



wwPDB NMR Structure Validation Summary Report ⓘ

Aug 10, 2026 – 05:12 pm BST

PDB ID : 9S9X / pdb_00009s9x
BMRB ID : 35012
Title : Human WASP/WIP complex
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Deposited on : 2025-08-06

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 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

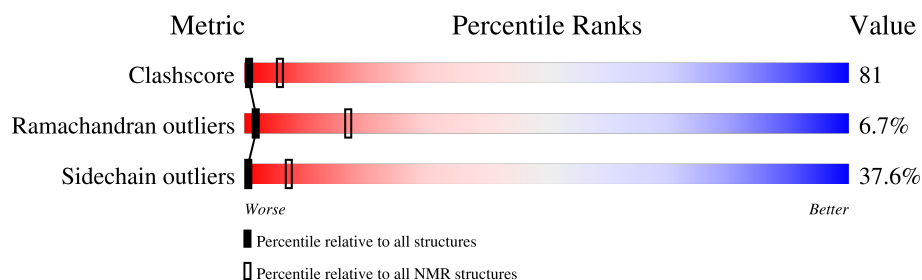
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 41%.

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	141	
2	B	53	

2 Ensemble composition and analysis

This entry contains 24 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:24-A:149, B:444-B:481 (164)	0.83	1

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 5 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 9, 15, 18, 19, 21, 22, 23
2	7, 8, 11, 12, 17
3	4, 6, 13, 24
4	5, 20
5	14, 16
Single-model clusters	10

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3081 atoms, of which 1507 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Actin nucleation-promoting factor WAS.

Mol	Chain	Residues	Atoms						Trace
1	A	141	Total	C	H	N	O	S	0
			2248	718	1109	204	212	5	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	SER	-	expression tag	UNP P42768
A	19	GLY	-	expression tag	UNP P42768

- Molecule 2 is a protein called WAS/WASL-interacting protein family member 1.

Mol	Chain	Residues	Atoms						Trace
2	B	53	Total	C	H	N	O	S	0
			833	267	398	77	90	1	

There are 2 discrepancies between the modelled and reference sequences:

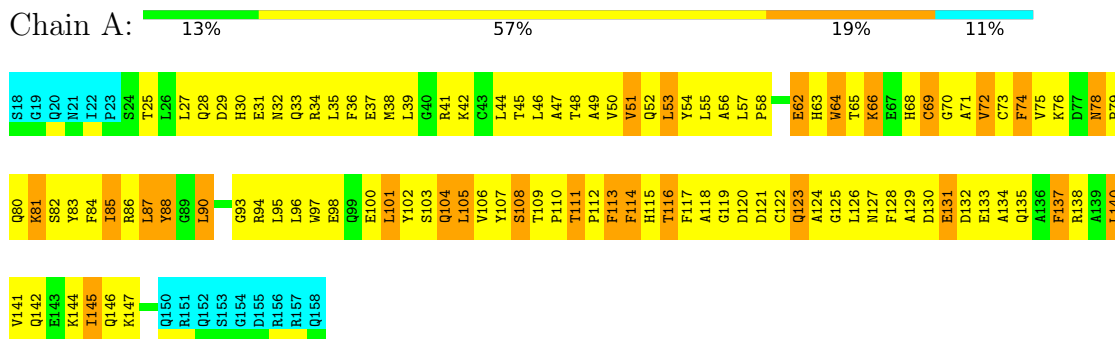
Chain	Residue	Modelled	Actual	Comment	Reference
B	440	SER	-	expression tag	UNP O43516
B	441	GLY	-	expression tag	UNP O43516

4 Residue-property plots

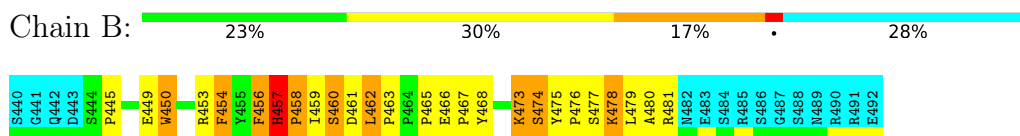
4.1 Average score per residue in the NMR ensemble

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: Actin nucleation-promoting factor WAS



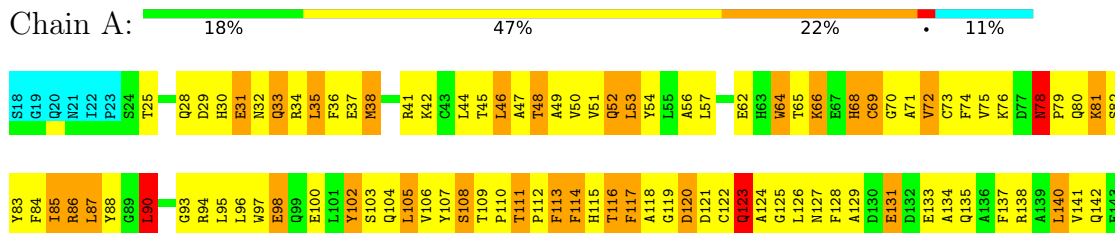
- Molecule 2: WAS/WASL-interacting protein family member 1

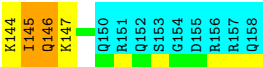


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

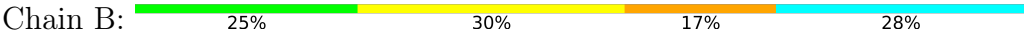
The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Actin nucleation-promoting factor WAS





● Molecule 2: WAS/WASL-interacting protein family member 1



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 24 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure calculation	
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	1256
Number of shifts mapped to atoms	1256
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	41%

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	0.45±0.01	0±0/1044 (0.0± 0.0%)	0.74±0.01	0±0/1416 (0.0± 0.0%)
2	B	0.48±0.01	0±0/333 (0.0± 0.0%)	0.96±0.03	2±1/458 (0.4± 0.2%)
All	All	0.45	0/33048 (0.0%)	0.80	40/44976 (0.1%)

There are no bond-length outliers.

All 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
2	B	457	HIS	CA-C-N	6.34	127.77	119.84	18	20
2	B	457	HIS	C-N-CA	6.34	127.77	119.84	18	20

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1018	992	988	182±10
2	B	318	295	294	60±6
All	All	32064	30888	30768	5066

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 81.

5 of 1438 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:VAL:HG13	1:A:145:ILE:HD12	1.06	1.27	6	3
1:A:35:LEU:HD11	1:A:75:VAL:HG22	1.01	1.30	10	22
1:A:109:THR:HG23	1:A:128:PHE:CE2	1.00	1.92	2	2
2:B:459:ILE:HD11	2:B:462:LEU:HD13	0.99	1.31	19	2
1:A:106:VAL:HA	1:A:145:ILE:HD11	0.94	1.37	10	4

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	126/141 (89%)	89±3 (71±2%)	29±3 (23±3%)	8±1 (6±1%)	2	19
2	B	38/53 (72%)	29±1 (76±4%)	6±2 (16±4%)	3±1 (9±2%)	1	12
All	All	3936/4656 (85%)	2823 (72%)	848 (22%)	265 (7%)	2	17

5 of 30 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	458	PRO	24
1	A	131	GLU	23
2	B	457	HIS	23
1	A	78	ASN	21
1	A	123	GLN	18

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	107/120 (89%)	65±5 (61±5%)	42±5 (39±5%)	0	6
2	B	37/50 (74%)	24±2 (66±5%)	12±2 (34±5%)	1	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3456/4080 (85%)	2156 (62%)	1300 (38%)	0 7

5 of 119 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	53	LEU	24
1	A	64	TRP	24
1	A	66	LYS	24
1	A	72	VAL	24
1	A	81	LYS	24

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 41% for the well-defined parts and 40% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1256
Number of shifts mapped to atoms	1256
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

- Can not parse the chemical shift value. First 5 (of 202) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	20	GLN	HB2	2.02	0.01	.
1	A	20	GLN	HB3	1.87	0.01	.
1	A	21	ASN	HB2	2.86	0.01	.
1	A	21	ASN	HB3	2.86	0.01	.
1	A	23	PRO	HB2	2.10	0.01	.
1	A	23	PRO	HB3	2.10	0.01	.
1	A	24	SER	HB2	3.52	0.01	.
1	A	24	SER	HB3	3.52	0.01	.
1	A	26	LEU	HB2	1.55	0.01	.
1	A	26	LEU	HB3	1.55	0.01	.
1	A	27	LEU	HB2	1.74	0.01	.
1	A	27	LEU	HB3	1.55	0.01	.
1	A	30	HIS	HB2	3.15	0.01	.
1	A	30	HIS	HB3	3.15	0.01	.
1	A	31	GLU	HB2	1.85	0.01	.
1	A	31	GLU	HB3	1.85	0.01	.
1	A	32	ASN	HB2	2.48	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	32	ASN	HB3	1.83	0.01	.
1	A	33	GLN	HB2	1.95	0.01	.
1	A	33	GLN	HB3	1.95	0.01	.
1	A	34	ARG	HB2	1.90	0.01	.
1	A	34	ARG	HB3	1.90	0.01	.
1	A	40	GLY	HA2	3.75	0.01	.
1	A	40	GLY	HA3	3.75	0.01	.
1	A	41	ARG	HB2	1.80	0.01	.
1	A	41	ARG	HB3	1.80	0.01	.
1	A	42	LYS	HB2	2.12	0.01	.
1	A	42	LYS	HB3	1.88	0.01	.
1	A	44	LEU	HB2	1.36	0.01	.
1	A	44	LEU	HB3	1.36	0.01	.
1	A	46	LEU	HB2	1.84	0.01	.
1	A	46	LEU	HB3	1.84	0.01	.
1	A	54	TYR	HB2	1.90	0.01	.
1	A	54	TYR	HB3	1.90	0.01	.
1	A	55	LEU	HB2	1.66	0.01	.
1	A	55	LEU	HB3	1.66	0.01	.
1	A	60	GLY	HA2	4.50	0.01	.
1	A	60	GLY	HA3	3.87	0.01	.
1	A	62	GLU	HB2	1.82	0.01	.
1	A	62	GLU	HB3	1.82	0.01	.
1	A	63	HIS	HB2	3.05	0.01	.
1	A	63	HIS	HB3	3.05	0.01	.
1	A	64	TRP	HB2	3.37	0.01	.
1	A	64	TRP	HB3	2.93	0.01	.
1	A	68	HIS	HB2	2.16	0.01	.
1	A	68	HIS	HB3	2.16	0.01	.
1	A	69	CYS	HB2	2.83	0.01	.
1	A	69	CYS	HB3	2.83	0.01	.
1	A	70	GLY	HA2	4.52	0.01	.
1	A	70	GLY	HA3	2.96	0.01	.
1	A	73	CYS	HB2	3.40	0.01	.
1	A	73	CYS	HB3	2.81	0.01	.
1	A	74	PHE	HB2	3.00	0.01	.
1	A	74	PHE	HB3	2.44	0.01	.
1	A	76	LYS	HB2	2.03	0.01	.
1	A	76	LYS	HB3	1.53	0.01	.
1	A	77	ASP	HB2	2.10	0.01	.
1	A	77	ASP	HB3	2.10	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	79	PRO	HB2	2.33	0.01	.
1	A	79	PRO	HB3	1.86	0.01	.
1	A	81	LYS	HB2	1.90	0.01	.
1	A	81	LYS	HB3	1.75	0.01	.
1	A	82	SER	HB2	3.54	0.01	.
1	A	82	SER	HB3	3.54	0.01	.
1	A	83	TYR	HB2	2.58	0.01	.
1	A	83	TYR	HB3	2.42	0.01	.
1	A	84	PHE	HB2	2.65	0.01	.
1	A	84	PHE	HB3	2.51	0.01	.
1	A	86	ARG	HB2	1.63	0.01	.
1	A	86	ARG	HB3	1.63	0.01	.
1	A	87	LEU	HB2	2.20	0.01	.
1	A	87	LEU	HB3	2.20	0.01	.
1	A	88	TYR	HB2	2.74	0.01	.
1	A	88	TYR	HB3	2.74	0.01	.
1	A	89	GLY	HA2	4.00	0.01	.
1	A	89	GLY	HA3	3.51	0.01	.
1	A	91	GLN	HB2	2.66	0.01	.
1	A	91	GLN	HB3	2.05	0.01	.
1	A	94	ARG	HB2	1.85	0.01	.
1	A	94	ARG	HB3	1.61	0.01	.
1	A	96	LEU	HB2	1.05	0.01	.
1	A	96	LEU	HB3	0.20	0.01	.
1	A	97	TRP	HB2	3.28	0.01	.
1	A	97	TRP	HB3	2.64	0.01	.
1	A	101	LEU	HB2	2.00	0.01	.
1	A	101	LEU	HB3	1.16	0.01	.
1	A	107	TYR	HB2	3.00	0.01	.
1	A	107	TYR	HB3	2.21	0.01	.
1	A	108	SER	HB2	3.84	0.01	.
1	A	108	SER	HB3	3.84	0.01	.
1	A	110	PRO	HB2	2.50	0.01	.
1	A	110	PRO	HB3	2.04	0.01	.
1	A	112	PRO	HB2	2.50	0.01	.
1	A	112	PRO	HB3	1.92	0.01	.
1	A	113	PHE	HB2	4.10	0.01	.
1	A	113	PHE	HB3	2.84	0.01	.
1	A	114	PHE	HB2	2.62	0.01	.
1	A	114	PHE	HB3	2.62	0.01	.
1	A	115	HIS	HB2	3.18	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	115	HIS	HB3	2.97	0.01	.
1	A	117	PHE	HB2	3.00	0.01	.
1	A	117	PHE	HB3	3.00	0.01	.
1	A	119	GLY	HA2	4.92	0.01	.
1	A	119	GLY	HA3	4.59	0.01	.
1	A	120	ASP	HB2	2.79	0.01	.
1	A	120	ASP	HB3	2.79	0.01	.
1	A	121	ASP	HB2	2.63	0.01	.
1	A	121	ASP	HB3	2.63	0.01	.
1	A	125	GLY	HA2	4.45	0.01	.
1	A	125	GLY	HA3	2.33	0.01	.
1	A	126	LEU	HB2	1.72	0.01	.
1	A	126	LEU	HB3	1.72	0.01	.
1	A	127	ASN	HB2	2.56	0.01	.
1	A	127	ASN	HB3	2.56	0.01	.
1	A	130	ASP	HB2	2.81	0.01	.
1	A	130	ASP	HB3	2.54	0.01	.
1	A	132	ASP	HB2	3.16	0.01	.
1	A	132	ASP	HB3	2.74	0.01	.
1	A	133	GLU	HB2	1.80	0.01	.
1	A	133	GLU	HB3	1.80	0.01	.
1	A	135	GLN	HB2	2.30	0.01	.
1	A	135	GLN	HB3	2.30	0.01	.
1	A	140	LEU	HB2	1.50	0.01	.
1	A	140	LEU	HB3	1.05	0.01	.
1	A	142	GLN	HB2	2.06	0.01	.
1	A	142	GLN	HB3	2.06	0.01	.
1	A	146	GLN	HB2	2.17	0.01	.
1	A	146	GLN	HB3	2.17	0.01	.
1	A	147	LYS	HB2	1.89	0.01	.
1	A	147	LYS	HB3	1.89	0.01	.
1	A	148	ARG	HB2	1.96	0.01	.
1	A	148	ARG	HB3	1.96	0.01	.
1	A	149	ASN	HB2	2.88	0.01	.
1	A	149	ASN	HB3	2.57	0.01	.
1	A	153	SER	HB2	3.90	0.01	.
1	A	153	SER	HB3	3.90	0.01	.
1	A	154	GLY	HA2	4.00	0.01	.
1	A	154	GLY	HA3	4.00	0.01	.
1	A	155	ASP	HB2	2.70	0.01	.
1	A	155	ASP	HB3	2.70	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	156	ARG	HB2	1.86	0.01	.
1	A	156	ARG	HB3	1.86	0.01	.
1	B	442	GLN	HB2	2.11	0.01	.
1	B	442	GLN	HB3	1.97	0.01	.
1	B	443	ASP	HB2	2.67	0.01	.
1	B	443	ASP	HB3	2.67	0.01	.
1	B	445	PRO	HB2	2.30	0.01	.
1	B	445	PRO	HB3	1.96	0.01	.
1	B	446	CYS	HB2	3.00	0.01	.
1	B	446	CYS	HB3	3.00	0.01	.
1	B	448	ASP	HB2	2.73	0.01	.
1	B	448	ASP	HB3	2.73	0.01	.
1	B	449	GLU	HB2	2.16	0.01	.
1	B	449	GLU	HB3	2.16	0.01	.
1	B	450	TRP	HB2	3.63	0.01	.
1	B	450	TRP	HB3	3.63	0.01	.
1	B	451	GLU	HB2	2.30	0.01	.
1	B	451	GLU	HB3	2.30	0.01	.
1	B	452	SER	HB2	4.00	0.01	.
1	B	452	SER	HB3	4.00	0.01	.
1	B	453	ARG	HB2	0.89	0.01	.
1	B	453	ARG	HB3	0.89	0.01	.
1	B	455	TYR	HB2	2.75	0.01	.
1	B	455	TYR	HB3	2.75	0.01	.
1	B	458	PRO	HB2	2.31	0.01	.
1	B	458	PRO	HB3	2.24	0.01	.
1	B	460	SER	HB2	4.08	0.01	.
1	B	460	SER	HB3	3.86	0.01	.
1	B	461	ASP	HB2	3.00	0.01	.
1	B	461	ASP	HB3	2.84	0.01	.
1	B	465	PRO	HB2	2.16	0.01	.
1	B	465	PRO	HB3	2.16	0.01	.
1	B	467	PRO	HB2	2.27	0.01	.
1	B	467	PRO	HB3	1.73	0.01	.
1	B	468	TYR	HB2	2.96	0.01	.
1	B	468	TYR	HB3	2.75	0.01	.
1	B	470	GLN	HB2	2.03	0.01	.
1	B	470	GLN	HB3	2.03	0.01	.
1	B	474	SER	HB2	3.86	0.01	.
1	B	474	SER	HB3	3.86	0.01	.
1	B	476	PRO	HB2	2.20	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	476	PRO	HB3	2.20	0.01	.
1	B	478	LYS	HB2	2.08	0.01	.
1	B	478	LYS	HB3	2.08	0.01	.
1	B	479	LEU	HB2	1.74	0.01	.
1	B	479	LEU	HB3	1.74	0.01	.
1	B	481	ARG	HB2	1.35	0.01	.
1	B	481	ARG	HB3	1.35	0.01	.
1	B	482	ASN	HB2	2.88	0.01	.
1	B	482	ASN	HB3	2.21	0.01	.
1	B	483	GLU	HB2	2.04	0.01	.
1	B	483	GLU	HB3	2.04	0.01	.
1	B	486	SER	HB2	3.91	0.01	.
1	B	486	SER	HB3	3.91	0.01	.
1	B	487	GLY	HA2	4.04	0.01	.
1	B	487	GLY	HA3	4.04	0.01	.
1	B	489	ASN	HB2	2.14	0.01	.
1	B	489	ASN	HB3	2.14	0.01	.
1	B	490	ARG	HB2	1.82	0.01	.
1	B	490	ARG	HB3	1.82	0.01	.
1	B	491	ARG	HB2	1.84	0.01	.
1	B	491	ARG	HB3	1.84	0.01	.

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
$^{13}\text{C}_\alpha$	185	-0.04 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	174	0.06 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}'$	167	0.31 ± 0.10	None needed (< 0.5 ppm)
^{15}N	167	-0.11 ± 0.29	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 41%, i.e. 929 atoms were assigned a chemical shift out of a possible 2270. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	728/803 (91%)	275/323 (85%)	307/328 (94%)	146/152 (96%)

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	Total	¹ H	¹³ C	¹⁵ N
Sidechain	201/1219 (16%)	50/789 (6%)	151/382 (40%)	0/48 (0%)
Aromatic	0/248 (0%)	0/120 (0%)	0/115 (0%)	0/13 (0%)
Overall	929/2270 (41%)	325/1232 (26%)	458/825 (56%)	146/213 (69%)

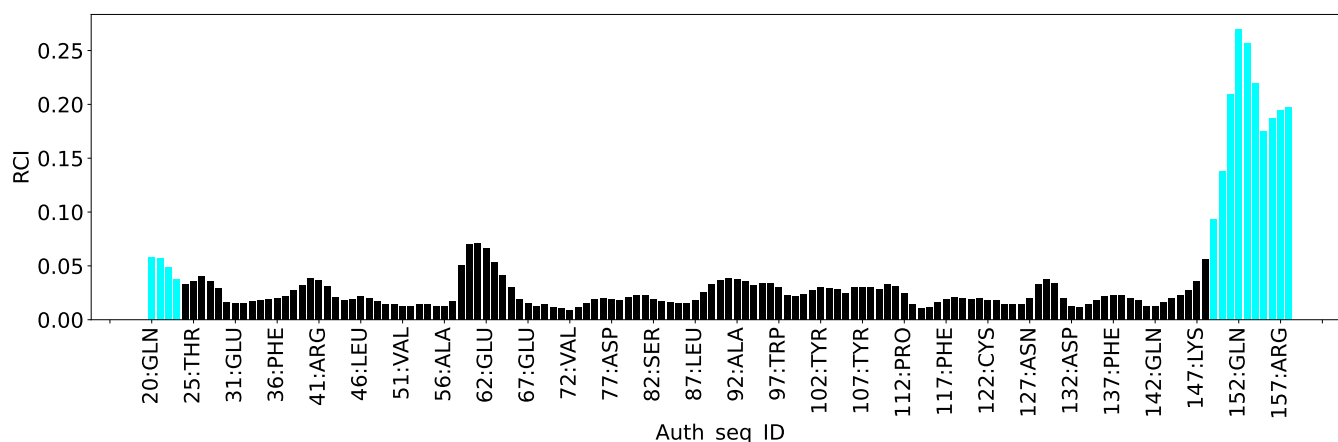
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

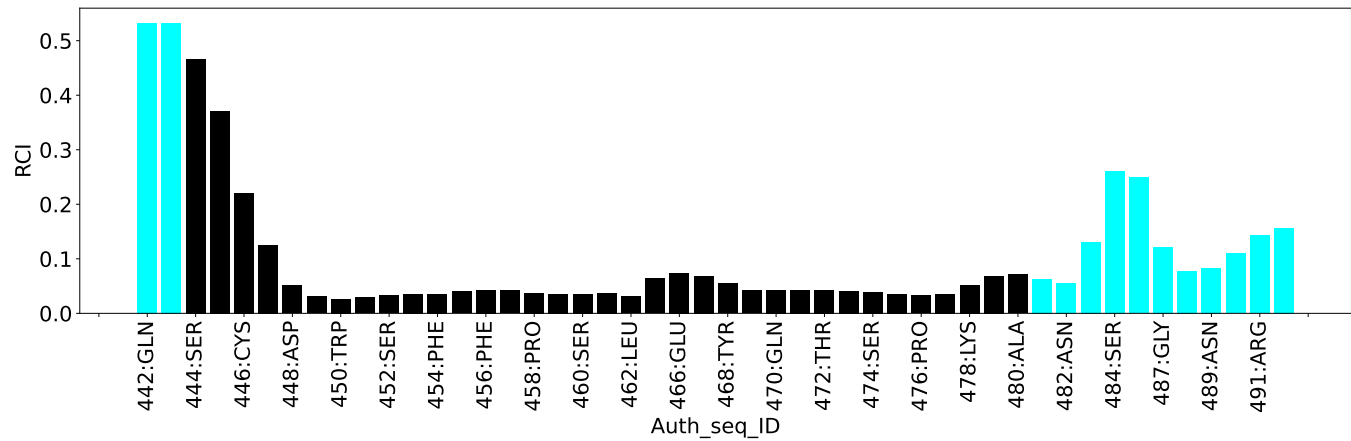
7.1.5 Random Coil Index (RCI) plots [i](#)

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:



Random coil index (RCI) for chain B:



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	1151
Intra-residue ($ i-j =0$)	4
Sequential ($ i-j =1$)	494
Medium range ($ i-j >1$ and $ i-j <5$)	192
Long range ($ i-j \geq 5$)	266
Inter-chain	63
Hydrogen bond restraints	132
Disulfide bond restraints	0
Total dihedral-angle restraints	308
Number of unmapped restraints	0
Number of restraints per residue	7.5
Number of long range restraints per residue ¹	1.7

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)	56.5	0.2
0.2-0.5 (Medium)	30.7	0.49
>0.5 (Large)	0.4	0.83

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)	43.2	8.07
10.0-20.0 (Medium)	0.2	15.94
>20.0 (Large)	1.5	95.73

9 Distance violation analysis ⓘ

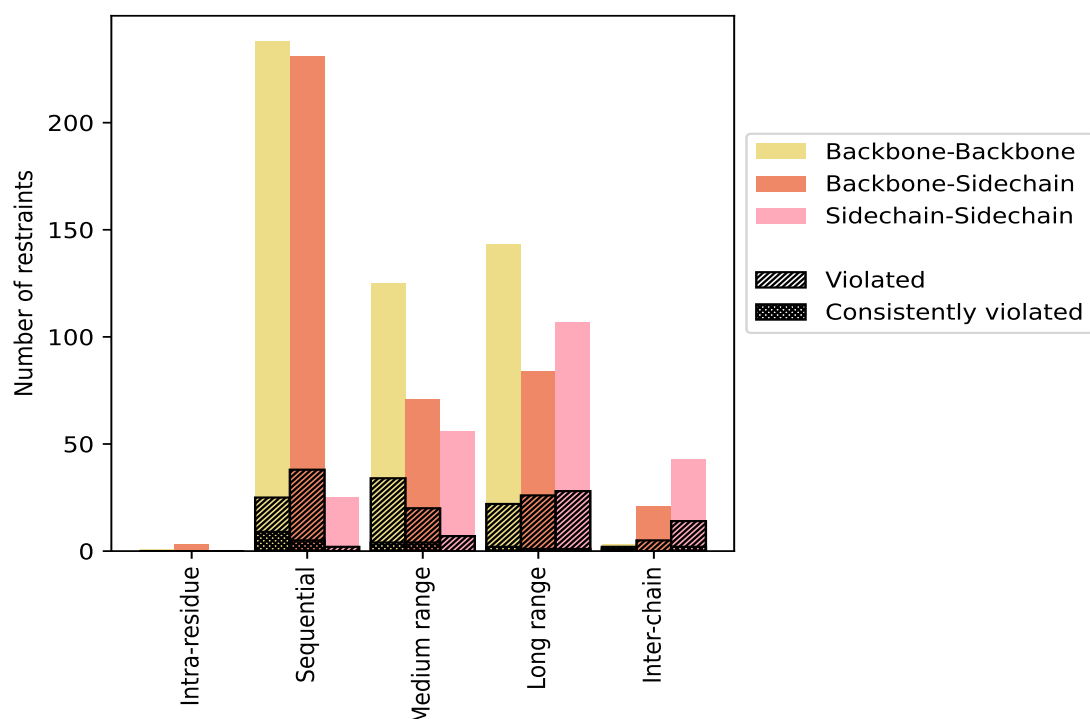
9.1 Summary of distance violations ⓘ

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)	4	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	3	0.3	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)	494	42.9	65	13.2	5.6	14	2.8	1.2
Backbone-Backbone	238	20.7	25	10.5	2.2	9	3.8	0.8
Backbone-Sidechain	231	20.1	38	16.5	3.3	5	2.2	0.4
Sidechain-Sidechain	25	2.2	2	8.0	0.2	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	192	16.7	47	24.5	4.1	7	3.6	0.6
Backbone-Backbone	65	5.6	20	30.8	1.7	3	4.6	0.3
Backbone-Sidechain	71	6.2	20	28.2	1.7	4	5.6	0.3
Sidechain-Sidechain	56	4.9	7	12.5	0.6	0	0.0	0.0
Long range (i-j ≥5)	266	23.1	64	24.1	5.6	4	1.5	0.3
Backbone-Backbone	75	6.5	10	13.3	0.9	2	2.7	0.2
Backbone-Sidechain	84	7.3	26	31.0	2.3	1	1.2	0.1
Sidechain-Sidechain	107	9.3	28	26.2	2.4	1	0.9	0.1
Inter-chain	63	5.5	21	33.3	1.8	3	4.8	0.3
Backbone-Backbone	3	0.3	2	66.7	0.2	1	33.3	0.1
Backbone-Sidechain	21	1.8	5	23.8	0.4	0	0.0	0.0
Sidechain-Sidechain	39	3.4	14	35.9	1.2	2	5.1	0.2
Hydrogen bond	132	11.5	26	19.7	2.3	1	0.8	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1151	100.0	223	19.4	19.4	29	2.5	2.5
Backbone-Backbone	510	44.3	83	16.3	7.2	16	3.1	1.4
Backbone-Sidechain	410	35.6	89	21.7	7.7	10	2.4	0.9
Sidechain-Sidechain	231	20.1	51	22.1	4.4	3	1.3	0.3

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	37	21	33	8	99	0.19	0.45	0.09	0.16
2	0	36	22	35	9	102	0.2	0.77	0.11	0.16
3	0	28	18	37	6	89	0.19	0.44	0.09	0.16
4	0	30	21	38	6	95	0.19	0.45	0.09	0.16
5	0	30	20	36	9	95	0.21	0.79	0.11	0.18
6	0	33	27	36	7	103	0.19	0.46	0.09	0.16
7	0	31	20	26	7	84	0.2	0.44	0.09	0.16
8	0	32	18	31	5	86	0.2	0.49	0.1	0.16
9	0	31	24	34	9	98	0.19	0.44	0.09	0.16
10	0	31	16	31	13	91	0.2	0.46	0.09	0.17

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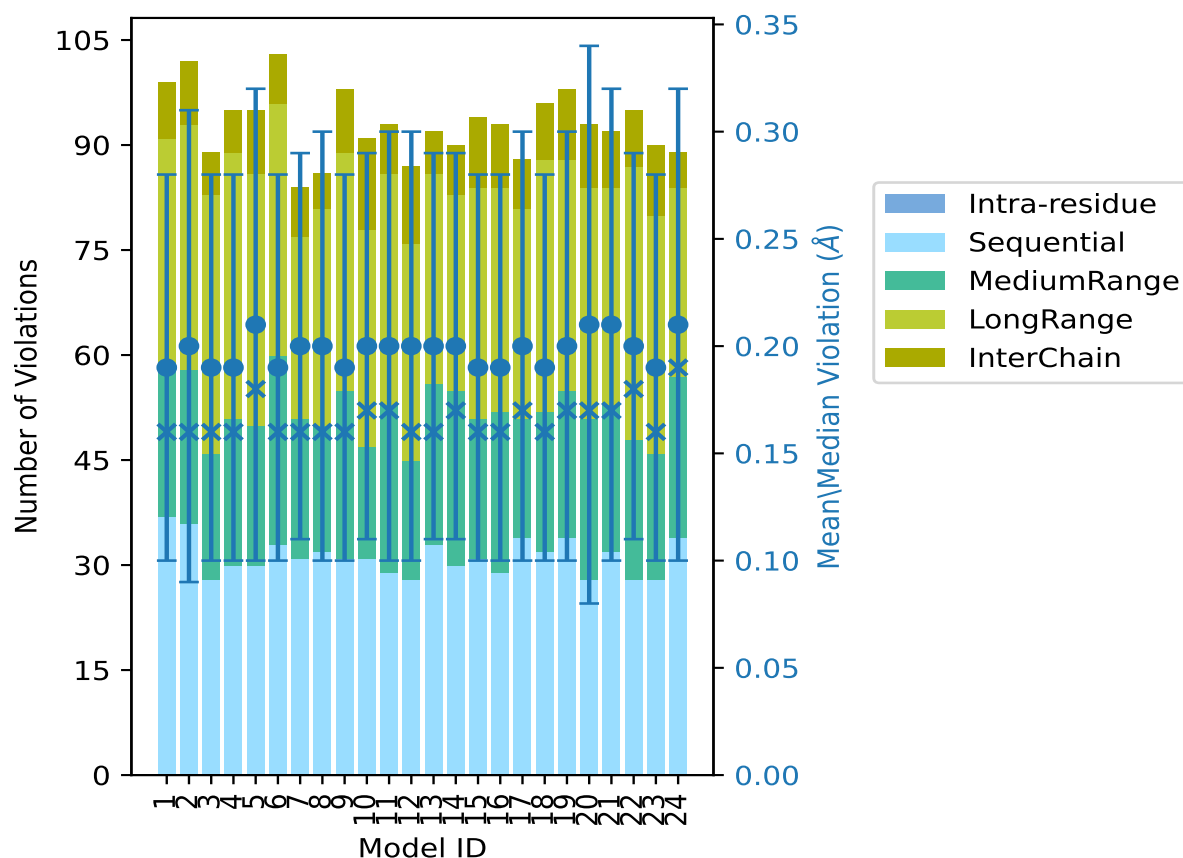
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	29	24	33	7	93	0.2	0.68	0.1	0.17
12	0	28	17	31	11	87	0.2	0.45	0.1	0.16
13	0	33	23	30	6	92	0.2	0.47	0.09	0.16
14	0	30	25	28	7	90	0.2	0.46	0.09	0.17
15	0	31	20	33	10	94	0.19	0.49	0.09	0.16
16	0	29	23	32	9	93	0.19	0.52	0.09	0.16
17	0	34	17	30	7	88	0.2	0.64	0.1	0.17
18	0	32	20	36	8	96	0.19	0.45	0.09	0.16
19	0	34	21	33	10	98	0.2	0.47	0.1	0.17
20	0	28	23	33	9	93	0.21	0.83	0.13	0.17
21	0	32	21	31	8	92	0.21	0.7	0.11	0.17
22	0	28	20	39	8	95	0.2	0.45	0.09	0.18
23	0	28	18	34	10	90	0.19	0.46	0.09	0.16
24	0	34	23	27	5	89	0.21	0.83	0.11	0.19

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 822(IR:4, SQ:429, MR:145, LR:202, IC:42) 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	8	11	4	3	26	1	4.2
0	7	0	9	2	18	2	8.3
0	6	4	3	0	13	3	12.5
0	2	3	5	3	13	4	16.7
0	4	5	5	1	15	5	20.8
0	0	2	3	1	6	6	25.0

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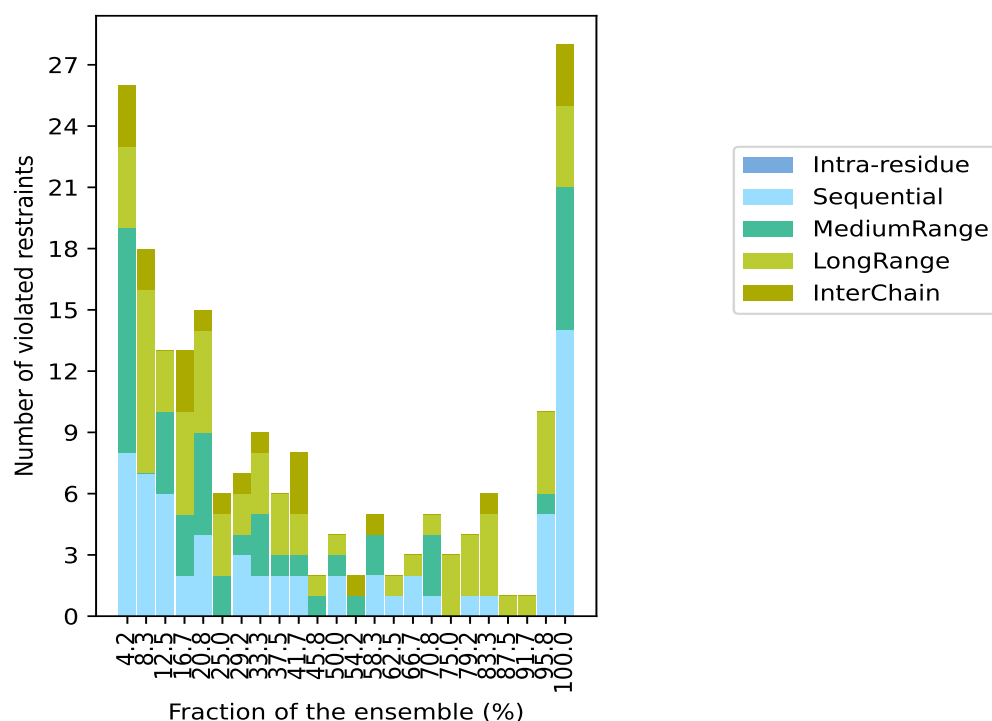
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	3	1	2	1	7	7	29.2
0	2	3	3	1	9	8	33.3
0	2	1	3	0	6	9	37.5
0	2	1	2	3	8	10	41.7
0	0	1	1	0	2	11	45.8
0	2	1	1	0	4	12	50.0
0	0	1	0	1	2	13	54.2
0	2	2	0	1	5	14	58.3
0	1	0	1	0	2	15	62.5
0	2	0	1	0	3	16	66.7
0	1	3	1	0	5	17	70.8
0	0	0	3	0	3	18	75.0
0	1	0	3	0	4	19	79.2
0	1	0	4	1	6	20	83.3
0	0	0	1	0	1	21	87.5
0	0	0	1	0	1	22	91.7
0	5	1	4	0	10	23	95.8
0	14	7	4	3	28	24	100.0

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

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

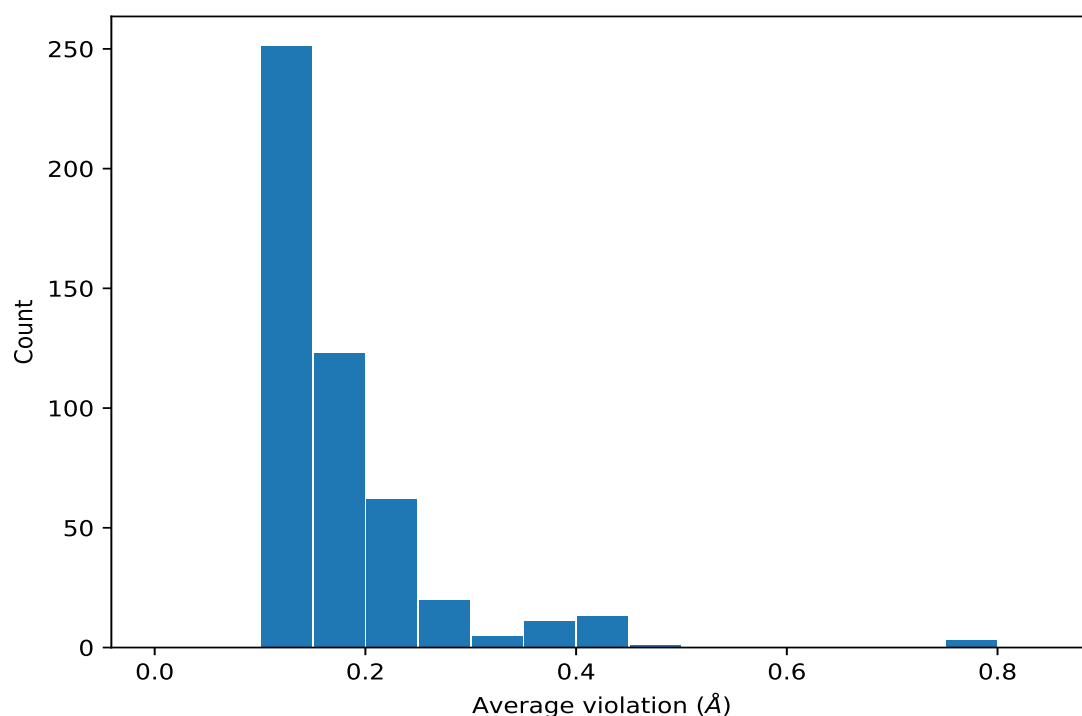
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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.

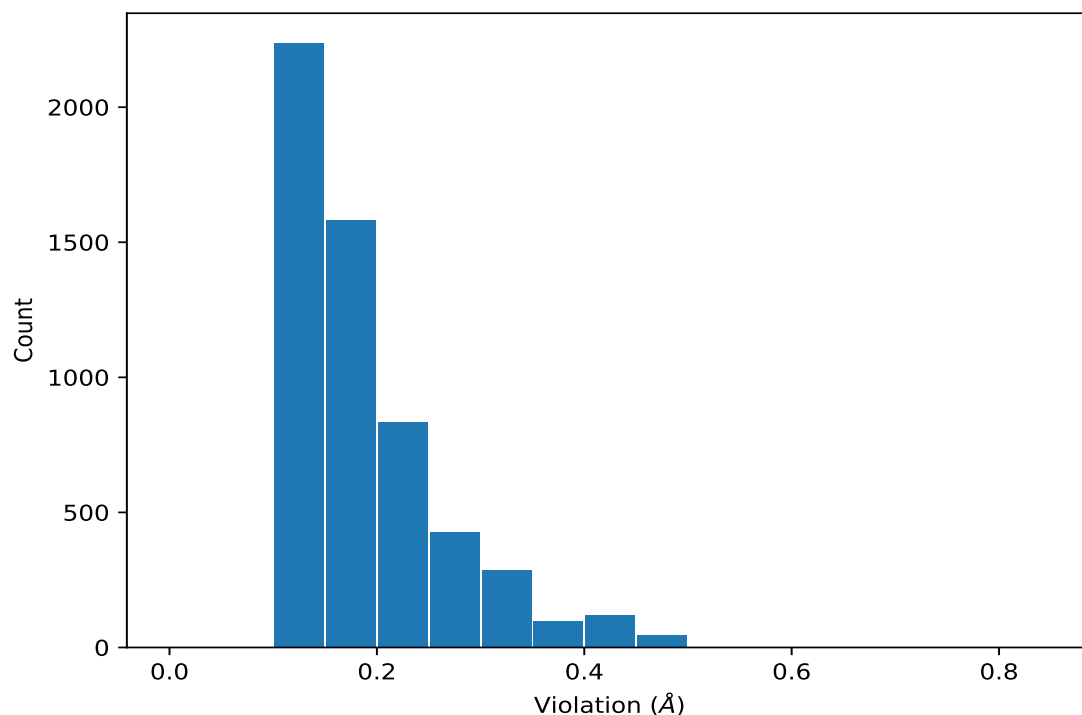
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,553)	2:450:B:TRP:H	2:449:B:GLU:HA	24	0.45	0.01	0.45
(1,787)	1:83:A:TYR:HA	1:85:A:ILE:HB	24	0.43	0.03	0.43
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG2	24	0.42	0.01	0.42
(1,582)	2:466:B:GLU:H	2:465:B:PRO:HG3	24	0.42	0.01	0.42
(1,551)	2:449:B:GLU:H	2:448:B:ASP:HA	24	0.4	0.01	0.4
(1,612)	2:479:B:LEU:H	2:475:B:TYR:HA	24	0.38	0.04	0.4
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG23	24	0.38	0.02	0.37
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG21	24	0.38	0.02	0.37
(1,396)	1:57:A:LEU:H	1:65:A:THR:HG22	24	0.38	0.02	0.37
(1,101)	1:62:A:GLU:H	1:61:A:ALA:HA	24	0.35	0.01	0.35
(1,75)	1:51:A:VAL:H	1:50:A:VAL:H	24	0.32	0.03	0.33
(1,191)	1:95:A:LEU:H	1:94:A:ARG:H	24	0.32	0.04	0.33
(1,167)	1:86:A:ARG:H	1:85:A:ILE:HB	24	0.32	0.02	0.32

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)
(1,734)	1:65:A:THR:HG23	1:63:A:HIS:HD1	20	0.83
(1,660)	1:45:A:THR:HG21	1:47:A:ALA:HA	24	0.83
(1,660)	1:45:A:THR:HG1	1:47:A:ALA:HA	5	0.79
(1,734)	1:65:A:THR:HG21	1:63:A:HIS:HD1	2	0.77
(1,735)	1:65:A:THR:HG22	1:67:A:GLU:HA	20	0.74
(1,734)	1:65:A:THR:HG22	1:63:A:HIS:HD1	21	0.7
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG21	11	0.68
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG23	17	0.64
(1,1015)	2:475:B:TYR:HE2	1:102:A:TYR:HE1	2	0.57
(1,69)	1:49:A:ALA:H	1:48:A:THR:HG23	16	0.52

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

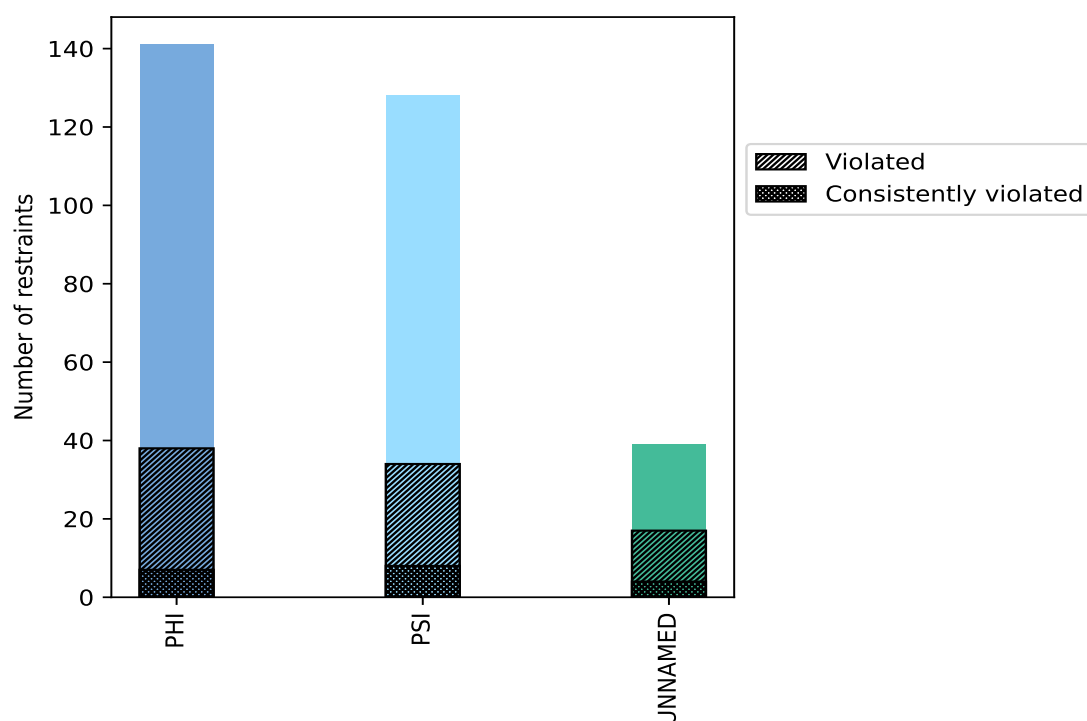
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	141	45.8	38	27.0	12.3	7	5.0	2.3
PSI	128	41.6	34	26.6	11.0	8	6.2	2.6
UNNAMED	39	12.7	17	43.6	5.5	4	10.3	1.3
Total	308	100.0	89	28.9	28.9	19	6.2	6.2

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](#)



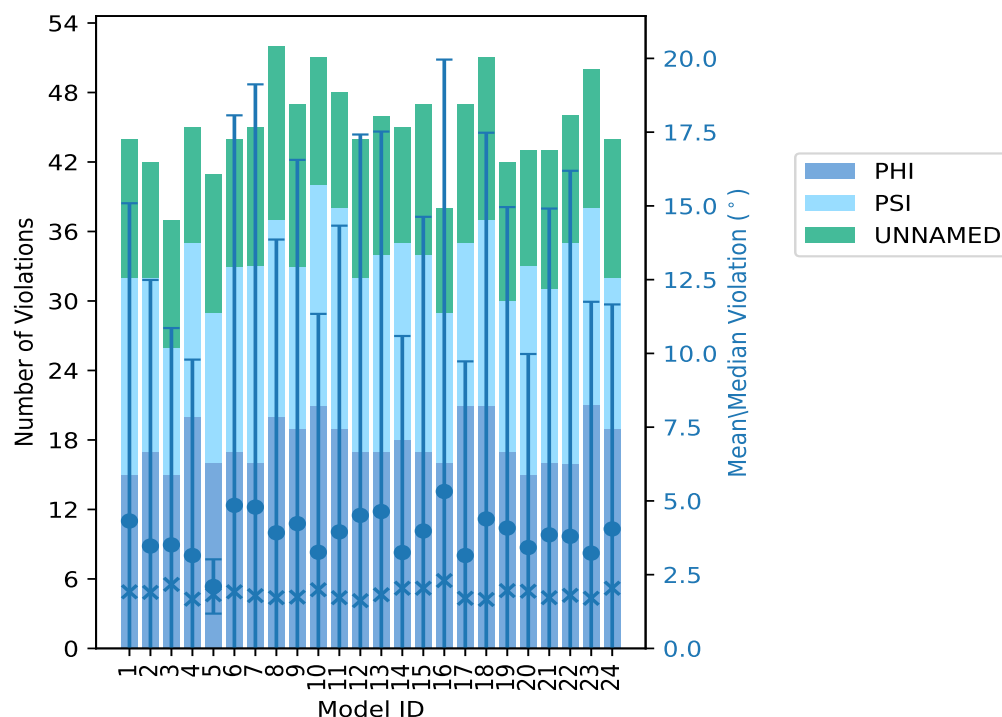
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PHI	PSI	UNNAMED	Total				
1	15	17	12	44	4.32	59.41	10.77	1.92
2	17	15	10	42	3.47	61.02	9.02	1.9
3	15	11	11	37	3.51	47.23	7.35	2.17
4	20	15	10	45	3.15	45.55	6.64	1.67
5	16	13	12	41	2.1	4.88	0.92	1.82
6	17	16	11	44	4.85	79.34	13.22	1.92
7	16	17	12	45	4.79	95.73	14.33	1.79
8	20	17	15	52	3.92	60.38	9.94	1.72
9	19	14	14	47	4.23	83.93	12.33	1.74
10	21	19	11	51	3.26	60.05	8.08	1.99
11	19	19	10	48	3.95	71.57	10.38	1.72
12	17	15	12	44	4.51	85.72	12.91	1.62
13	17	17	12	46	4.64	81.12	12.88	1.82
14	18	17	10	45	3.25	51.57	7.34	2.04
15	17	17	13	47	3.98	74.72	10.65	2.04
16	16	13	9	38	5.32	88.16	14.64	2.3
17	21	14	12	47	3.15	46.31	6.58	1.7
18	21	16	14	51	4.39	87.3	13.09	1.66
19	17	13	12	42	4.08	72.76	10.88	1.96
20	15	18	10	43	3.42	40.2	6.56	1.94
21	16	15	12	43	3.85	75.07	11.06	1.72
22	16	19	11	46	3.8	86.7	12.39	1.8
23	21	17	12	50	3.23	62.55	8.52	1.7
24	19	13	12	44	4.05	38.34	7.61	2.04

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

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

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints				Fraction of the ensemble	
PHI	PSI	UNNAMED	Total	Count ¹	%
7	5	0	12	1	4.2
1	4	2	7	2	8.3
2	1	1	4	3	12.5
2	1	0	3	4	16.7
0	2	1	3	5	20.8
4	1	0	5	6	25.0
0	1	0	1	7	29.2
2	2	1	5	8	33.3
2	1	0	3	9	37.5
0	2	0	2	10	41.7
2	0	0	2	11	45.8

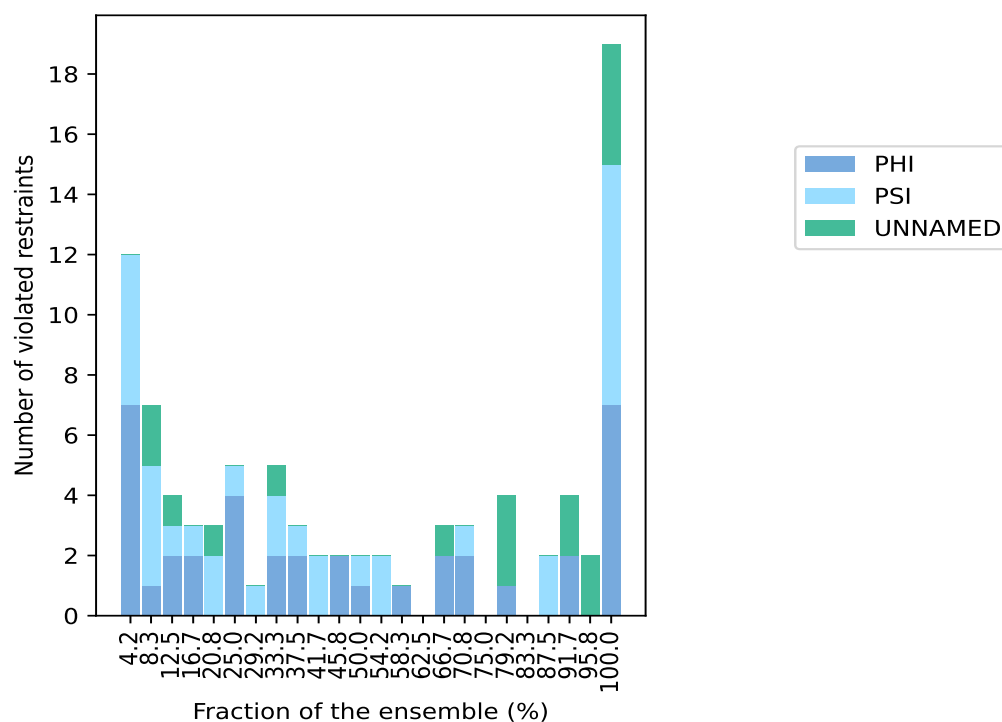
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Number of violated restraints				Fraction of the ensemble	
PHI	PSI	UNNAMED	Total	Count ¹	%
1	1	0	2	12	50.0
0	2	0	2	13	54.2
1	0	0	1	14	58.3
0	0	0	0	15	62.5
2	0	1	3	16	66.7
2	1	0	3	17	70.8
0	0	0	0	18	75.0
1	0	3	4	19	79.2
0	0	0	0	20	83.3
0	2	0	2	21	87.5
2	0	2	4	22	91.7
0	0	2	2	23	95.8
7	8	4	19	24	100.0

¹ Number of models with violations

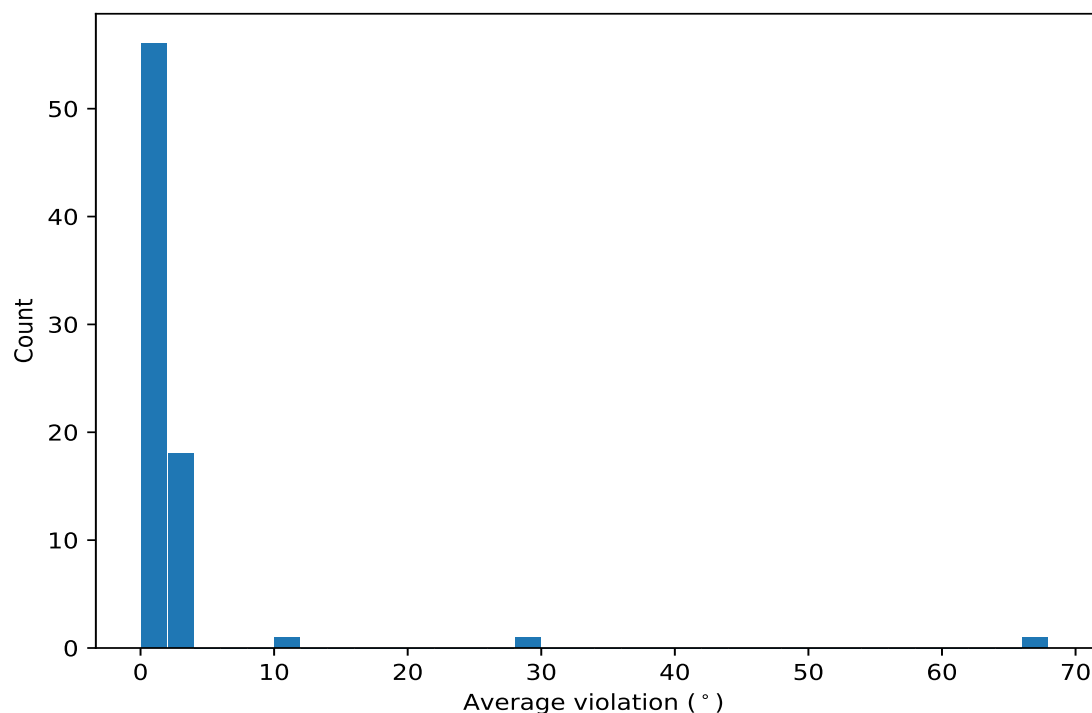
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ



10.4 Most violated dihedral-angle restraints in the ensemble [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.

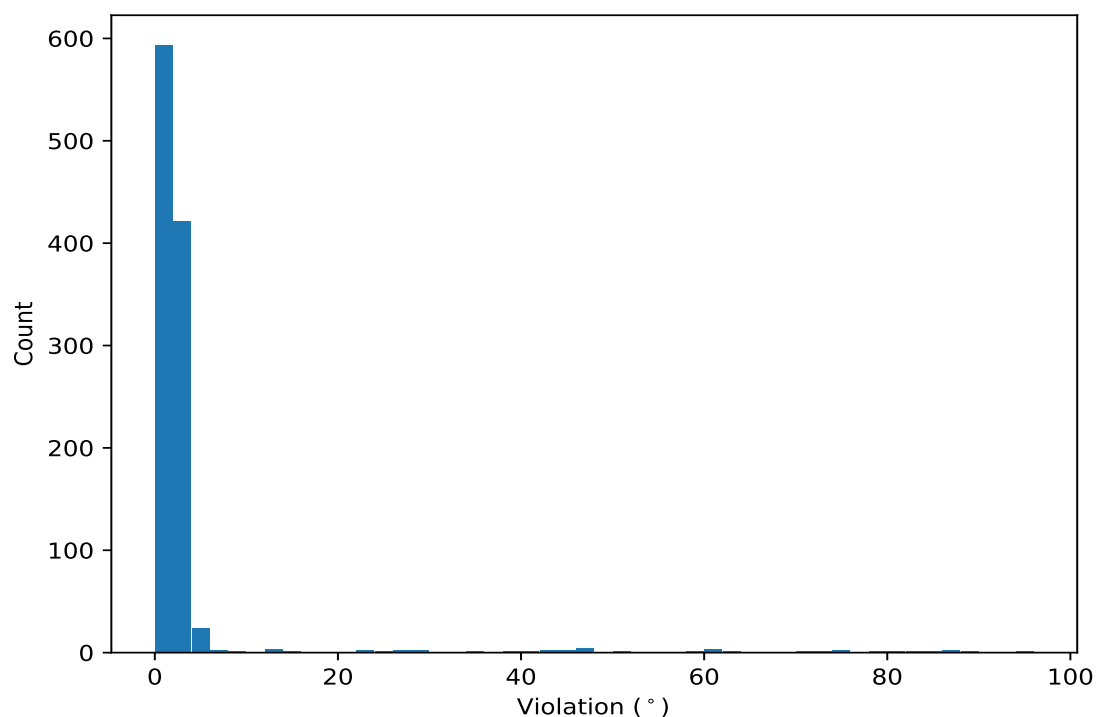
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,260)	2:452:B:SER:C	2:453:B:ARG:N	2:453:B:ARG:CA	2:453:B:ARG:C	24	3.93	0.29	3.88
(1,142)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:PHE:N	24	3.62	0.47	3.63
(1,279)	1:75:A:VAL:H	1:75:A:VAL:N	1:111:A:THR:N	1:111:A:THR:H	24	3.52	1.09	3.7
(1,242)	2:465:B:PRO:N	2:465:B:PRO:CA	2:465:B:PRO:C	2:466:B:GLU:N	24	3.35	0.33	3.28
(1,222)	2:474:B:SER:C	2:475:B:TYR:N	2:475:B:TYR:CA	2:475:B:TYR:C	24	3.25	0.59	3.28
(1,203)	2:450:B:TRP:C	2:451:B:GLU:N	2:451:B:GLU:CA	2:451:B:GLU:C	24	3.24	0.3	3.24
(1,167)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:ASP:N	24	2.84	0.35	2.76
(1,270)	1:51:A:VAL:H	1:51:A:VAL:N	1:60:A:GLY:N	1:60:A:GLY:H	24	2.77	0.72	2.77
(1,80)	1:129:A:ALA:C	1:130:A:ASP:N	1:130:A:ASP:CA	1:130:A:ASP:C	24	2.67	0.41	2.63
(1,231)	2:450:B:TRP:N	2:450:B:TRP:CA	2:450:B:TRP:C	2:451:B:GLU:N	24	2.66	0.33	2.66

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 (°)
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	7	95.73
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	16	88.16
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	18	87.3
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	22	86.7
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	12	85.72
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	9	83.93
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	13	81.12
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	6	79.34
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	21	75.07
(1,276)	1:64:A:TRP:H	1:64:A:TRP:N	1:75:A:VAL:N	1:75:A:VAL:H	15	74.72