



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2M38 / pdb_00002m38
BMRB ID : 17934
Title : PTB domain of AIDA1
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Deposited on : 2013-01-14

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

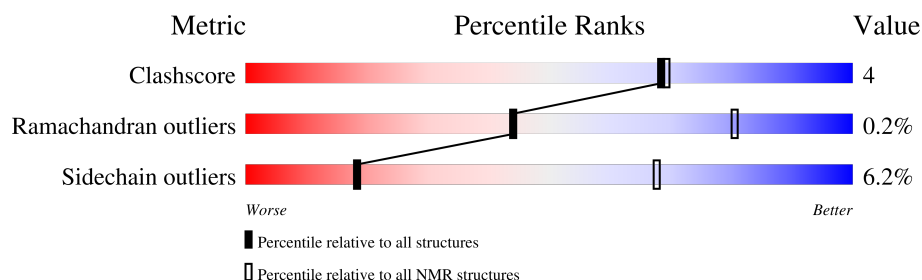
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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	153	

2 Ensemble composition and analysis

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:18-A:51, A:61-A:144 (118)	0.91	16

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1813 atoms, of which 765 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ankyrin repeat and sterile alpha motif domain-containing protein 1B.

Mol	Chain	Residues	Atoms						Trace
1	A	135	Total	C	H	N	O	S	0
			1813	660	765	177	203	8	

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	TYR	engineered mutation	UNP Q7Z6G8
A	16	ALA	PHE	engineered mutation	UNP Q7Z6G8
A	24	ALA	PHE	engineered mutation	UNP Q7Z6G8
A	70	ALA	TYR	engineered mutation	UNP Q7Z6G8
A	131	ALA	TYR	engineered mutation	UNP Q7Z6G8

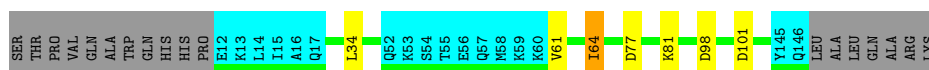
4 Residue-property plots [i](#)

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: Ankyrin repeat and sterile alpha motif domain-containing protein 1B

Chain A: 



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

The representative model is number 16. Colouring as in section 4.1 above.

- Molecule 1: Ankyrin repeat and sterile alpha motif domain-containing protein 1B

Chain A: 



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CYANA	structure solution	3
X-PLOR NIH	refinement	2.23

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	1553
Number of shifts mapped to atoms	1265
Number of unparsed shifts	0
Number of shifts with mapping errors	288
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	904	671	901	7±2
All	All	18080	13420	18020	135

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 4.

5 of 78 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:LEU:HD11	1:A:38:GLU:HB2	0.77	1.57	5	1
1:A:29:MET:HE3	1:A:47:MET:SD	0.75	2.22	20	7
1:A:64:ILE:HD11	1:A:75:PHE:HB3	0.63	1.69	7	9
1:A:77:ASP:O	1:A:81:LYS:HA	0.60	1.97	16	15
1:A:19:CYS:HB3	1:A:68:VAL:HG13	0.59	1.74	9	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	118/153 (77%)	114±1 (96±1%)	4±1 (4±1%)	0±1 (0±0%)	44 80
All	All	2360/3060 (77%)	2271 (96%)	84 (4%)	5 (0%)	44 80

All 3 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	61	VAL	3
1	A	70	ALA	1
1	A	32	LYS	1

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	98/129 (76%)	92±3 (94±3%)	6±3 (6±3%)	18 68
All	All	1960/2580 (76%)	1839 (94%)	121 (6%)	18 68

5 of 41 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	64	ILE	20
1	A	66	LEU	9
1	A	110	LYS	6
1	A	34	LEU	6
1	A	109	THR	5

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 79% for the well-defined parts and 77% 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	1553
Number of shifts mapped to atoms	1265
Number of unparsed shifts	0
Number of shifts with mapping errors	288
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 288) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	PRO	HA	4.407	0.0000	1
1	A	3	PRO	HB2	1.838	0.0000	2
1	A	3	PRO	HB3	2.258	0.0000	2
1	A	3	PRO	HD2	3.895	0.0000	2
1	A	3	PRO	HD3	3.724	0.0000	2
1	A	3	PRO	HG2	1.976	0.0000	2
1	A	3	PRO	HG3	1.976	0.0000	2
1	A	3	PRO	C	176.764	0.0000	1
1	A	3	PRO	CA	63.289	0.0000	1
1	A	3	PRO	CB	31.883	0.0000	1
1	A	3	PRO	CD	51.268	0.0000	1
1	A	3	PRO	CG	27.371	0.0000	1
1	A	4	VAL	H	8.093	0.0000	1
1	A	4	VAL	HA	3.97	0.0000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	VAL	HB	1.92	0.0000	1
1	A	4	VAL	HG11	0.82	0.0000	2
1	A	4	VAL	HG12	0.82	0.0000	2
1	A	4	VAL	HG13	0.82	0.0000	2
1	A	4	VAL	HG21	0.87	0.0000	2
1	A	4	VAL	HG22	0.87	0.0000	2
1	A	4	VAL	HG23	0.87	0.0000	2
1	A	4	VAL	C	176.173	0.0000	1
1	A	4	VAL	CA	63.289	0.0000	1
1	A	4	VAL	CB	32.82	0.0000	1
1	A	4	VAL	CG1	21.07	0.0000	1
1	A	4	VAL	CG2	20.674	0.0000	1
1	A	4	VAL	N	120.487	0.0000	1
1	A	5	GLN	H	8.217	0.0000	1
1	A	5	GLN	HA	4.187	0.0000	1
1	A	5	GLN	HB2	1.7	0.0000	2
1	A	5	GLN	HB3	1.782	0.0000	2
1	A	5	GLN	HG2	2.19	0.0000	2
1	A	5	GLN	HG3	2.19	0.0000	2
1	A	5	GLN	C	176.232	0.0000	1
1	A	5	GLN	CA	55.32	0.0000	1
1	A	5	GLN	CB	29.07	0.0000	1
1	A	5	GLN	CG	33.686	0.0000	1
1	A	5	GLN	N	123.719	0.0000	1
1	A	6	ALA	H	8.147	0.0000	1
1	A	6	ALA	HA	4.202	0.0000	1
1	A	6	ALA	HB1	1.25	0.0000	1
1	A	6	ALA	HB2	1.25	0.0000	1
1	A	6	ALA	HB3	1.25	0.0000	1
1	A	6	ALA	C	177.27	0.0000	1
1	A	6	ALA	CA	52.508	0.0000	1
1	A	6	ALA	CB	19.081	0.0000	1
1	A	6	ALA	N	125.128	0.0000	1
1	A	7	TRP	H	7.81	0.0000	1
1	A	7	TRP	HA	4.68	0.0000	1
1	A	7	TRP	HB2	3.22	0.0000	2
1	A	7	TRP	HB3	3.16	0.0000	2
1	A	7	TRP	HD1	7.176	0.0000	1
1	A	7	TRP	HE1	10.19	0.0000	1
1	A	7	TRP	HE3	7.537	0.0000	1
1	A	7	TRP	HH2	7.122	0.0000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	TRP	HZ2	7.409	0.0000	1
1	A	7	TRP	HZ3	7.08	0.0000	1
1	A	7	TRP	C	176.468	0.0000	1
1	A	7	TRP	CA	56.35	0.0000	1
1	A	7	TRP	CB	29.85	0.0000	1
1	A	7	TRP	CD1	126.937	0.0000	1
1	A	7	TRP	CE3	120.939	0.0000	1
1	A	7	TRP	CH2	124.438	0.0000	1
1	A	7	TRP	CZ2	114.441	0.0000	1
1	A	7	TRP	CZ3	121.939	0.0000	1
1	A	7	TRP	N	119.157	0.0000	1
1	A	7	TRP	NE1	129.492	0.0000	1
1	A	11	PRO	HA	4.114	0.0000	1
1	A	11	PRO	HB2	1.932	0.0000	2
1	A	11	PRO	HB3	2.247	0.0000	2
1	A	11	PRO	HD2	2.64	0.0000	2
1	A	11	PRO	HD3	2.86	0.0000	2
1	A	11	PRO	C	177.575	0.0000	1
1	A	11	PRO	CA	65.164	0.0000	1
1	A	11	PRO	CB	31.883	0.0000	1
1	A	11	PRO	CG	27.644	0.0000	1
1	A	12	GLU	H	9.56	0.0000	1
1	A	12	GLU	HB2	2.059	0.0000	2
1	A	12	GLU	HB3	2.059	0.0000	2
1	A	12	GLU	HG2	2.302	0.0000	2
1	A	12	GLU	HG3	2.302	0.0000	2
1	A	20	ASP	HB2	2.19	0.0000	2
1	A	20	ASP	HB3	2.4	0.0000	2
1	A	21	TYR	HD2	6.97	0.0000	3
1	A	21	TYR	HE2	6.53	0.0000	3
1	A	22	LYS	HB2	1.795	0.0000	2
1	A	22	LYS	HB3	1.795	0.0000	2
1	A	22	LYS	HG2	1.381	0.0000	2
1	A	22	LYS	HG3	1.381	0.0000	2
1	A	25	TYR	HD1	6.65	0.0000	3
1	A	25	TYR	HE1	6.59	0.0000	3
1	A	31	ILE	HG13	1.03	0.0000	1
1	A	32	LYS	HB2	1.691	0.0000	2
1	A	32	LYS	HB3	1.796	0.0000	2
1	A	32	LYS	HD2	1.161	0.0000	2
1	A	32	LYS	HD3	1.161	0.0000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	32	LYS	HG2	1.357	0.0000	2
1	A	32	LYS	HG3	1.357	0.0000	2
1	A	33	GLU	HB2	1.83	0.0000	2
1	A	33	GLU	HB3	1.788	0.0000	2
1	A	33	GLU	HG2	2.07	0.0000	2
1	A	33	GLU	HG3	2.131	0.0000	2
1	A	35	ARG	HB2	1.978	0.0000	2
1	A	35	ARG	HB3	1.493	0.0000	2
1	A	35	ARG	HD2	3.106	0.0000	2
1	A	35	ARG	HD3	3.106	0.0000	2
1	A	35	ARG	HG2	1.424	0.0000	2
1	A	35	ARG	HG3	1.424	0.0000	2
1	A	38	GLU	HB2	2.137	0.0000	2
1	A	38	GLU	HB3	2.137	0.0000	2
1	A	38	GLU	HG2	2.222	0.0000	2
1	A	38	GLU	HG3	2.357	0.0000	2
1	A	42	ASP	HB2	2.641	0.0000	2
1	A	42	ASP	HB3	2.824	0.0000	2
1	A	46	LYS	HB2	1.728	0.0000	2
1	A	46	LYS	HB3	1.797	0.0000	2
1	A	46	LYS	HG2	1.488	0.0000	2
1	A	46	LYS	HG3	1.488	0.0000	2
1	A	48	ARG	HB2	1.813	0.0000	2
1	A	48	ARG	HB3	1.813	0.0000	2
1	A	56	GLU	HB2	2.02	0.0000	2
1	A	56	GLU	HB3	2.27	0.0000	2
1	A	56	GLU	HG2	2.292	0.0000	2
1	A	56	GLU	HG3	2.292	0.0000	2
1	A	59	LYS	HB2	1.863	0.0000	2
1	A	59	LYS	HB3	1.863	0.0000	2
1	A	59	LYS	HD2	1.43	0.0000	2
1	A	59	LYS	HD3	1.521	0.0000	2
1	A	59	LYS	HG2	1.688	0.0000	2
1	A	59	LYS	HG3	1.688	0.0000	2
1	A	60	LYS	HB2	1.771	0.0000	2
1	A	60	LYS	HB3	1.902	0.0000	2
1	A	60	LYS	HD2	1.393	0.0000	2
1	A	60	LYS	HD3	1.491	0.0000	2
1	A	60	LYS	HG2	1.674	0.0000	2
1	A	60	LYS	HG3	1.674	0.0000	2
1	A	64	ILE	HG13	0.98	0.0000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	65	ILE	HG13	1.07	0.0000	1
1	A	71	LYS	HB2	1.864	0.0000	2
1	A	71	LYS	HB3	1.605	0.0000	2
1	A	71	LYS	HG2	1.437	0.0000	2
1	A	71	LYS	HG3	1.437	0.0000	2
1	A	74	LYS	HB2	1.696	0.0000	2
1	A	74	LYS	HB3	1.696	0.0000	2
1	A	74	LYS	HD2	1.24	0.0000	2
1	A	74	LYS	HD3	1.407	0.0000	2
1	A	74	LYS	HG2	1.553	0.0000	2
1	A	74	LYS	HG3	1.553	0.0000	2
1	A	75	PHE	HD2	6.59	0.0000	3
1	A	75	PHE	HE2	6.71	0.0000	3
1	A	76	ILE	HG13	1.07	0.0000	1
1	A	77	ASP	HB2	3.198	0.0000	2
1	A	77	ASP	HB3	2.584	0.0000	2
1	A	83	ILE	HG13	0.95	0.0000	1
1	A	84	ILE	HG13	1.07	0.0000	1
1	A	88	GLU	HB2	2.33	0.0000	2
1	A	88	GLU	HB3	2.33	0.0000	2
1	A	88	GLU	HG2	2.434	0.0000	2
1	A	88	GLU	HG3	2.434	0.0000	2
1	A	89	ILE	HG13	0.97	0.0000	1
1	A	90	ARG	HB2	1.759	0.0000	2
1	A	90	ARG	HB3	1.759	0.0000	2
1	A	100	GLU	HB2	1.801	0.0000	2
1	A	100	GLU	HB3	2.106	0.0000	2
1	A	100	GLU	HG2	2.264	0.0000	2
1	A	100	GLU	HG3	2.264	0.0000	2
1	A	101	ASP	HB2	2.438	0.0000	2
1	A	101	ASP	HB3	2.503	0.0000	2
1	A	105	PHE	HD2	7.05	0.0000	3
1	A	105	PHE	HE2	6.69	0.0000	3
1	A	107	TYR	HD2	6.89	0.0000	3
1	A	107	TYR	HE2	6.67	0.0000	3
1	A	108	ILE	HG13	0.95	0.0000	1
1	A	110	LYS	HB2	1.597	0.0000	2
1	A	110	LYS	HB3	1.769	0.0000	2
1	A	110	LYS	HD3	1.052	0.0000	2
1	A	110	LYS	HG2	1.597	0.0000	2
1	A	110	LYS	HG3	1.597	0.0000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	111	ASP	HB2	2.622	0.0000	2
1	A	111	ASP	HB3	3.028	0.0000	2
1	A	113	LYS	HB2	1.939	0.0000	2
1	A	113	LYS	HB3	1.939	0.0000	2
1	A	113	LYS	HD2	1.385	0.0000	2
1	A	113	LYS	HD3	1.484	0.0000	2
1	A	118	TYR	HD1	6.75	0.0000	3
1	A	118	TYR	HE1	6.7	0.0000	3
1	A	122	PHE	HD1	6.54	0.0000	3
1	A	122	PHE	HE1	6.9	0.0000	3
1	A	125	PHE	HD2	7.28	0.0000	3
1	A	125	PHE	HE2	7.28	0.0000	3
1	A	126	ASP	HB2	2.897	0.0000	2
1	A	126	ASP	HB3	2.705	0.0000	2
1	A	132	GLU	HB2	2.16	0.0000	2
1	A	132	GLU	HB3	1.493	0.0000	2
1	A	133	ILE	HG13	0.88	0.0000	1
1	A	134	ILE	HG13	1.37	0.0000	1
1	A	141	PHE	HD2	7.32	0.0000	3
1	A	142	GLU	HB2	2.236	0.0000	2
1	A	142	GLU	HB3	2.292	0.0000	2
1	A	142	GLU	HG2	2.51	0.0000	2
1	A	142	GLU	HG3	2.437	0.0000	2
1	A	145	TYR	HD2	7.13	0.0000	3
1	A	145	TYR	HE2	6.83	0.0000	3
1	A	147	LEU	H	8.375	0.0000	1
1	A	147	LEU	HA	4.1	0.0000	1
1	A	147	LEU	HB2	1.89	0.0000	2
1	A	147	LEU	HB3	1.54	0.0000	2
1	A	147	LEU	HD11	0.82	0.0000	2
1	A	147	LEU	HD12	0.82	0.0000	2
1	A	147	LEU	HD13	0.82	0.0000	2
1	A	147	LEU	HD21	0.82	0.0000	2
1	A	147	LEU	HD22	0.82	0.0000	2
1	A	147	LEU	HD23	0.82	0.0000	2
1	A	147	LEU	C	179.6	0.0000	1
1	A	147	LEU	CA	57.66	0.0000	1
1	A	147	LEU	CB	42.19	0.0000	1
1	A	147	LEU	CD1	22.82	0.0000	1
1	A	147	LEU	CD2	25.58	0.0000	1
1	A	147	LEU	CG	26.7	0.0000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	147	LEU	N	119.811	0.0000	1
1	A	148	ALA	H	7.73	0.0000	1
1	A	148	ALA	HA	4.14	0.0000	1
1	A	148	ALA	HB1	1.42	0.0000	1
1	A	148	ALA	HB2	1.42	0.0000	1
1	A	148	ALA	HB3	1.42	0.0000	1
1	A	148	ALA	C	179.873	0.0000	1
1	A	148	ALA	CA	54.1	0.0000	1
1	A	148	ALA	CB	17.86	0.0000	1
1	A	148	ALA	N	121.919	0.0000	1
1	A	149	LEU	H	7.7	0.0000	1
1	A	149	LEU	HA	4.08	0.0000	1
1	A	149	LEU	HB2	1.72	0.0000	2
1	A	149	LEU	HB3	1.57	0.0000	2
1	A	149	LEU	HD11	0.77	0.0000	2
1	A	149	LEU	HD12	0.77	0.0000	2
1	A	149	LEU	HD13	0.77	0.0000	2
1	A	149	LEU	HD21	0.76	0.0000	2
1	A	149	LEU	HD22	0.76	0.0000	2
1	A	149	LEU	HD23	0.76	0.0000	2
1	A	149	LEU	C	179.173	0.0000	1
1	A	149	LEU	CA	56.9	0.0000	1
1	A	149	LEU	CB	42.09	0.0000	1
1	A	149	LEU	CD1	24.89	0.0000	1
1	A	149	LEU	CD2	23.17	0.0000	1
1	A	149	LEU	CG	26.63	0.0000	1
1	A	149	LEU	N	119.142	0.0000	1
1	A	150	GLN	H	7.748	0.0000	1
1	A	150	GLN	HA	4.149	0.0000	1
1	A	150	GLN	HB2	2.071	0.0000	2
1	A	150	GLN	HB3	2.16	0.0000	2
1	A	150	GLN	HG2	2.505	0.0000	2
1	A	150	GLN	HG3	2.428	0.0000	2
1	A	150	GLN	C	176.588	0.0000	1
1	A	150	GLN	CA	57.195	0.0000	1
1	A	150	GLN	CB	29.07	0.0000	1
1	A	150	GLN	CG	34.017	0.0000	1
1	A	150	GLN	N	117.673	0.0000	1
1	A	151	ALA	H	7.72	0.0000	1
1	A	151	ALA	HA	4.25	0.0000	1
1	A	151	ALA	HB1	1.42	0.0000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	151	ALA	HB2	1.42	0.0000	1
1	A	151	ALA	HB3	1.42	0.0000	1
1	A	151	ALA	C	177.855	0.0000	1
1	A	151	ALA	CA	52.86	0.0000	1
1	A	151	ALA	CB	18.66	0.0000	1
1	A	151	ALA	N	122.082	0.0000	1
1	A	152	ARG	H	7.786	0.0000	1
1	A	152	ARG	HA	4.263	0.0000	1
1	A	152	ARG	HB2	1.873	0.0000	2
1	A	152	ARG	HB3	1.873	0.0000	2
1	A	152	ARG	HD2	3.174	0.0000	2
1	A	152	ARG	HD3	3.174	0.0000	2
1	A	152	ARG	HG2	1.632	0.0000	2
1	A	152	ARG	HG3	1.69	0.0000	2
1	A	152	ARG	C	176.133	0.0000	1
1	A	152	ARG	CA	56.258	0.0000	1
1	A	152	ARG	CB	30.945	0.0000	1
1	A	152	ARG	CD	43.553	0.0000	1
1	A	152	ARG	CG	27.02	0.0000	1
1	A	152	ARG	N	118.752	0.0000	1
1	A	153	LYS	H	8.091	0.0000	1
1	A	153	LYS	C	176.23	0.0000	1
1	A	153	LYS	CA	56.258	0.0000	1
1	A	153	LYS	CB	33.289	0.0000	1
1	A	153	LYS	CD	29.131	0.0000	1
1	A	153	LYS	CE	42.197	0.0000	1
1	A	153	LYS	CG	24.837	0.0000	1
1	A	153	LYS	N	122.047	0.0000	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
$^{13}\text{C}_\alpha$	142	-0.26 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	135	-0.07 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	127	-0.09 ± 0.06	None needed (< 0.5 ppm)
^{15}N	133	0.16 ± 0.37	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 79%, i.e. 1227 atoms were assigned a chemical shift out of a possible 1555. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	544/590 (92%)	219/238 (92%)	216/236 (92%)	109/116 (94%)
Sidechain	650/855 (76%)	442/561 (79%)	208/268 (78%)	0/26 (0%)
Aromatic	33/110 (30%)	17/57 (30%)	16/53 (30%)	0/0 (—%)
Overall	1227/1555 (79%)	678/856 (79%)	440/557 (79%)	109/142 (77%)

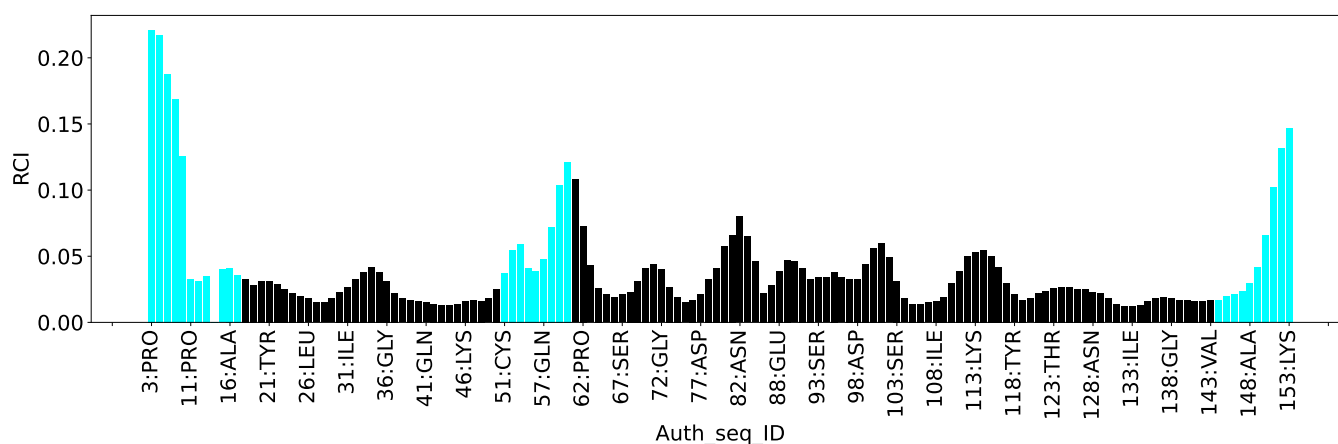
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	611
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	179
Medium range ($ i-j >1$ and $ i-j <5$)	65
Long range ($ i-j \geq 5$)	251
Inter-chain	0
Hydrogen bond restraints	116
Disulfide bond restraints	0
Total dihedral-angle restraints	192
Number of unmapped restraints	1
Number of restraints per residue	5.2
Number of long range restraints per residue ¹	2.0

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)	23.5	0.2
0.2-0.5 (Medium)	6.5	0.44
>0.5 (Large)	0.1	0.54

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)	0.2	3.53
10.0-20.0 (Medium)	None	None
>20.0 (Large)	4.0	119.93

9 Distance violation analysis ⓘ

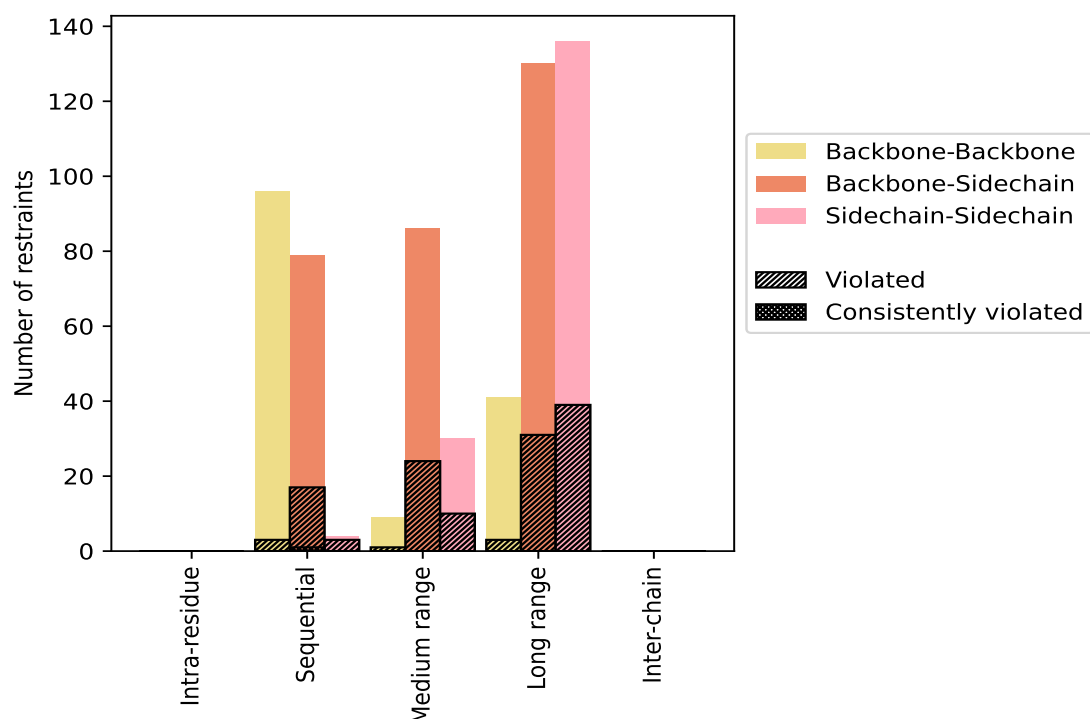
9.1 Summary of distance violations ⓘ

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$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	179	29.3	23	12.8	3.8	1	0.6	0.2
Backbone-Backbone	96	15.7	3	3.1	0.5	0	0.0	0.0
Backbone-Sidechain	79	12.9	17	21.5	2.8	1	1.3	0.2
Sidechain-Sidechain	4	0.7	3	75.0	0.5	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	65	10.6	18	27.7	2.9	0	0.0	0.0
Backbone-Backbone	9	1.5	1	11.1	0.2	0	0.0	0.0
Backbone-Sidechain	26	4.3	7	26.9	1.1	0	0.0	0.0
Sidechain-Sidechain	30	4.9	10	33.3	1.6	0	0.0	0.0
Long range ($ i-j \geq 5$)	251	41.1	59	23.5	9.7	0	0.0	0.0
Backbone-Backbone	41	6.7	3	7.3	0.5	0	0.0	0.0
Backbone-Sidechain	74	12.1	17	23.0	2.8	0	0.0	0.0
Sidechain-Sidechain	136	22.3	39	28.7	6.4	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	116	19.0	31	26.7	5.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	611	100.0	131	21.4	21.4	1	0.2	0.2
Backbone-Backbone	146	23.9	7	4.8	1.1	0	0.0	0.0
Backbone-Sidechain	295	48.3	72	24.4	11.8	1	0.3	0.2
Sidechain-Sidechain	170	27.8	52	30.6	8.5	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	6	8	20	0	34	0.17	0.3	0.06	0.15
2	0	8	8	13	0	29	0.17	0.35	0.06	0.15
3	0	10	8	10	0	28	0.16	0.27	0.04	0.16
4	0	10	10	14	0	34	0.16	0.28	0.05	0.14
5	0	7	8	21	0	36	0.16	0.31	0.06	0.14
6	0	8	8	15	0	31	0.16	0.29	0.05	0.14
7	0	10	13	14	0	37	0.16	0.28	0.05	0.14
8	0	6	6	18	0	30	0.17	0.33	0.06	0.15
9	0	9	9	21	0	39	0.17	0.34	0.06	0.14
10	0	5	10	15	0	30	0.15	0.26	0.04	0.14

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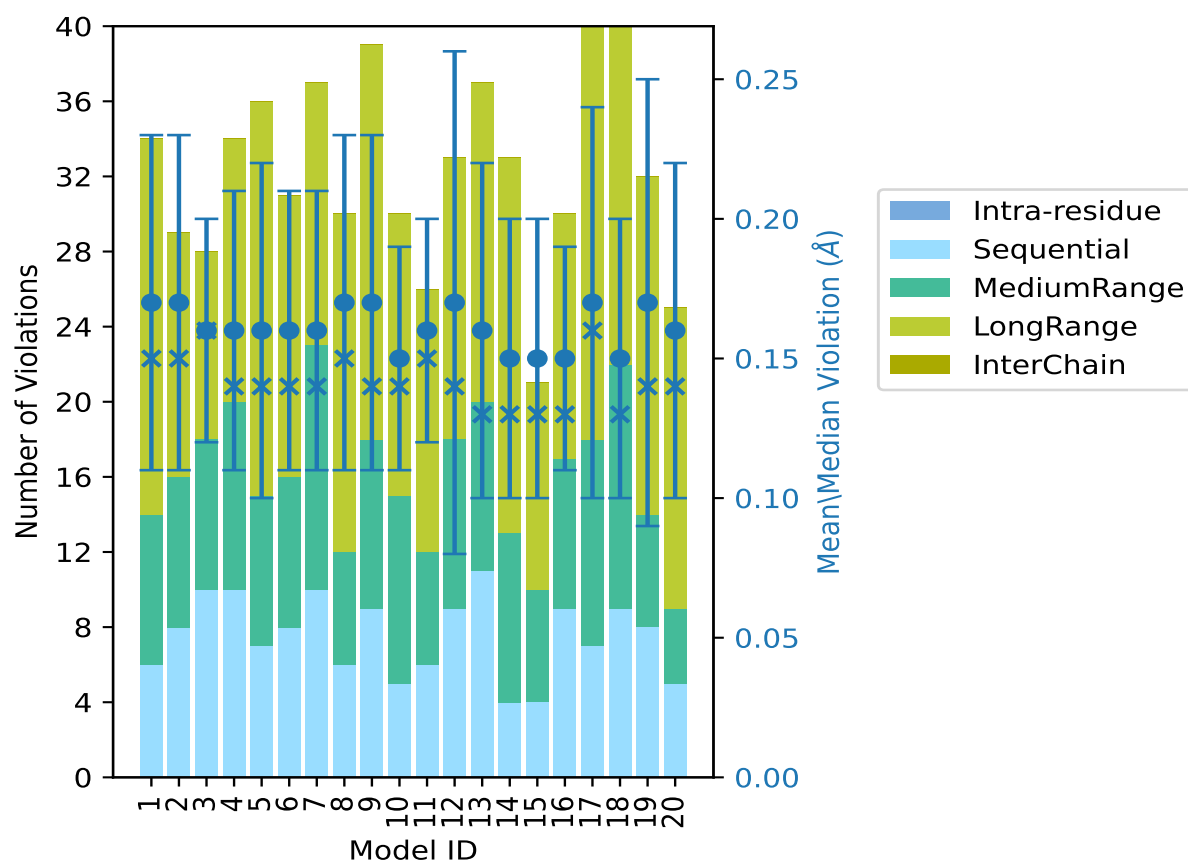
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	6	6	14	0	26	0.16	0.25	0.04	0.15
12	0	9	9	15	0	33	0.17	0.54	0.09	0.14
13	0	11	9	17	0	37	0.16	0.31	0.06	0.13
14	0	4	9	20	0	33	0.15	0.33	0.05	0.13
15	0	4	6	11	0	21	0.15	0.26	0.05	0.13
16	0	9	8	13	0	30	0.15	0.26	0.04	0.13
17	0	7	11	22	0	40	0.17	0.44	0.07	0.16
18	0	9	13	18	0	40	0.15	0.28	0.05	0.13
19	0	8	6	18	0	32	0.17	0.36	0.08	0.14
20	0	5	4	16	0	25	0.16	0.31	0.06	0.14

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble ⓘ

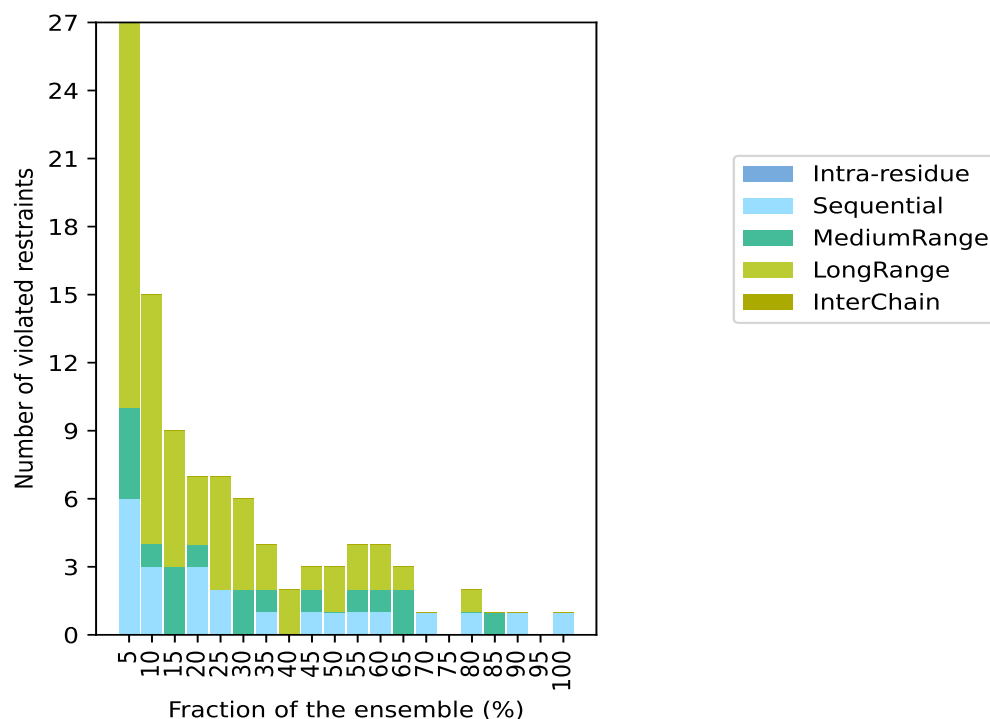
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 395(IR:0, SQ:156, MR:47, LR:192, IC:0) restraints are not 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	6	4	17	0	27	1	5.0
0	3	1	11	0	15	2	10.0
0	0	3	6	0	9	3	15.0
0	3	1	3	0	7	4	20.0
0	2	0	5	0	7	5	25.0
0	0	2	4	0	6	6	30.0
0	1	1	2	0	4	7	35.0
0	0	0	2	0	2	8	40.0
0	1	1	1	0	3	9	45.0
0	1	0	2	0	3	10	50.0
0	1	1	2	0	4	11	55.0
0	1	1	2	0	4	12	60.0
0	0	2	1	0	3	13	65.0
0	1	0	0	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	1	0	1	0	2	16	80.0
0	0	1	0	0	1	17	85.0
0	1	0	0	0	1	18	90.0
0	0	0	0	0	0	19	95.0
0	1	0	0	0	1	20	100.0

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

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

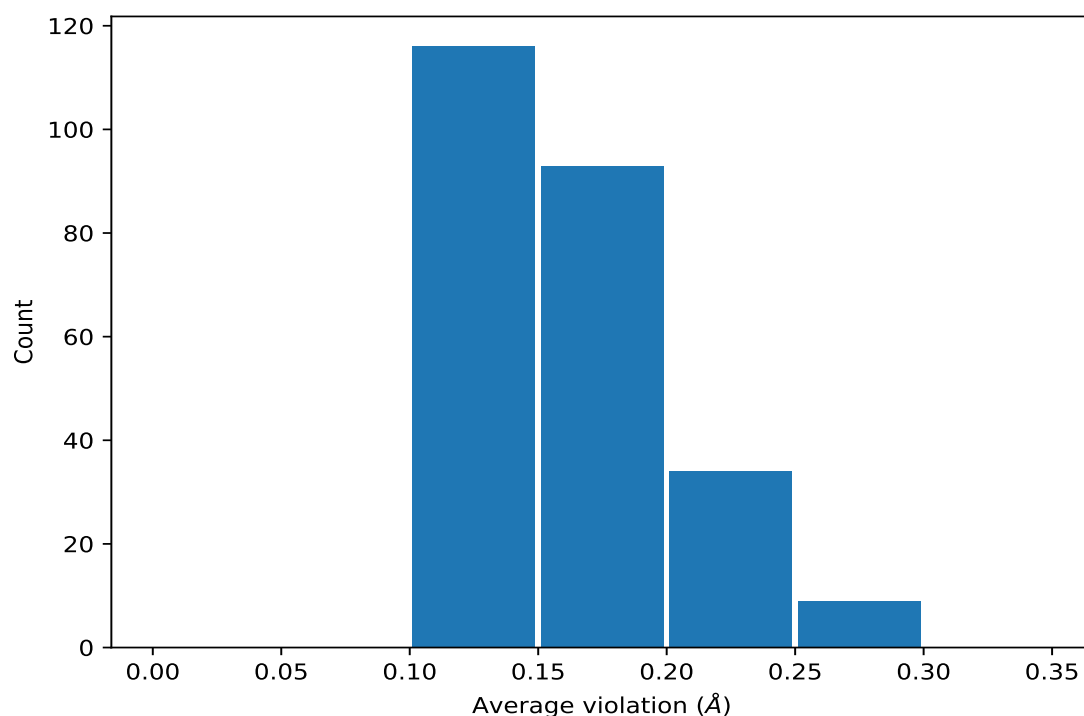
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,252)	1:30:A:LEU:HA	1:31:A:ILE:HD11	20	0.22	0.05	0.22
(1,252)	1:30:A:LEU:HA	1:31:A:ILE:HD12	20	0.22	0.05	0.22
(1,252)	1:30:A:LEU:HA	1:31:A:ILE:HD13	20	0.22	0.05	0.22
(1,191)	1:67:A:SER:HB2	1:68:A:VAL:H	18	0.24	0.06	0.24
(1,239)	1:27:A:GLY:H	1:29:A:MET:HE1	17	0.22	0.07	0.24
(1,239)	1:27:A:GLY:H	1:29:A:MET:HE2	17	0.22	0.07	0.24
(1,239)	1:27:A:GLY:H	1:29:A:MET:HE3	17	0.22	0.07	0.24
(1,199)	1:108:A:ILE:HD11	1:109:A:THR:H	16	0.17	0.03	0.18
(1,199)	1:108:A:ILE:HD12	1:109:A:THR:H	16	0.17	0.03	0.18
(1,199)	1:108:A:ILE:HD13	1:109:A:THR:H	16	0.17	0.03	0.18
(2,107)	1:94:A:CYS:H	1:108:A:ILE:O	16	0.14	0.02	0.14
(1,167)	1:17:A:GLN:HA	1:18:A:SER:H	14	0.18	0.04	0.18
(1,270)	1:55:A:THR:HB	1:58:A:MET:HE1	13	0.2	0.07	0.2
(1,270)	1:55:A:THR:HB	1:58:A:MET:HE2	13	0.2	0.07	0.2
(1,270)	1:55:A:THR:HB	1:58:A:MET:HE3	13	0.2	0.07	0.2
(1,290)	1:64:A:ILE:HD11	1:66:A:LEU:HD11	13	0.17	0.04	0.17

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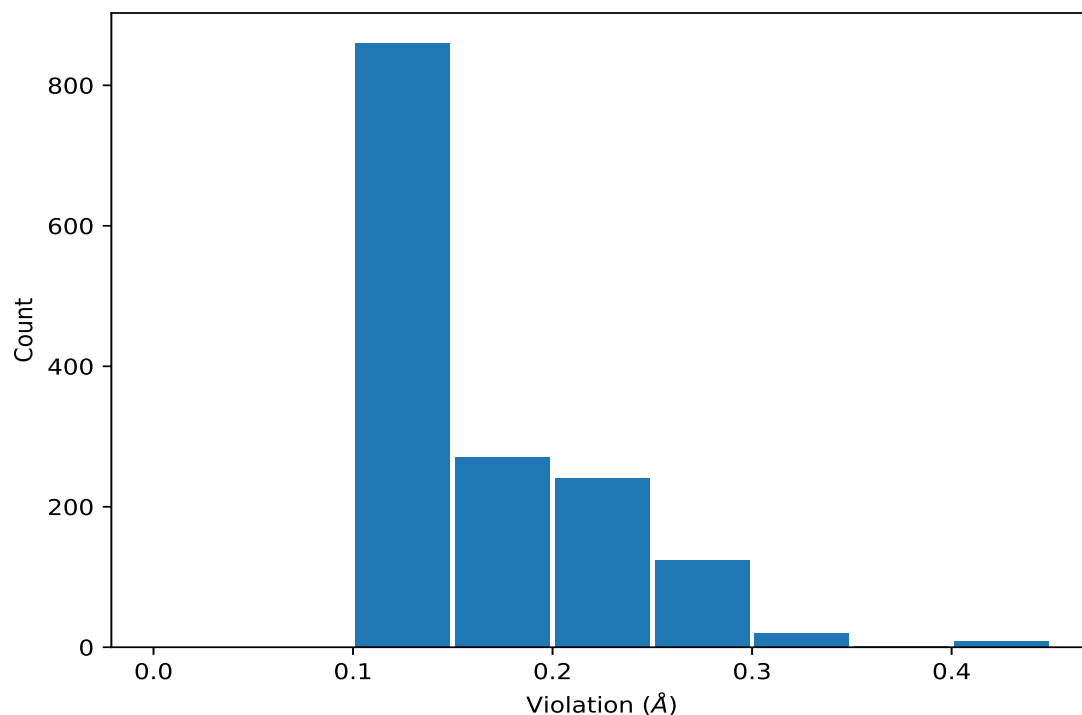
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,290)	1:64:A:ILE:HD11	1:66:A:LEU:HD12	13	0.17	0.04	0.17
(1,290)	1:64:A:ILE:HD11	1:66:A:LEU:HD13	13	0.17	0.04	0.17
(1,290)	1:64:A:ILE:HD12	1:66:A:LEU:HD11	13	0.17	0.04	0.17
(1,290)	1:64:A:ILE:HD12	1:66:A:LEU:HD12	13	0.17	0.04	0.17
(1,290)	1:64:A:ILE:HD12	1:66:A:LEU:HD13	13	0.17	0.04	0.17
(1,290)	1:64:A:ILE:HD13	1:66:A:LEU:HD11	13	0.17	0.04	0.17
(1,290)	1:64:A:ILE:HD13	1:66:A:LEU:HD12	13	0.17	0.04	0.17
(1,290)	1:64:A:ILE:HD13	1:66:A:LEU:HD13	13	0.17	0.04	0.17
(2,75)	1:27:A:GLY:H	1:121:A:VAL:O	13	0.13	0.02	0.13
(1,327)	1:82:A:ASN:HB3	1:84:A:ILE:HD11	12	0.18	0.05	0.19

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)
(1,220)	1:23:A:ALA:HB1	1:66:A:LEU:HD11	17	0.44
(1,220)	1:23:A:ALA:HB1	1:66:A:LEU:HD12	17	0.44
(1,220)	1:23:A:ALA:HB1	1:66:A:LEU:HD13	17	0.44
(1,220)	1:23:A:ALA:HB2	1:66:A:LEU:HD11	17	0.44
(1,220)	1:23:A:ALA:HB2	1:66:A:LEU:HD12	17	0.44
(1,220)	1:23:A:ALA:HB2	1:66:A:LEU:HD13	17	0.44
(1,220)	1:23:A:ALA:HB3	1:66:A:LEU:HD11	17	0.44
(1,220)	1:23:A:ALA:HB3	1:66:A:LEU:HD12	17	0.44
(1,220)	1:23:A:ALA:HB3	1:66:A:LEU:HD13	17	0.44
(1,191)	1:67:A:SER:HB2	1:68:A:VAL:H	19	0.36
(1,239)	1:27:A:GLY:H	1:29:A:MET:HE1	2	0.35
(1,239)	1:27:A:GLY:H	1:29:A:MET:HE2	2	0.35
(1,239)	1:27:A:GLY:H	1:29:A:MET:HE3	2	0.35
(1,270)	1:55:A:THR:HB	1:58:A:MET:HE1	19	0.34
(1,270)	1:55:A:THR:HB	1:58:A:MET:HE2	19	0.34
(1,270)	1:55:A:THR:HB	1:58:A:MET:HE3	19	0.34
(1,252)	1:30:A:LEU:HA	1:31:A:ILE:HD11	14	0.33
(1,252)	1:30:A:LEU:HA	1:31:A:ILE:HD12	14	0.33
(1,252)	1:30:A:LEU:HA	1:31:A:ILE:HD13	14	0.33
(1,379)	1:26:A:LEU:HD11	1:123:A:THR:HG21	19	0.32
(1,379)	1:26:A:LEU:HD11	1:123:A:THR:HG22	19	0.32
(1,379)	1:26:A:LEU:HD11	1:123:A:THR:HG23	19	0.32
(1,379)	1:26:A:LEU:HD12	1:123:A:THR:HG21	19	0.32
(1,379)	1:26:A:LEU:HD12	1:123:A:THR:HG22	19	0.32
(1,379)	1:26:A:LEU:HD12	1:123:A:THR:HG23	19	0.32
(1,379)	1:26:A:LEU:HD13	1:123:A:THR:HG21	19	0.32
(1,379)	1:26:A:LEU:HD13	1:123:A:THR:HG22	19	0.32
(1,379)	1:26:A:LEU:HD13	1:123:A:THR:HG23	19	0.32
(1,191)	1:67:A:SER:HB2	1:68:A:VAL:H	12	0.32
(1,191)	1:67:A:SER:HB2	1:68:A:VAL:H	9	0.31
(1,458)	1:34:A:LEU:HD11	1:108:A:ILE:HG21	17	0.3
(1,458)	1:34:A:LEU:HD11	1:108:A:ILE:HG22	17	0.3
(1,458)	1:34:A:LEU:HD11	1:108:A:ILE:HG23	17	0.3
(1,458)	1:34:A:LEU:HD12	1:108:A:ILE:HG21	17	0.3
(1,458)	1:34:A:LEU:HD12	1:108:A:ILE:HG22	17	0.3
(1,458)	1:34:A:LEU:HD12	1:108:A:ILE:HG23	17	0.3
(1,458)	1:34:A:LEU:HD13	1:108:A:ILE:HG21	17	0.3
(1,458)	1:34:A:LEU:HD13	1:108:A:ILE:HG22	17	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,458)	1:34:A:LEU:HD13	1:108:A:ILE:HG23	17	0.3
(1,381)	1:26:A:LEU:HD21	1:48:A:ARG:HA	13	0.3

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

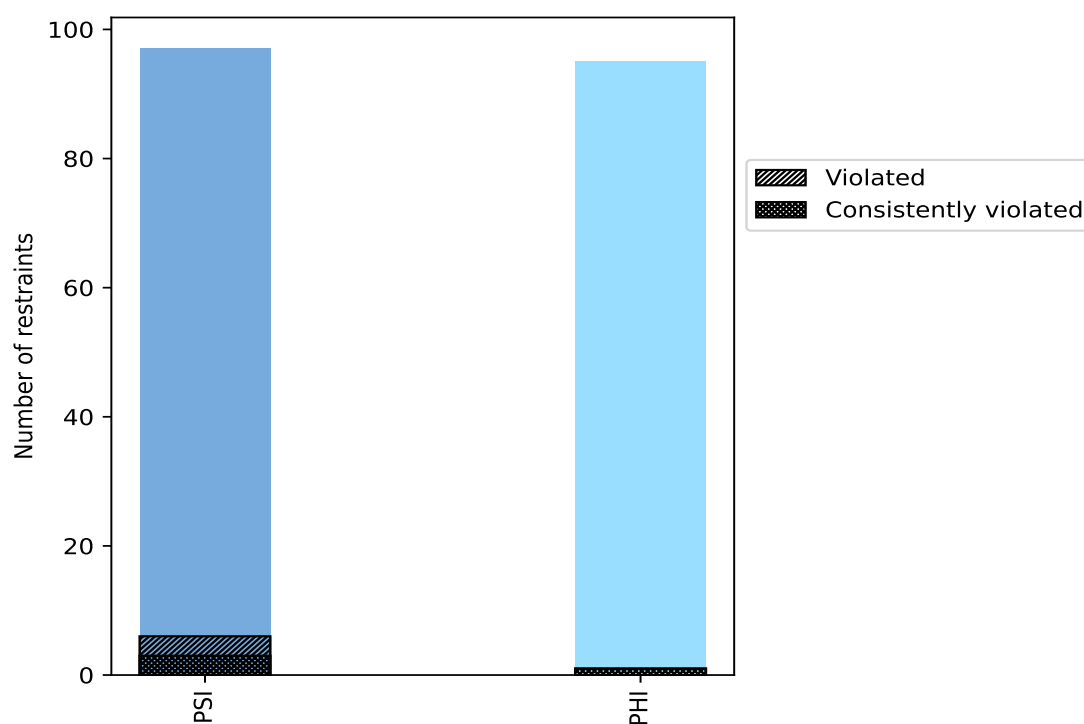
10.1 Summary of dihedral-angle violations [i](#)

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	97	50.5	6	6.2	3.1	3	3.1	1.6
PHI	95	49.5	1	1.1	0.5	1	1.1	0.5
Total	192	100.0	7	3.6	3.6	4	2.1	2.1

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

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



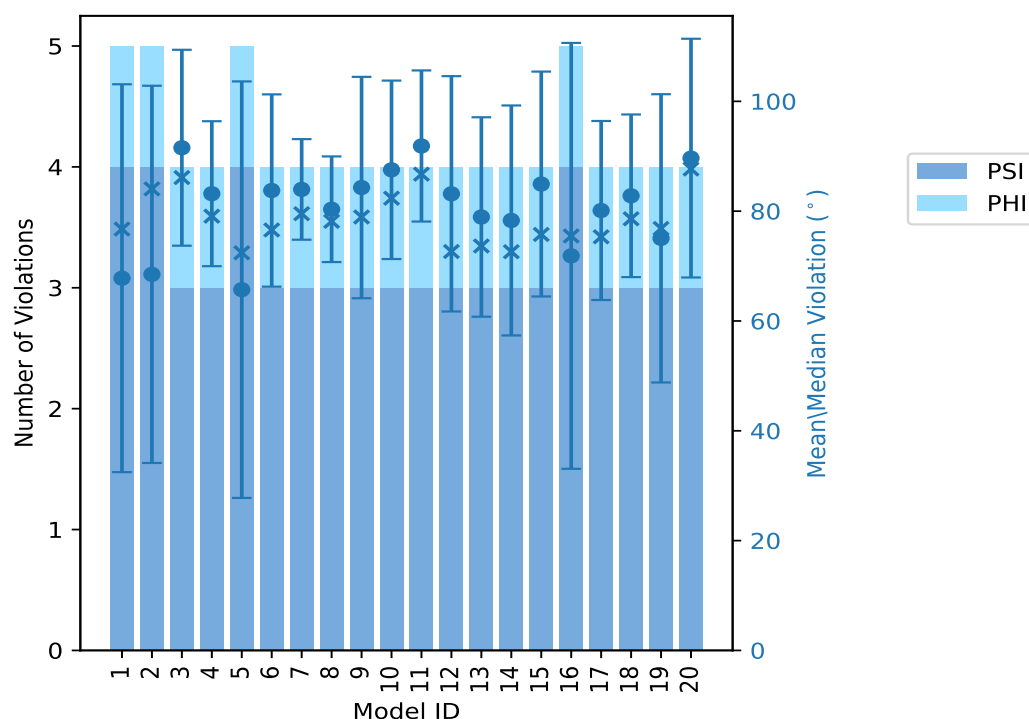
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	4	1	5	67.79	105.88	35.32	76.74
2	4	1	5	68.49	100.52	34.35	84.06
3	3	1	4	91.55	119.11	17.84	86.12
4	3	1	4	83.18	104.7	13.2	79.09
5	4	1	5	65.7	114.18	37.93	72.42
6	3	1	4	83.76	112.61	17.51	76.58
7	3	1	4	83.96	99.73	9.16	79.54
8	3	1	4	80.35	95.13	9.62	78.15
9	3	1	4	84.3	116.86	20.16	78.94
10	3	1	4	87.53	114.28	16.25	82.36
11	3	1	4	91.87	114.85	13.76	86.74
12	3	1	4	83.16	119.93	21.43	72.65
13	3	1	4	78.94	108.65	18.16	73.66
14	3	1	4	78.31	109.24	20.94	72.62
15	3	1	4	84.94	119.41	20.48	75.76
16	4	1	5	71.86	118.55	38.78	75.48
17	3	1	4	80.12	104.66	16.3	75.33
18	3	1	4	82.8	104.78	14.81	78.61
19	3	1	4	75.05	109.34	26.25	76.85
20	3	1	4	89.66	119.9	21.74	87.68

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

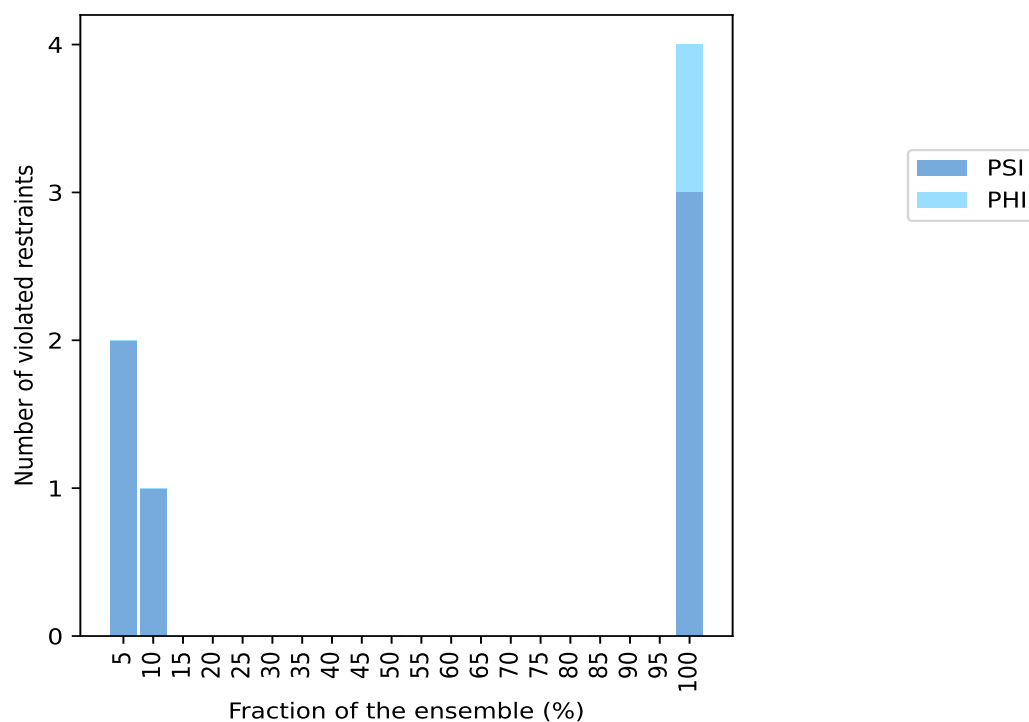
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
3	1	4	20	100.0

¹ Number of models with violations

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

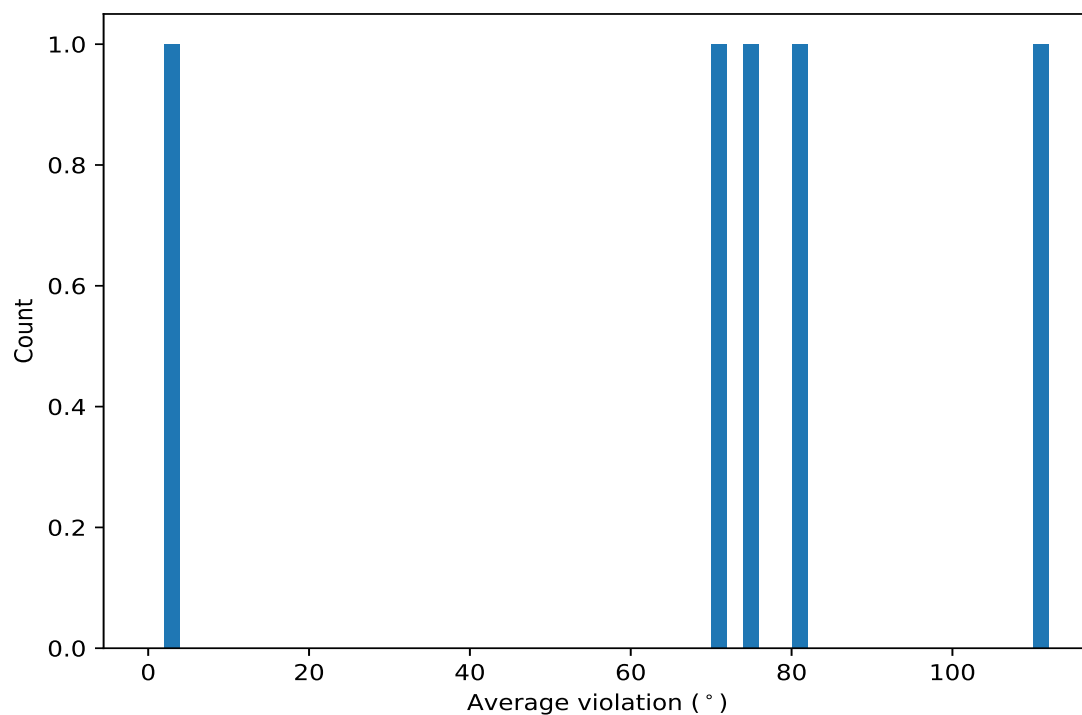


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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 violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

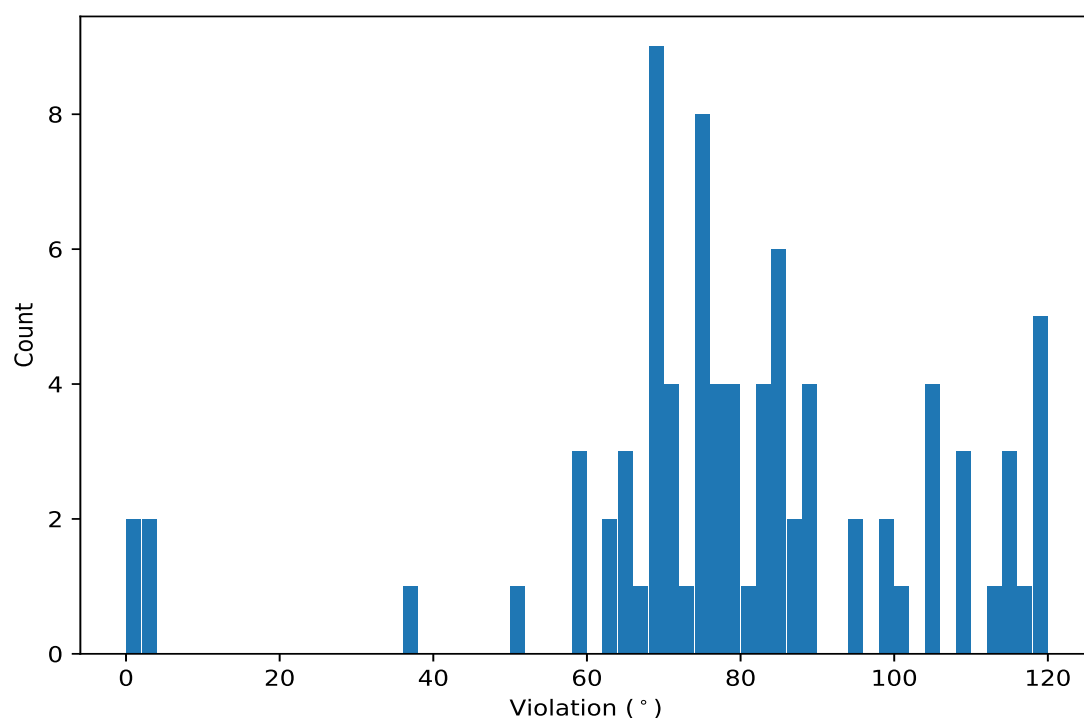
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,92)	1:84:A:ILE:C	1:85:A:ALA:N	1:85:A:ALA:CA	1:85:A:ALA:C	20	110.62	7.3	110.98
(1,118)	1:105:A:PHE:N	1:105:A:PHE:CA	1:105:A:PHE:C	1:106:A:ALA:N	20	80.28	8.28	82.68
(1,142)	1:118:A:TYR:N	1:118:A:TYR:CA	1:118:A:TYR:C	1:119:A:CYS:N	20	74.65	9.69	71.34
(1,140)	1:117:A:HIS:N	1:117:A:HIS:CA	1:117:A:HIS:C	1:118:A:TYR:N	20	70.39	11.29	72.55
(1,136)	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	1:115:A:ASN:N	2	2.78	0.75	2.78

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 (°)
(1,92)	1:84:A:ILE:C	1:85:A:ALA:N	1:85:A:ALA:CA	1:85:A:ALA:C	12	119.93
(1,92)	1:84:A:ILE:C	1:85:A:ALA:N	1:85:A:ALA:CA	1:85:A:ALA:C	20	119.9
(1,92)	1:84:A:ILE:C	1:85:A:ALA:N	1:85:A:ALA:CA	1:85:A:ALA:C	15	119.41
(1,92)	1:84:A:ILE:C	1:85:A:ALA:N	1:85:A:ALA:CA	1:85:A:ALA:C	3	119.11
(1,92)	1:84:A:ILE:C	1:85:A:ALA:N	1:85:A:ALA:CA	1:85:A:ALA:C	16	118.55
(1,92)	1:84:A:ILE:C	1:85:A:ALA:N	1:85:A:ALA:CA	1:85:A:ALA:C	9	116.86
(1,92)	1:84:A:ILE:C	1:85:A:ALA:N	1:85:A:ALA:CA	1:85:A:ALA:C	11	114.85
(1,92)	1:84:A:ILE:C	1:85:A:ALA:N	1:85:A:ALA:CA	1:85:A:ALA:C	10	114.28
(1,92)	1:84:A:ILE:C	1:85:A:ALA:N	1:85:A:ALA:CA	1:85:A:ALA:C	5	114.18
(1,92)	1:84:A:ILE:C	1:85:A:ALA:N	1:85:A:ALA:CA	1:85:A:ALA:C	6	112.61