



wwPDB NMR Structure Validation Summary Report ⓘ

Sep 9, 2026 – 10:17 AM JST

PDB ID : 9WKT / pdb_00009wkt
BMRB ID : 36783
Title : mature Mba1, UniProt P38300, residues 34-278, *Saccharomyces cerevisiae*
Authors : Yang, J.; Ruan, M.S.; Wang, J.F.; Li, Y.Y.
Deposited on : 2025-09-01

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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 : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2.1
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

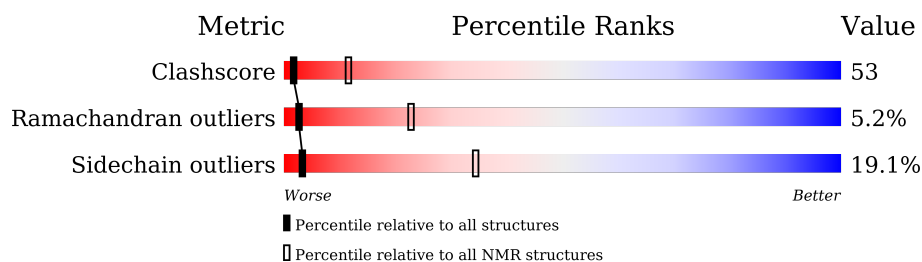
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 51%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	210	

2 Ensemble composition and analysis

This entry contains 15 models. Model 3 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:78-A:103, A:116-A:177, A:190-A:208, A:213-A:231, A:235-A:243 (135)	1.40	3

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, 3, 4, 5, 12, 13
2	7, 8, 14
3	11, 15
Single-model clusters	2; 6; 9; 10

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3435 atoms, of which 1746 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Inner membrane mitoribosome receptor MBA1, mitochondrial.

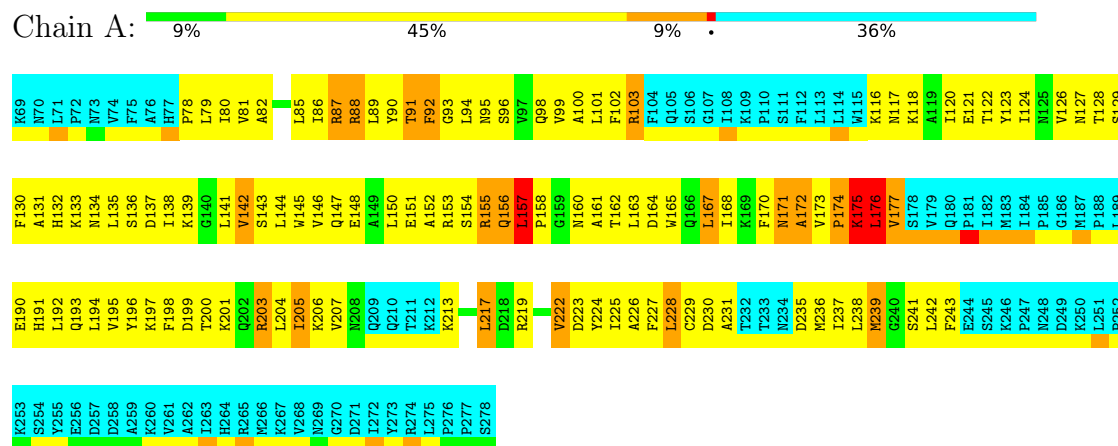
Mol	Chain	Residues	Atoms						Trace
1	A	210	Total	C	H	N	O	S	0
			3435	1092	1746	290	301	6	

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.

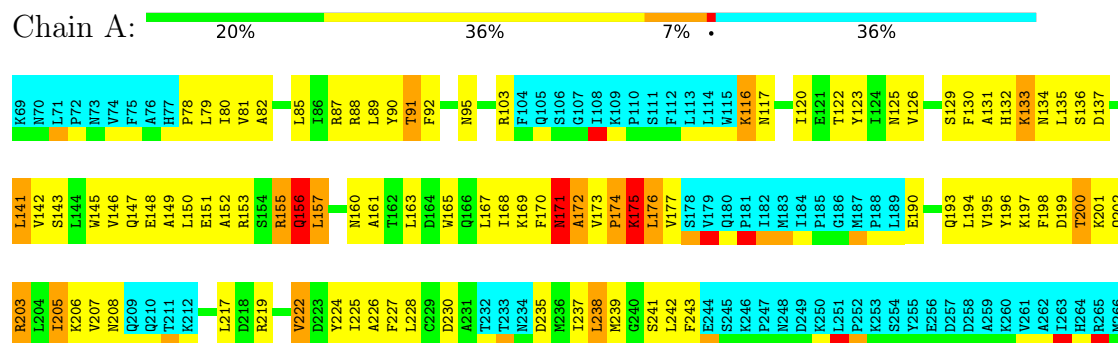
- Molecule 1: Inner membrane mitoribosome receptor MBA1, mitochondrial



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

The representative model is number 3. Colouring as in section 4.1 above.

- Molecule 1: Inner membrane mitoribosome receptor MBA1, mitochondrial



N267
N268
N269
G270
D271
I272
V273
R274
L275
P276
P277
S278

5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 15 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 calculation	2.19
X-PLOR NIH	refinement	2.19

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	1586
Number of shifts mapped to atoms	1469
Number of unparsed shifts	0
Number of shifts with mapping errors	117
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	51%

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	1.50±0.02	2±1/1110 (0.2± 0.1%)	1.95±0.08	17±2/1504 (1.1± 0.1%)
All	All	1.50	37/16650 (0.2%)	1.95	259/22560 (1.1%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	9.5±1.1
All	All	0	142

5 of 8 unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	176	LEU	C-N	13.62	1.52	1.33	9	9
1	A	175	LYS	C-N	12.27	1.50	1.33	13	15
1	A	177	VAL	CA-CB	8.36	1.65	1.54	7	1
1	A	175	LYS	N-CA	8.29	1.55	1.46	3	6
1	A	176	LEU	N-CA	6.82	1.54	1.46	8	1

5 of 29 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	177	VAL	N-CA-C	27.22	145.56	108.27	1	8
1	A	176	LEU	N-CA-C	26.39	152.42	109.40	14	15
1	A	175	LYS	N-CA-C	22.66	145.49	108.32	13	15
1	A	176	LEU	CA-C-N	-13.17	104.64	122.94	15	15
1	A	176	LEU	C-N-CA	-13.17	104.64	122.94	15	15

There are no chirality outliers.

5 of 10 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	87	ARG	Sidechain	15
1	A	88	ARG	Sidechain	15
1	A	103	ARG	Sidechain	15
1	A	153	ARG	Sidechain	15
1	A	155	ARG	Sidechain	15

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	1090	1135	1135	117±19
All	All	16350	17025	17025	1757

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 53.

5 of 1143 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:LEU:HD22	1:A:196:TYR:CD2	1.01	1.90	1	2
1:A:126:VAL:HG21	1:A:238:LEU:HD13	1.01	1.22	5	1
1:A:144:LEU:HD13	1:A:145:TRP:N	1.00	1.71	13	1
1:A:122:THR:HG21	1:A:236:MET:HE1	0.99	1.33	5	1
1:A:242:LEU:O	1:A:242:LEU:HD13	0.99	1.58	11	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	135/210 (64%)	115±2 (85±2%)	13±3 (10±2%)	7±2 (5±1%)	3	23
All	All	2025/3150 (64%)	1722 (85%)	197 (10%)	106 (5%)	3	23

5 of 22 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	156	GLN	13
1	A	157	LEU	13
1	A	172	ALA	11
1	A	158	PRO	10
1	A	142	VAL	9

6.3.2 Protein sidechains ⓘ

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	120/189 (63%)	97±4 (81±3%)	23±4 (19±3%)	3	34
All	All	1800/2835 (63%)	1456 (81%)	344 (19%)	3	34

5 of 90 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	167	LEU	13
1	A	157	LEU	11
1	A	204	LEU	11
1	A	242	LEU	11
1	A	79	LEU	11

6.3.3 RNA ⓘ

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 51% for the well-defined parts and 49% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	1586
Number of shifts mapped to atoms	1469
Number of unparsed shifts	0
Number of shifts with mapping errors	117
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 117) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	35	LYS	H	8.249	0.001	1
1	A	35	LYS	HA	4.297	.	1
1	A	35	LYS	HB2	1.895	.	1
1	A	35	LYS	HD2	1.74	.	1
1	A	35	LYS	HG2	1.404	.	1
1	A	35	LYS	C	175.731	.	1
1	A	35	LYS	CA	55.542	.	1
1	A	35	LYS	CB	31.445	.	1
1	A	35	LYS	N	123.012	0.065	1
1	A	36	GLU	H	7.998	0.002	1
1	A	36	GLU	HA	4.021	.	1
1	A	36	GLU	HB2	1.972	.	1
1	A	36	GLU	HG2	2.248	.	1
1	A	36	GLU	C	178.519	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	36	GLU	CA	56.261	.	1
1	A	36	GLU	CB	28.282	.	1
1	A	36	GLU	N	119.073	0.067	1
1	A	37	SER	H	8.257	0.004	1
1	A	37	SER	HA	4.452	.	1
1	A	37	SER	HB2	3.866	.	1
1	A	37	SER	C	174.298	.	1
1	A	37	SER	CA	57.76	.	1
1	A	37	SER	CB	62.721	.	1
1	A	37	SER	N	116.674	0.057	1
1	A	39	THR	H	8.133	0.005	1
1	A	39	THR	HA	4.367	.	1
1	A	39	THR	HB	4.021	.	1
1	A	39	THR	HG21	1.15	0.004	1
1	A	39	THR	HG22	1.15	0.004	1
1	A	39	THR	HG23	1.15	0.004	1
1	A	39	THR	C	174.573	.	1
1	A	39	THR	CA	61.627	0.0	1
1	A	39	THR	CB	68.559	0.018	1
1	A	39	THR	CG2	19.385	.	1
1	A	39	THR	N	114.601	0.056	1
1	A	44	ASP	H	8.25	0.002	1
1	A	44	ASP	HA	4.297	.	1
1	A	44	ASP	HB2	2.558	.	1
1	A	44	ASP	C	175.855	.	1
1	A	44	ASP	CA	53.373	.	1
1	A	44	ASP	CB	40.321	.	1
1	A	44	ASP	N	122.094	0.01	1
1	A	48	GLN	H	8.183	0.002	1
1	A	48	GLN	HA	3.93	.	1
1	A	48	GLN	HB2	2.015	.	1
1	A	48	GLN	C	174.959	.	1
1	A	48	GLN	CA	54.96	0.062	1
1	A	48	GLN	CB	27.981	0.028	1
1	A	48	GLN	N	120.807	0.029	1
1	A	51	PHE	H	8.207	0.004	1
1	A	51	PHE	HA	4.331	.	1
1	A	51	PHE	HB2	3.049	.	1
1	A	51	PHE	C	173.911	.	1
1	A	51	PHE	CA	56.527	0.011	1
1	A	51	PHE	CB	38.253	0.002	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	51	PHE	N	120.857	0.054	1
1	A	52	ASN	H	8.216	0.001	1
1	A	52	ASN	HA	4.443	.	1
1	A	52	ASN	HB2	2.678	.	1
1	A	52	ASN	C	173.057	.	1
1	A	52	ASN	CA	49.954	.	1
1	A	52	ASN	CB	38.1	.	1
1	A	52	ASN	N	122.645	0.048	1
1	A	55	HIS	H	7.599	0.004	1
1	A	55	HIS	HA	4.409	.	1
1	A	55	HIS	HB2	3.238	.	1
1	A	55	HIS	C	175.193	.	1
1	A	55	HIS	CA	56.599	.	1
1	A	55	HIS	CB	28.465	.	1
1	A	55	HIS	N	119.437	0.072	1
1	A	57	GLY	H	8.215	0.011	1
1	A	57	GLY	HA2	3.996	.	2
1	A	57	GLY	HA3	3.915	.	2
1	A	57	GLY	C	174.146	.	1
1	A	57	GLY	CA	44.845	0.001	1
1	A	57	GLY	N	108.255	0.101	1
1	A	58	VAL	H	7.91	0.004	1
1	A	58	VAL	HA	3.944	.	1
1	A	58	VAL	HB	2.127	.	1
1	A	58	VAL	HG11	0.945	0.012	1
1	A	58	VAL	HG12	0.945	0.012	1
1	A	58	VAL	HG13	0.945	0.012	1
1	A	58	VAL	C	175.646	.	1
1	A	58	VAL	CA	61.967	.	1
1	A	58	VAL	CB	31.009	.	1
1	A	58	VAL	CG1	18.386	.	1
1	A	58	VAL	N	119.622	0.012	1
1	A	59	ALA	H	7.897	0.004	1
1	A	59	ALA	HA	4.297	.	1
1	A	59	ALA	HB1	1.348	0.005	1
1	A	59	ALA	HB2	1.348	0.005	1
1	A	59	ALA	HB3	1.348	0.005	1
1	A	59	ALA	C	177.126	.	1
1	A	59	ALA	CA	52.288	.	1
1	A	59	ALA	CB	17.446	.	1
1	A	59	ALA	N	123.04	0.106	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	62	ILE	H	7.628	0.009	1
1	A	62	ILE	HA	4.169	.	1
1	A	62	ILE	HB	1.762	.	1
1	A	62	ILE	HD11	0.659	.	1
1	A	62	ILE	HD12	0.659	.	1
1	A	62	ILE	HD13	0.659	.	1
1	A	62	ILE	HG21	0.865	0.001	1
1	A	62	ILE	HG22	0.865	0.001	1
1	A	62	ILE	HG23	0.865	0.001	1
1	A	62	ILE	C	174.94	.	1
1	A	62	ILE	CA	60.948	0.015	1
1	A	62	ILE	CB	37.072	0.003	1
1	A	62	ILE	CG2	15.186	.	1
1	A	62	ILE	N	117.534	0.082	1
1	A	64	ILE	HG12	1.14	.	1
1	A	68	TYR	H	7.795	0.002	1
1	A	68	TYR	HA	4.224	.	1
1	A	68	TYR	HB2	2.914	.	1
1	A	68	TYR	CA	57.35	0.016	1
1	A	68	TYR	CB	37.045	0.002	1
1	A	68	TYR	N	116.155	0.039	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	162	0.59 ± 0.16	Should be checked
$^{13}\text{C}_\beta$	153	1.54 ± 0.09	Should be checked
$^{13}\text{C}'$	140	0.56 ± 0.10	Should be applied
^{15}N	189	0.19 ± 0.16	None needed (< 0.5 ppm)

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 51%, i.e. 991 atoms were assigned a chemical shift out of a possible 1959. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	507/673 (75%)	224/271 (83%)	171/270 (63%)	112/132 (85%)

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	Total	¹ H	¹³ C	¹⁵ N
Sidechain	484/1142 (42%)	329/747 (44%)	155/349 (44%)	0/46 (0%)
Aromatic	0/144 (0%)	0/71 (0%)	0/69 (0%)	0/4 (0%)
Overall	991/1959 (51%)	553/1089 (51%)	326/688 (47%)	112/182 (62%)

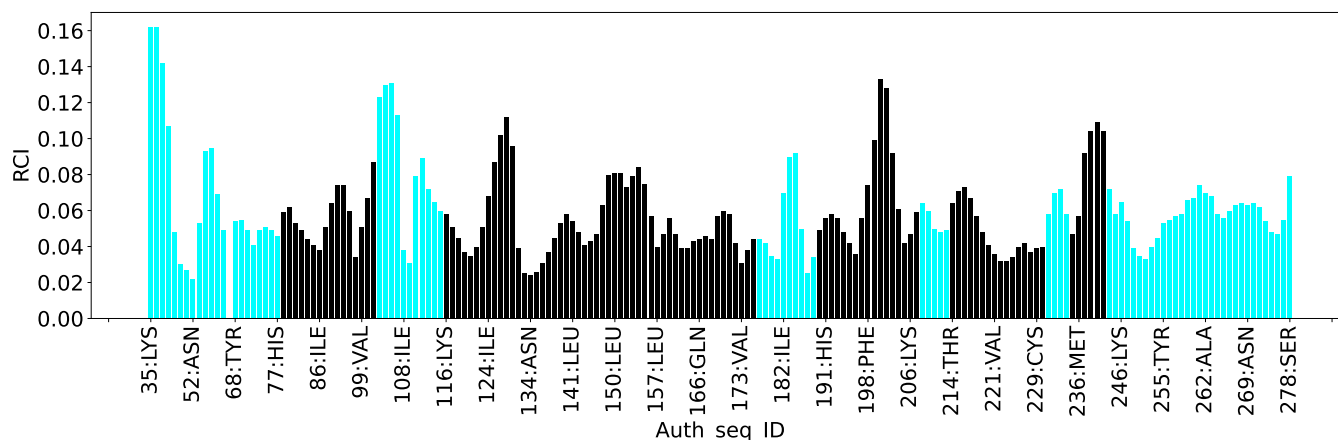
7.1.4 Statistically unusual chemical shifts [i](#)

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	399
Intra-residue ($ i-j =0$)	1
Sequential ($ i-j =1$)	216
Medium range ($ i-j >1$ and $ i-j <5$)	63
Long range ($ i-j \geq 5$)	119
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	264
Number of unmapped restraints	0
Number of restraints per residue	3.2
Number of long range restraints per residue ¹	0.6

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)	1.6	0.2
0.2-0.5 (Medium)	6.1	0.5
>0.5 (Large)	88.3	48.03

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)	16.4	9.96
10.0-20.0 (Medium)	3.5	19.75
>20.0 (Large)	39.6	159.91

9 Distance violation analysis ⓘ

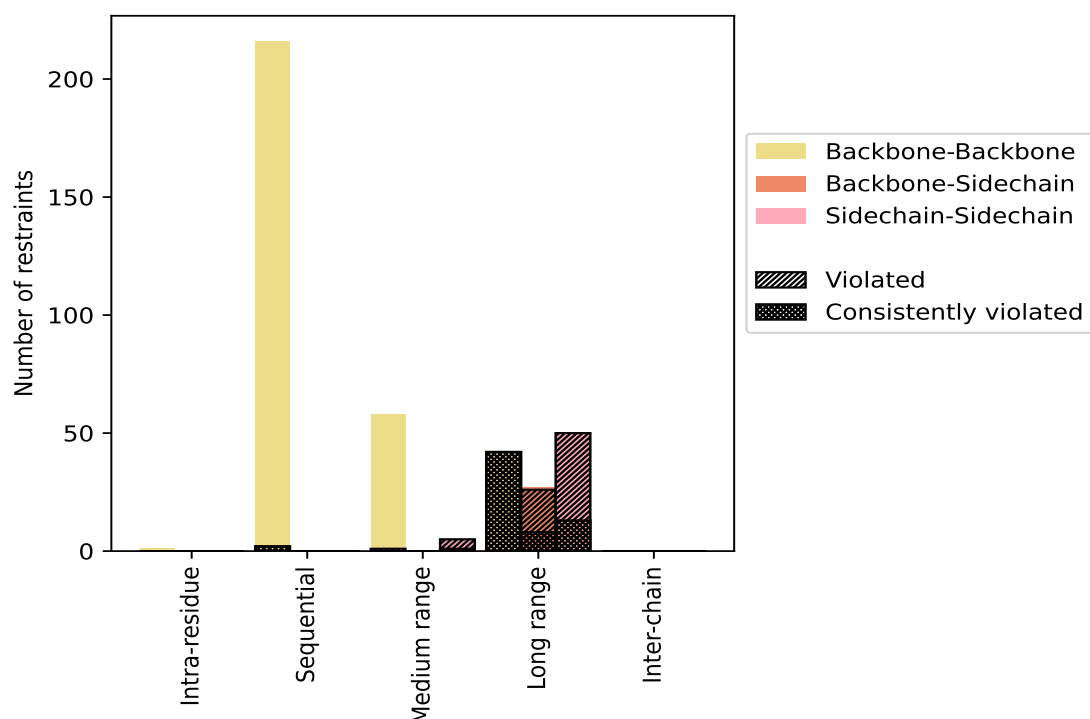
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	1	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	1	0.3	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
Sequential ($i-j =1$)	216	54.1	2	0.9	0.5	2	0.9	0.5
Backbone-Backbone	216	54.1	2	0.9	0.5	2	0.9	0.5
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
Medium range ($i-j >1$ & $i-j <5$)	63	15.8	6	9.5	1.5	1	1.6	0.3
Backbone-Backbone	58	14.5	1	1.7	0.3	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	5	1.3	5	100.0	1.3	1	20.0	0.3
Long range ($i-j \geq 5$)	119	29.8	118	99.2	29.6	63	52.9	15.8
Backbone-Backbone	42	10.5	42	100.0	10.5	42	100.0	10.5
Backbone-Sidechain	27	6.8	26	96.3	6.5	8	29.6	2.0
Sidechain-Sidechain	50	12.5	50	100.0	12.5	13	26.0	3.3
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	399	100.0	126	31.6	31.6	66	16.5	16.5
Backbone-Backbone	317	79.4	45	14.2	11.3	44	13.9	11.0
Backbone-Sidechain	27	6.8	26	96.3	6.5	8	29.6	2.0
Sidechain-Sidechain	55	13.8	55	100.0	13.8	14	25.5	3.5

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	2	2	85	0	89	12.51	41.97	10.38	13.9
2	0	2	2	91	0	95	10.99	31.34	9.46	12.31
3	0	2	3	92	0	97	11.58	33.48	9.96	12.61
4	0	2	4	93	0	99	10.98	34.78	9.66	10.13
5	0	2	4	90	0	96	11.2	39.92	10.03	9.04
6	0	2	4	94	0	100	10.6	30.01	9.11	8.92
7	0	2	2	89	0	93	11.96	40.79	10.3	13.46
8	0	2	4	93	0	99	11.04	36.57	10.06	9.56
9	0	2	4	91	0	97	11.17	37.7	10.06	11.77
10	0	2	3	90	0	95	11.47	38.88	9.85	11.68

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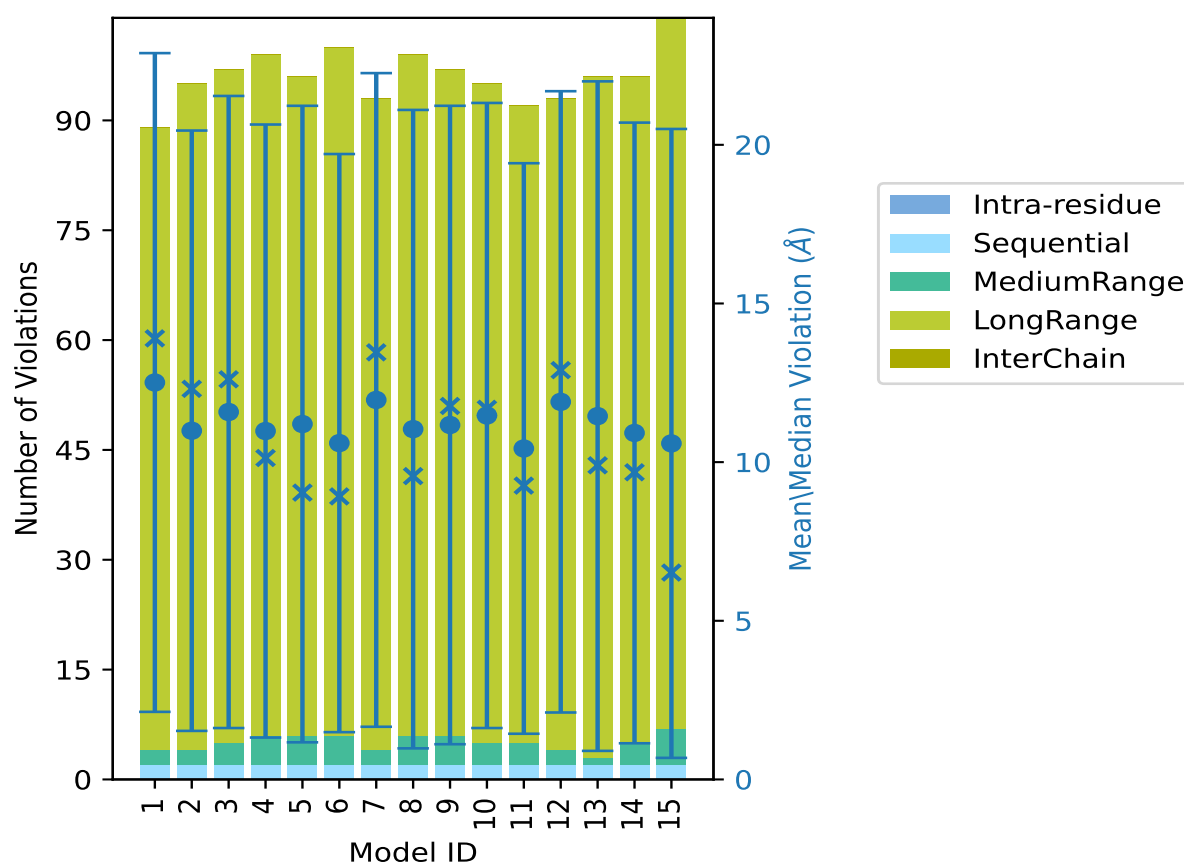
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	2	3	87	0	92	10.43	31.04	8.99	9.26
12	0	2	2	89	0	93	11.9	36.06	9.79	12.9
13	0	2	1	93	0	96	11.45	48.03	10.55	9.9
14	0	2	3	91	0	96	10.92	37.4	9.78	9.68
15	0	2	5	97	0	104	10.59	33.89	9.91	6.52

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 ⓘ

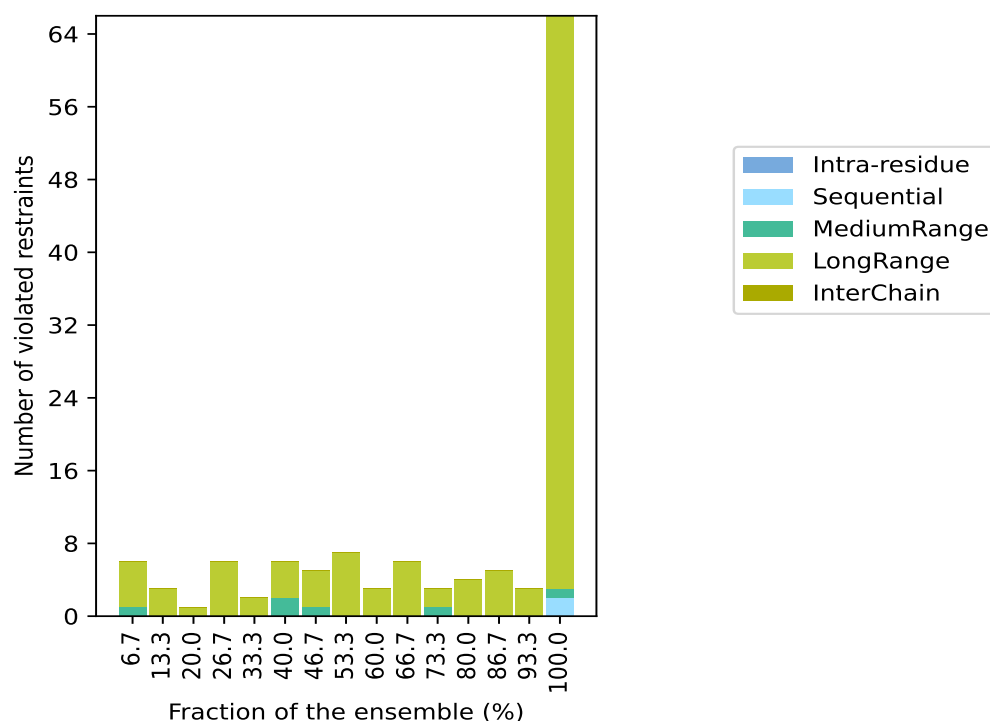
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 273(IR:1, SQ:214, MR:57, LR:1, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	1	5	0	6	1	6.7
0	0	0	3	0	3	2	13.3
0	0	0	1	0	1	3	20.0
0	0	0	6	0	6	4	26.7
0	0	0	2	0	2	5	33.3
0	0	2	4	0	6	6	40.0
0	0	1	4	0	5	7	46.7
0	0	0	7	0	7	8	53.3
0	0	0	3	0	3	9	60.0
0	0	0	6	0	6	10	66.7
0	0	1	2	0	3	11	73.3
0	0	0	4	0	4	12	80.0
0	0	0	5	0	5	13	86.7
0	0	0	3	0	3	14	93.3
0	2	1	63	0	66	15	100.0

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

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

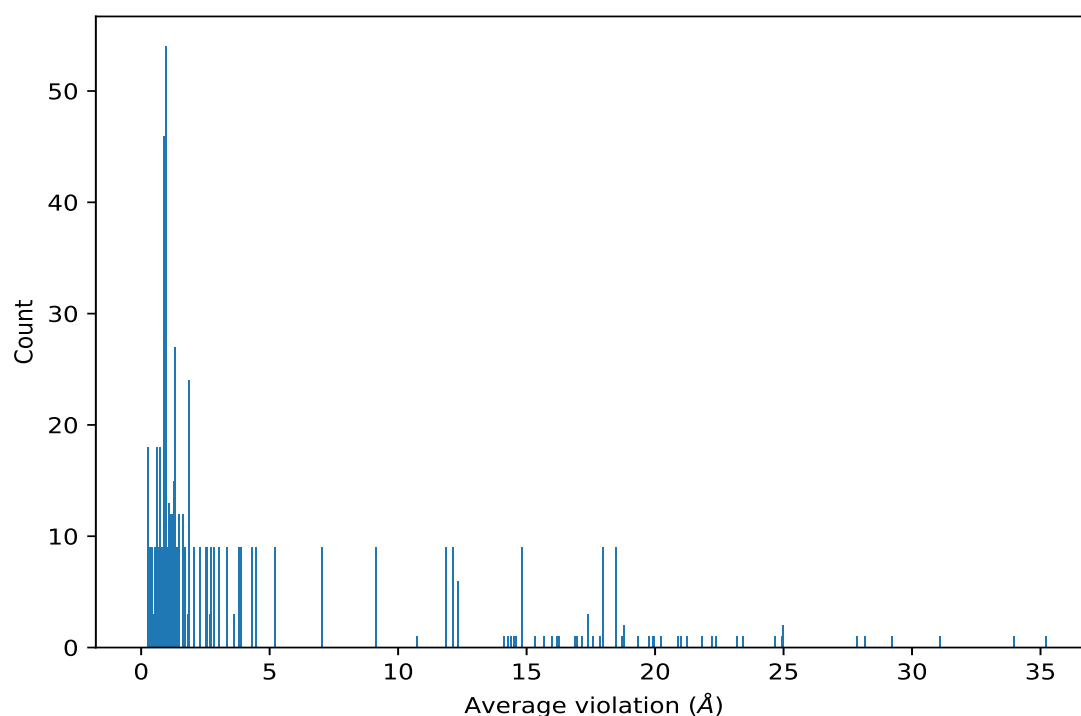
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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.

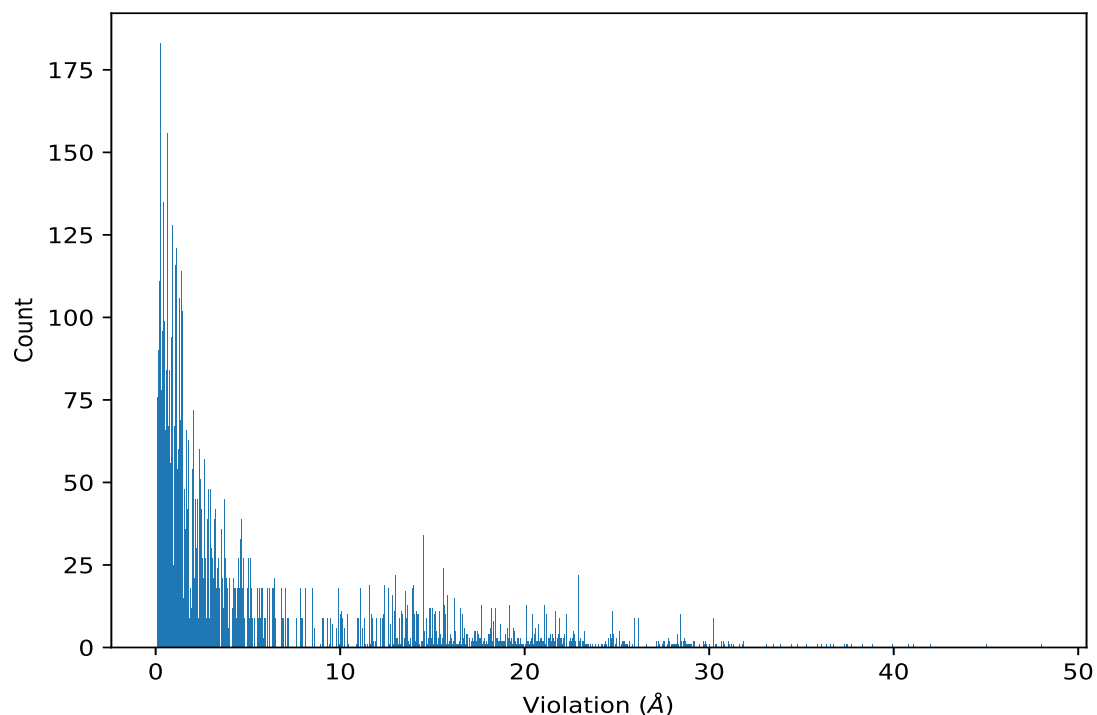
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	15	35.22	7.48	36.57
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	15	33.96	6.95	35.89
(1,53)	1:129:A:SER:HA	1:97:A:VAL:H	15	31.09	0.53	31.04
(1,51)	1:129:A:SER:H	1:97:A:VAL:H	15	29.21	0.41	29.16
(1,46)	1:94:A:LEU:H	1:129:A:SER:H	15	28.16	0.45	28.25
(1,48)	1:95:A:ASN:H	1:129:A:SER:H	15	27.88	0.59	27.85
(1,52)	1:129:A:SER:H	1:98:A:GLN:H	15	24.98	0.33	24.97
(1,258)	1:233:A:THR:HA	1:201:A:LYS:H	15	24.97	2.92	24.38
(1,50)	1:95:A:ASN:HA	1:129:A:SER:H	15	24.93	0.41	24.83
(1,298)	1:259:A:ALA:HA	1:227:A:PHE:H	15	24.65	3.18	23.65

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)
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	13	48.03
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	13	45.0
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	1	41.97
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	1	41.09
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	7	40.79
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	5	39.92
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	10	38.88
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	5	38.3
(1,317)	1:241:A:SER:HA	1:275:A:LEU:H	9	37.7
(1,316)	1:241:A:SER:H	1:275:A:LEU:H	7	37.47

10 Dihedral-angle violation analysis ⓘ

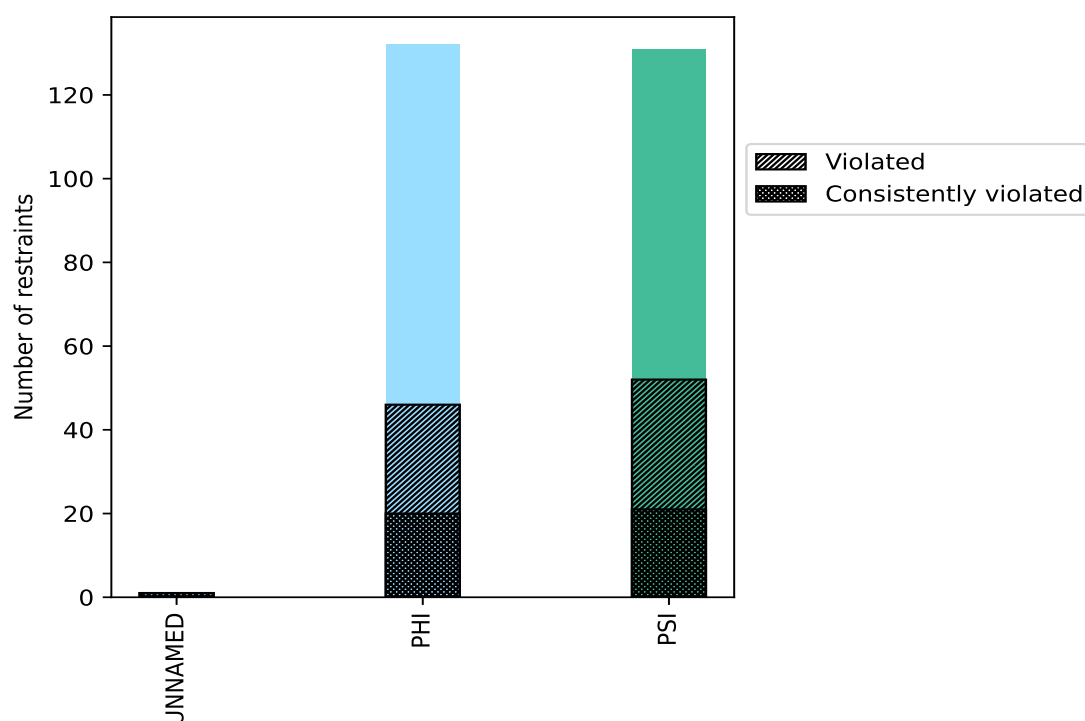
10.1 Summary of dihedral-angle violations ⓘ

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
UNNAMED	1	0.4	1	100.0	0.4	1	100.0	0.4
PHI	132	50.0	46	34.8	17.4	20	15.2	7.6
PSI	131	49.6	52	39.7	19.7	21	16.0	8.0
Total	264	100.0	99	37.5	37.5	42	15.9	15.9

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 ⓘ



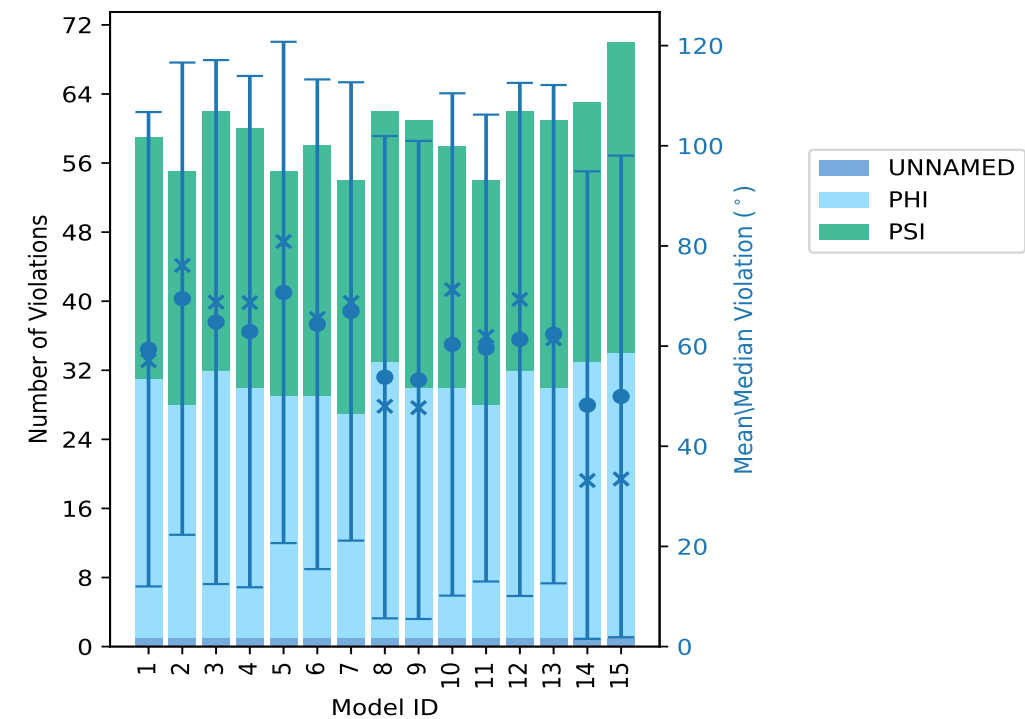
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	UNNAMED	PHI	PSI	Total				
1	1	30	28	59	59.37	157.94	47.36	57.08
2	1	27	27	55	69.47	158.63	47.15	76.11
3	1	31	30	62	64.8	154.25	52.31	68.78
4	1	29	30	60	62.89	159.91	51.05	68.68
5	1	28	26	55	70.71	157.27	50.05	80.89
6	1	28	29	58	64.36	154.67	48.89	65.51
7	1	26	27	54	66.92	156.29	45.76	68.72
8	1	32	29	62	53.79	156.18	48.15	47.99
9	1	29	31	61	53.24	155.36	47.73	47.7
10	1	29	28	58	60.33	154.44	50.15	71.29
11	1	27	26	54	59.61	158.15	46.61	61.94
12	1	31	30	62	61.33	158.65	51.23	69.34
13	1	29	31	61	62.38	155.87	49.75	61.46
14	1	32	30	63	48.22	149.38	46.67	33.16
15	1	33	36	70	49.95	157.54	48.08	33.47

10.2.1 Bar graph : Dihedral 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

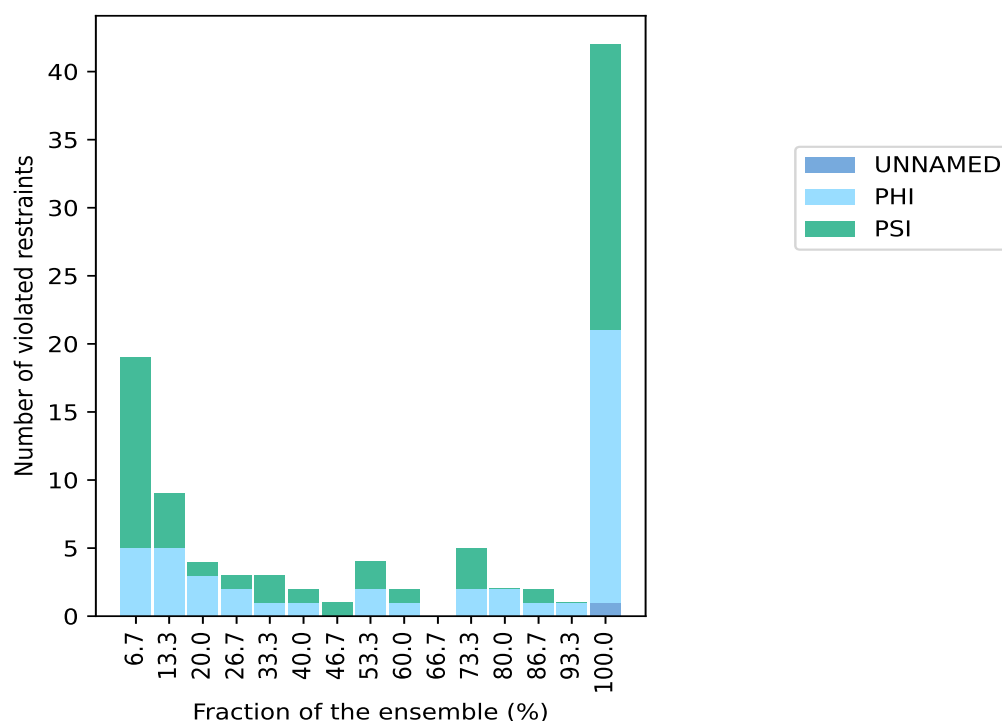
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	
UNNAMED	PHI	PSI	Total	Count ¹	%
0	5	14	19	1	6.7
0	5	4	9	2	13.3
0	3	1	4	3	20.0
0	2	1	3	4	26.7
0	1	2	3	5	33.3
0	1	1	2	6	40.0
0	0	1	1	7	46.7
0	2	2	4	8	53.3
0	1	1	2	9	60.0
0	0	0	0	10	66.7
0	2	3	5	11	73.3
0	2	0	2	12	80.0
0	1	1	2	13	86.7
0	1	0	1	14	93.3
1	20	21	42	15	100.0

¹ Number of models with violations

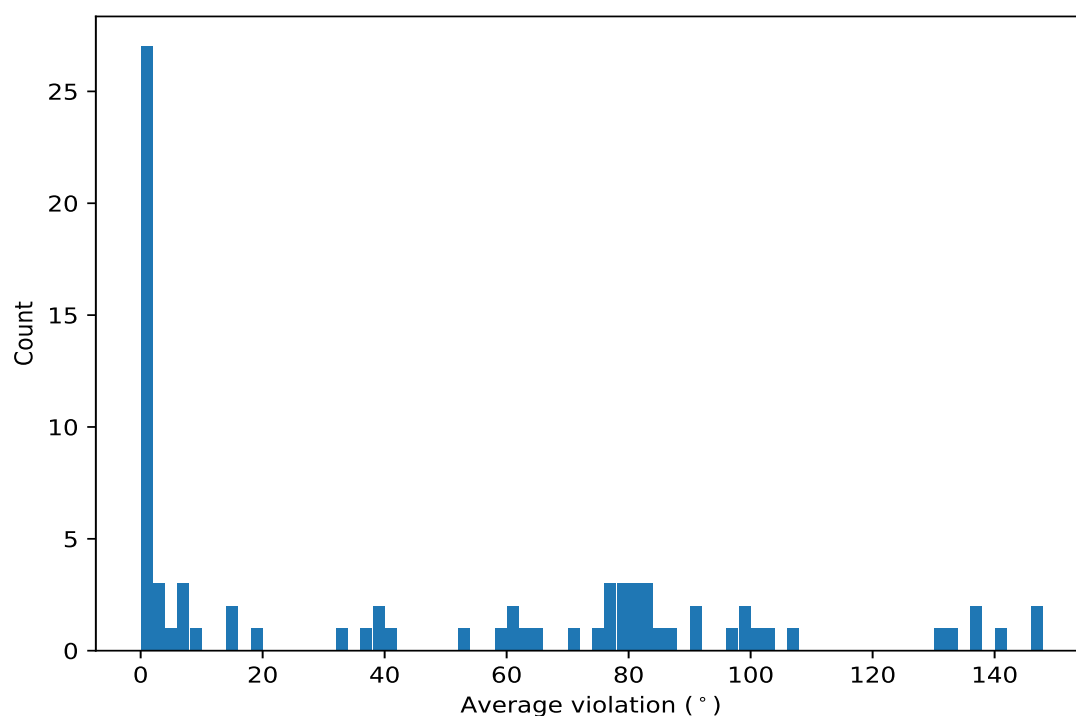
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

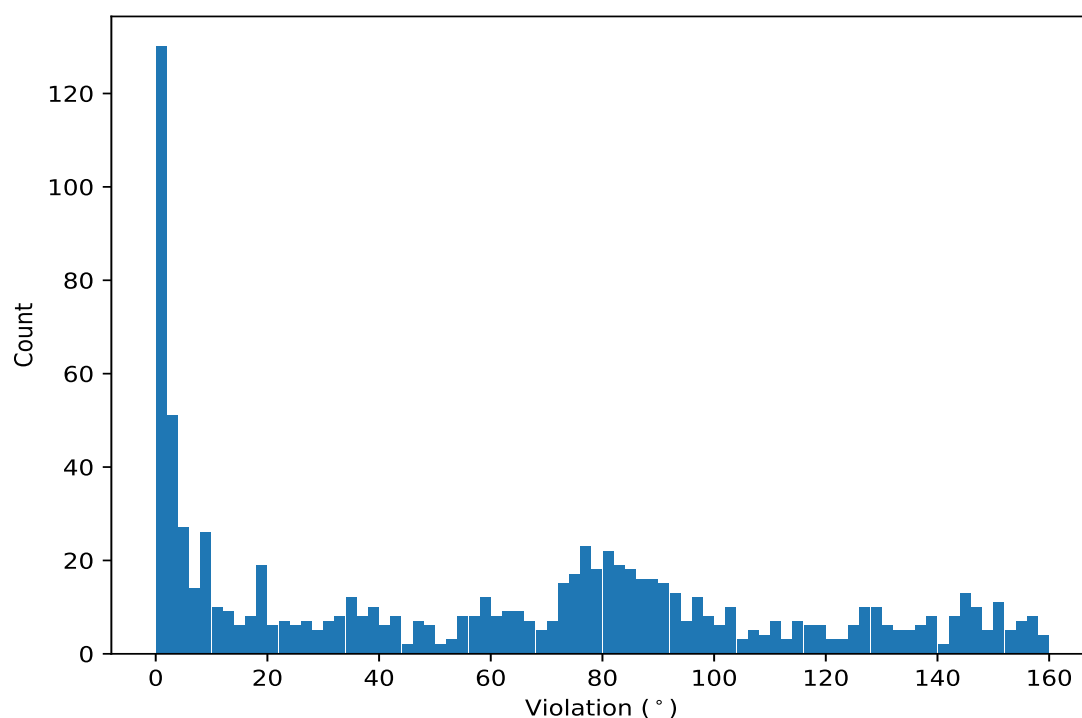
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	15	147.24	7.3	146.93
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	15	146.51	9.14	150.12
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	15	140.87	17.99	145.11
(1,41)	1:95:A:ASN:C	1:129:A:SER:N	1:129:A:SER:CA	1:129:A:SER:C	15	137.35	8.48	139.51
(1,115)	1:180:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	15	136.14	8.36	134.54
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	15	133.15	15.64	130.34
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	15	130.93	19.33	139.44
(1,242)	1:259:A:ALA:N	1:259:A:ALA:CA	1:259:A:ALA:C	1:227:A:PHE:N	15	106.52	46.81	121.82
(1,198)	1:199:A:ASP:N	1:199:A:ASP:CA	1:199:A:ASP:C	1:233:A:THR:N	15	103.28	12.75	105.6
(1,67)	1:118:A:LYS:C	1:152:A:ALA:N	1:152:A:ALA:CA	1:152:A:ALA:C	15	101.92	10.72	102.33

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 (°)
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	4	159.91
(1,66)	1:118:A:LYS:N	1:118:A:LYS:CA	1:118:A:LYS:C	1:152:A:ALA:N	12	158.65
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	2	158.63
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	11	158.15
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	1	157.94
(1,32)	1:89:A:LEU:N	1:89:A:LEU:CA	1:89:A:LEU:C	1:123:A:TYR:N	15	157.54
(1,40)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:129:A:SER:N	5	157.27
(1,114)	1:180:A:GLN:N	1:180:A:GLN:CA	1:180:A:GLN:C	1:148:A:GLU:N	12	156.81
(1,82)	1:126:A:VAL:N	1:126:A:VAL:CA	1:126:A:VAL:C	1:160:A:ASN:N	12	156.7
(1,33)	1:89:A:LEU:C	1:123:A:TYR:N	1:123:A:TYR:CA	1:123:A:TYR:C	11	156.65