49	6.73	24.8	5.44	5.1
16	21	23	44	7.47	22.5	5.88	5.6
17	26	25	51	6.75	23.7	5.65	5.3
18	26	25	51	6.45	22.1	5.0	4.8
19	23	24	47	7.2	23.7	5.32	5.8
20	23	22	45	7.22	25.2	5.78	5.4

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

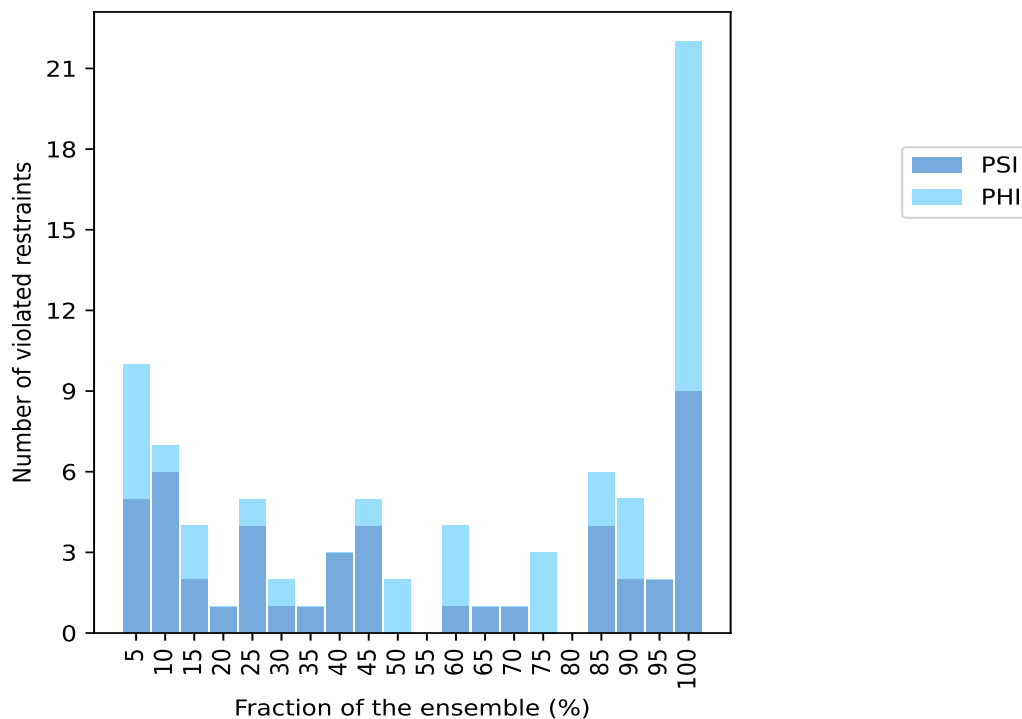
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
1	3	4	12	60.0
1	0	1	13	65.0
1	0	1	14	70.0
0	3	3	15	75.0
0	0	0	16	80.0
4	2	6	17	85.0
2	3	5	18	90.0
2	0	2	19	95.0
9	13	22	20	100.0

¹ Number of models with violations

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

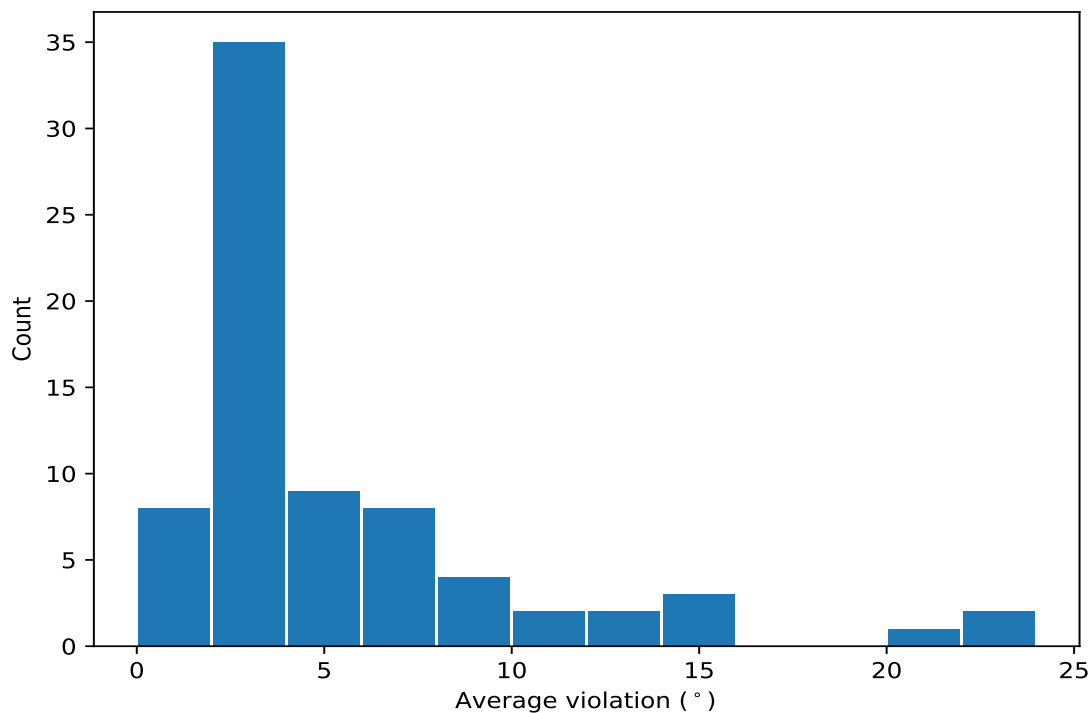


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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.

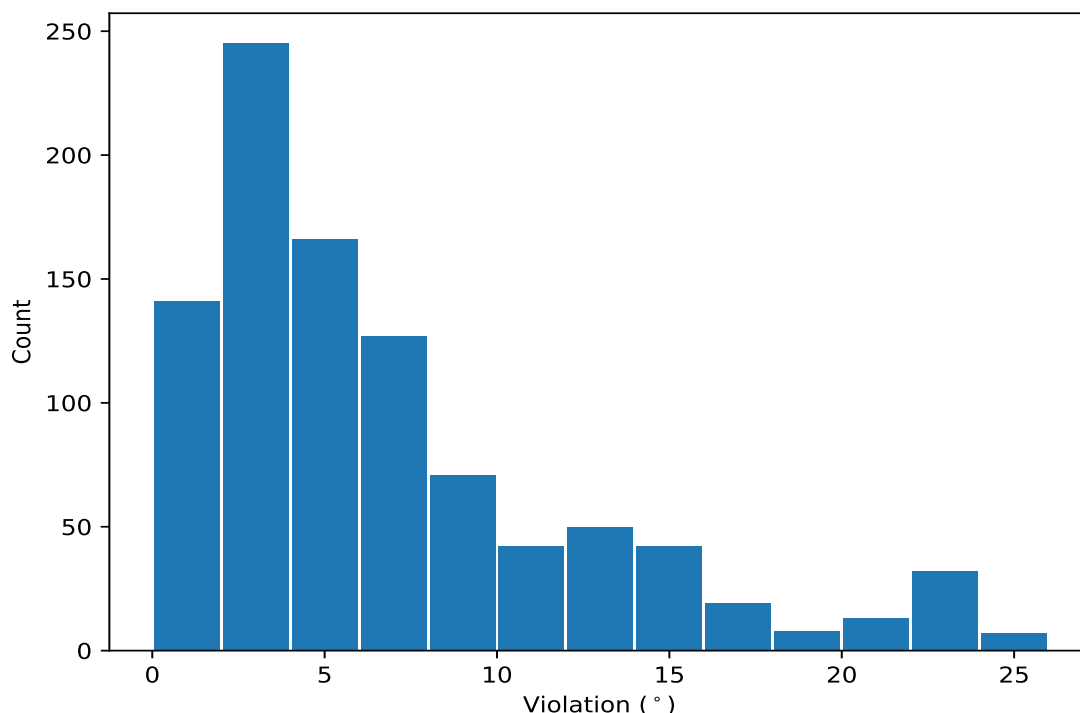
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,15)	1:A:413:PRO:N	1:A:413:PRO:CA	1:A:413:PRO:C	1:A:414:GLN:N	20	23.02	1.35	23.1
(1,17)	1:A:414:GLN:N	1:A:414:GLN:CA	1:A:414:GLN:C	1:A:415:GLU:N	20	22.91	1.2	22.8
(1,58)	1:A:436:VAL:N	1:A:436:VAL:CA	1:A:436:VAL:C	1:A:437:PHE:N	20	20.64	2.48	20.2
(1,18)	1:A:414:GLN:C	1:A:415:GLU:N	1:A:415:GLU:CA	1:A:415:GLU:C	20	14.5	2.37	15.25
(1,59)	1:A:436:VAL:C	1:A:437:PHE:N	1:A:437:PHE:CA	1:A:437:PHE:C	20	14.47	2.59	13.95
(1,16)	1:A:413:PRO:C	1:A:414:GLN:N	1:A:414:GLN:CA	1:A:414:GLN:C	20	14.32	1.13	14.15
(1,60)	1:A:437:PHE:N	1:A:437:PHE:CA	1:A:437:PHE:C	1:A:438:ILE:N	20	13.14	2.03	13.4
(1,1)	1:A:405:ALA:C	1:A:406:ASN:N	1:A:406:ASN:CA	1:A:406:ASN:C	20	12.5	2.24	12.35
(1,74)	1:A:444:LEU:N	1:A:444:LEU:CA	1:A:444:LEU:C	1:A:445:SER:N	20	11.08	2.86	11.2
(1,12)	1:A:411:HIS:N	1:A:411:HIS:CA	1:A:411:HIS:C	1:A:412:LEU:N	20	10.05	4.14	11.1

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 (°)
(1,17)	1:A:414:GLN:N	1:A:414:GLN:CA	1:A:414:GLN:C	1:A:415:GLU:N	9	25.9
(1,15)	1:A:413:PRO:N	1:A:413:PRO:CA	1:A:413:PRO:C	1:A:414:GLN:N	20	25.2
(1,17)	1:A:414:GLN:N	1:A:414:GLN:CA	1:A:414:GLN:C	1:A:415:GLU:N	1	24.9
(1,15)	1:A:413:PRO:N	1:A:413:PRO:CA	1:A:413:PRO:C	1:A:414:GLN:N	10	24.9
(1,15)	1:A:413:PRO:N	1:A:413:PRO:CA	1:A:413:PRO:C	1:A:414:GLN:N	15	24.8
(1,15)	1:A:413:PRO:N	1:A:413:PRO:CA	1:A:413:PRO:C	1:A:414:GLN:N	6	24.5
(1,15)	1:A:413:PRO:N	1:A:413:PRO:CA	1:A:413:PRO:C	1:A:414:GLN:N	13	24.3
(1,58)	1:A:436:VAL:N	1:A:436:VAL:CA	1:A:436:VAL:C	1:A:437:PHE:N	5	23.9
(1,58)	1:A:436:VAL:N	1:A:436:VAL:CA	1:A:436:VAL:C	1:A:437:PHE:N	13	23.9
(1,17)	1:A:414:GLN:N	1:A:414:GLN:CA	1:A:414:GLN:C	1:A:415:GLU:N	5	23.9