



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2LXM / pdb_00002lxm
BMRB ID : 18682
Title : Lip5-chmp5
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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
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

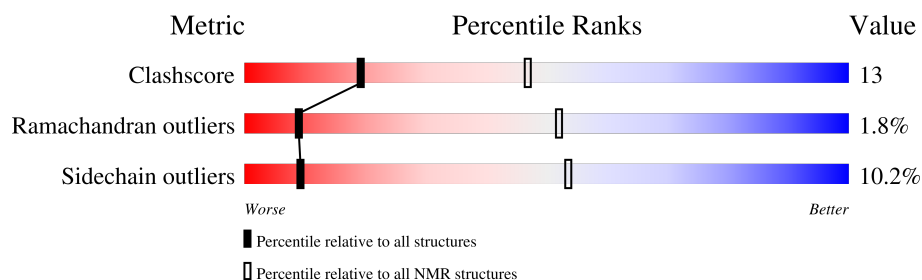
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 74%.

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	168	 79% 16% ...
2	B	59	 34% 14% 14% 39%

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 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:4-A:163, B:154-B:176, B:182-B:186 (188)	0.99	8

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 1 single-model cluster was found.

Cluster number	Models
1	1, 3, 5, 8, 10
2	2, 9
3	4, 7
Single-model clusters	6

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3132 atoms, of which 1548 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Vacuolar protein sorting-associated protein VTA1 homolog.

Mol	Chain	Residues	Atoms						Trace
1	A	163	Total	C	H	N	O	S	0
			2642	839	1323	232	238	10	

- Molecule 2 is a protein called Charged multivesicular body protein 5.

Mol	Chain	Residues	Atoms					Trace
2	B	36	Total	C	H	N	O	0
			490	158	225	36	71	

There are 2 discrepancies between the modelled and reference sequences:

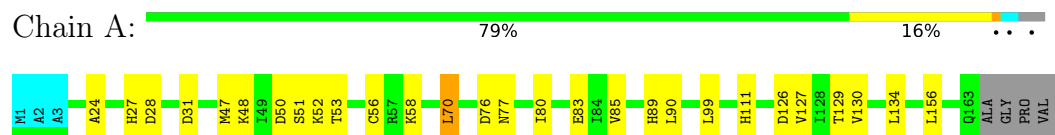
Chain	Residue	Modelled	Actual	Comment	Reference
B	137	GLY	-	expression tag	UNP Q9NZZ3
B	138	HIS	-	expression tag	UNP Q9NZZ3

4 Residue-property plots

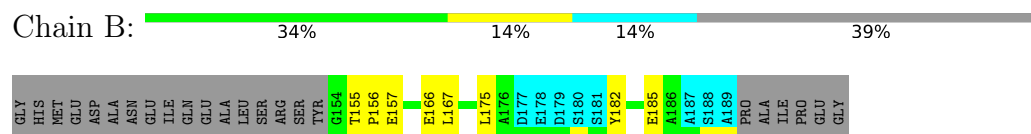
4.1 Average score per residue in the NMR ensemble

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: Vacuolar protein sorting-associated protein VTA1 homolog



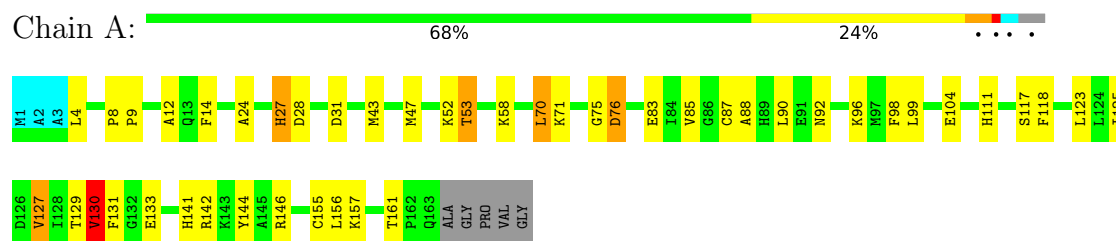
- Molecule 2: Charged multivesicular body protein 5



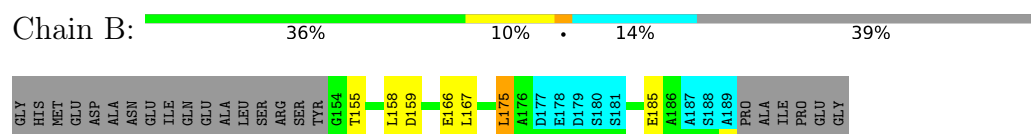
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 8. Colouring as in section 4.1 above.

- Molecule 1: Vacuolar protein sorting-associated protein VTA1 homolog



- Molecule 2: Charged multivesicular body protein 5



5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
XPLOR-NIH	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	2276
Number of shifts mapped to atoms	2009
Number of unparsed shifts	0
Number of shifts with mapping errors	267
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%

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	1301	1305	1305	34±6
2	B	212	186	185	5±3
All	All	15130	14910	14900	381

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 13.

5 of 250 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:VAL:O	1:A:130:VAL:HG22	0.71	1.85	1	10
1:A:129:THR:HG22	1:A:134:LEU:HD13	0.68	1.62	6	1
1:A:153:HIS:ND1	1:A:154:ASN:N	0.67	2.42	7	1
1:A:156:LEU:C	1:A:156:LEU:HD23	0.66	2.16	6	1
1:A:86:GLY:O	1:A:89:HIS:ND1	0.65	2.28	9	3

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	159/168 (95%)	148±2 (93±2%)	8±2 (5±1%)	3±2 (2±1%)	9	53
2	B	27/59 (46%)	26±0 (97±1%)	0±0 (1±2%)	1±0 (2±2%)	7	47
All	All	1860/2270 (82%)	1745 (94%)	82 (4%)	33 (2%)	9	52

5 of 15 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	156	PRO	6
1	A	77	ASN	5
1	A	51	SER	4
1	A	52	LYS	3
1	A	53	THR	2

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	140/143 (98%)	128±2 (91±1%)	12±2 (9±1%)	11	58
2	B	22/46 (48%)	18±1 (80±3%)	4±1 (20±3%)	3	33
All	All	1620/1890 (86%)	1454 (90%)	166 (10%)	9	53

5 of 67 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	70	LEU	10
2	B	166	GLU	10
2	B	167	LEU	10
1	A	85	VAL	8
1	A	90	LEU	7

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 74% for the well-defined parts and 74% 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	2276
Number of shifts mapped to atoms	2009
Number of unparsed shifts	0
Number of shifts with mapping errors	267
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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 267) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	H	8.486	0.000	1
1	A	164	ALA	H	8.743	0.000	1
1	A	164	ALA	HA	4.448	0.000	1
1	A	164	ALA	HB1	1.66	0.000	1
1	A	164	ALA	HB2	1.66	0.000	1
1	A	164	ALA	HB3	1.66	0.000	1
1	A	164	ALA	CA	53.205	0.000	1
1	A	164	ALA	CB	21.15	0.000	1
1	A	164	ALA	N	131.15	0.000	1
1	A	165	GLY	H	10.005	0.000	1
1	A	165	GLY	HA2	3.904	0.000	.
1	A	165	GLY	HA3	4.525	0.000	.
1	A	165	GLY	CA	45.303	0.029	1
1	A	165	GLY	N	110.726	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	166	PRO	HA	5.313	0.000	1
1	A	166	PRO	CA	63.48	0.000	1
1	A	167	VAL	H	7.741	0.000	1
1	A	167	VAL	HA	4.258	0.000	1
1	A	167	VAL	HB	1.566	0.000	1
1	A	167	VAL	HG11	0.642	0.000	.
1	A	167	VAL	HG12	0.642	0.000	.
1	A	167	VAL	HG13	0.642	0.000	.
1	A	167	VAL	HG21	0.782	0.000	.
1	A	167	VAL	HG22	0.782	0.000	.
1	A	167	VAL	HG23	0.782	0.000	.
1	A	167	VAL	CA	62.089	0.000	1
1	A	167	VAL	CB	32.74	0.000	1
1	A	167	VAL	CG1	21.085	0.000	.
1	A	167	VAL	CG2	21.293	0.000	.
1	A	167	VAL	N	117.266	0.000	1
1	A	168	GLY	H	8.003	0.000	1
1	A	168	GLY	HA2	3.716	0.000	.
1	A	168	GLY	HA3	3.809	0.000	.
1	A	168	GLY	CA	46.052	0.007	1
1	A	168	GLY	N	119.021	0.000	1
1	B	137	GLY	HA2	3.921	0.000	.
1	B	137	GLY	HA3	3.921	0.000	.
1	B	137	GLY	CA	43.559	0.000	1
1	B	138	HIS	HA	4.754	0.000	1
1	B	138	HIS	HB2	3.235	0.000	.
1	B	138	HIS	HB3	3.279	0.000	.
1	B	138	HIS	HE1	8.07	0.000	1
1	B	138	HIS	CA	56.557	0.000	1
1	B	138	HIS	CB	30.282	0.001	1
1	B	138	HIS	CE1	137.108	0.000	1
1	B	139	MET	H	8.658	0.000	1
1	B	139	MET	HA	4.466	0.000	1
1	B	139	MET	HB2	2.06	0.000	.
1	B	139	MET	HB3	2.133	0.000	.
1	B	139	MET	HE1	2.162	0.000	1
1	B	139	MET	HE2	2.162	0.000	1
1	B	139	MET	HE3	2.162	0.000	1
1	B	139	MET	HG2	2.531	0.000	.
1	B	139	MET	HG3	2.615	0.000	.
1	B	139	MET	CA	56.113	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	139	MET	CB	32.599	0.006	1
1	B	139	MET	CE	17.101	0.000	1
1	B	139	MET	CG	32.111	0.007	1
1	B	139	MET	N	121.904	0.000	1
1	B	140	GLU	H	8.592	0.000	1
1	B	140	GLU	HA	4.316	0.000	1
1	B	140	GLU	HB2	2.044	0.000	.
1	B	140	GLU	HB3	2.128	0.000	.
1	B	140	GLU	HG2	2.354	0.000	.
1	B	140	GLU	HG3	2.354	0.000	.
1	B	140	GLU	CA	57.447	0.000	1
1	B	140	GLU	CB	30.078	0.000	1
1	B	140	GLU	CG	36.597	0.000	1
1	B	140	GLU	N	121.409	0.000	1
1	B	141	ASP	H	8.343	0.000	1
1	B	141	ASP	HA	4.643	0.000	1
1	B	141	ASP	HB2	2.727	0.000	.
1	B	141	ASP	HB3	2.811	0.000	.
1	B	141	ASP	CA	54.639	0.000	1
1	B	141	ASP	CB	41.304	0.002	1
1	B	141	ASP	N	121.106	0.000	1
1	B	142	ALA	H	8.294	0.000	1
1	B	142	ALA	HA	4.35	0.000	1
1	B	142	ALA	HB1	1.485	0.000	1
1	B	142	ALA	HB2	1.485	0.000	1
1	B	142	ALA	HB3	1.485	0.000	1
1	B	142	ALA	CA	53.237	0.000	1
1	B	142	ALA	CB	19.154	0.000	1
1	B	142	ALA	N	124.241	0.000	1
1	B	143	ASN	H	8.455	0.000	1
1	B	143	ASN	HA	4.705	0.000	1
1	B	143	ASN	HB2	2.883	0.000	.
1	B	143	ASN	HB3	2.919	0.000	.
1	B	143	ASN	HD21	6.992	0.000	.
1	B	143	ASN	HD22	7.767	0.000	.
1	B	143	ASN	CA	54.179	0.000	1
1	B	143	ASN	CB	39.012	0.005	1
1	B	143	ASN	N	117.648	0.000	1
1	B	143	ASN	ND2	113.272	0.010	1
1	B	144	GLU	H	8.441	0.000	1
1	B	144	GLU	HA	4.279	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	144	GLU	HB2	2.127	0.000	.
1	B	144	GLU	HB3	2.127	0.000	.
1	B	144	GLU	HG2	2.362	0.018	.
1	B	144	GLU	CA	57.959	0.000	1
1	B	144	GLU	CB	30.044	0.000	1
1	B	144	GLU	CG	36.492	0.002	1
1	B	144	GLU	N	121.067	0.000	1
1	B	145	ILE	H	8.085	0.000	1
1	B	145	ILE	HA	4.085	0.000	1
1	B	145	ILE	HB	1.975	0.000	1
1	B	145	ILE	HD11	0.941	0.000	1
1	B	145	ILE	HD12	0.941	0.000	1
1	B	145	ILE	HD13	0.941	0.000	1
1	B	145	ILE	HG12	1.266	0.000	.
1	B	145	ILE	HG13	1.606	0.000	.
1	B	145	ILE	HG21	0.982	0.000	1
1	B	145	ILE	HG22	0.982	0.000	1
1	B	145	ILE	HG23	0.982	0.000	1
1	B	145	ILE	CA	62.47	0.000	1
1	B	145	ILE	CB	38.359	0.000	1
1	B	145	ILE	CD1	12.941	0.000	1
1	B	145	ILE	CG1	28.038	0.011	1
1	B	145	ILE	CG2	17.703	0.000	1
1	B	145	ILE	N	120.863	0.000	1
1	B	146	GLN	H	8.254	0.000	1
1	B	146	GLN	HA	4.269	0.000	1
1	B	146	GLN	HB2	2.138	0.000	.
1	B	146	GLN	HB3	2.197	0.000	.
1	B	146	GLN	HE21	6.909	0.000	.
1	B	146	GLN	HE22	7.59	0.000	.
1	B	146	GLN	HG2	2.484	0.000	.
1	B	146	GLN	HG3	2.484	0.000	.
1	B	146	GLN	CA	57.12	0.000	1
1	B	146	GLN	CB	29.156	0.000	1
1	B	146	GLN	CG	33.982	0.000	1
1	B	146	GLN	N	122.118	0.000	1
1	B	146	GLN	NE2	112.383	0.002	1
1	B	147	GLU	H	8.429	0.000	1
1	B	147	GLU	HA	4.224	0.000	1
1	B	147	GLU	HB2	2.119	0.000	.
1	B	147	GLU	HB3	2.119	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	147	GLU	HG2	2.361	0.000	.
1	B	147	GLU	HG3	2.361	0.000	.
1	B	147	GLU	CA	58.039	0.000	1
1	B	147	GLU	CB	29.98	0.000	1
1	B	147	GLU	CG	36.155	0.000	1
1	B	147	GLU	N	121.843	0.000	1
1	B	148	ALA	H	8.27	0.000	1
1	B	148	ALA	HA	4.322	0.000	1
1	B	148	ALA	HB1	1.563	0.000	1
1	B	148	ALA	HB2	1.563	0.000	1
1	B	148	ALA	HB3	1.563	0.000	1
1	B	148	ALA	CA	53.857	0.000	1
1	B	148	ALA	CB	18.956	0.000	1
1	B	148	ALA	N	123.185	0.000	1
1	B	149	LEU	H	8.099	0.000	1
1	B	149	LEU	HA	4.437	0.000	1
1	B	149	LEU	HB2	1.711	0.000	.
1	B	149	LEU	HB3	1.86	0.000	.
1	B	149	LEU	HD11	0.969	0.000	.
1	B	149	LEU	HD12	0.969	0.000	.
1	B	149	LEU	HD13	0.969	0.000	.
1	B	149	LEU	HD21	0.998	0.000	.
1	B	149	LEU	HD22	0.998	0.000	.
1	B	149	LEU	HD23	0.998	0.000	.
1	B	149	LEU	HG	1.857	0.000	1
1	B	149	LEU	CA	55.924	0.000	1
1	B	149	LEU	CB	42.255	0.002	1
1	B	149	LEU	CD1	23.32	0.000	.
1	B	149	LEU	CD2	25.388	0.000	.
1	B	149	LEU	CG	27.167	0.000	1
1	B	149	LEU	N	118.699	0.000	1
1	B	150	SER	H	8.032	0.000	1
1	B	150	SER	HA	4.575	0.000	1
1	B	150	SER	HB2	4.012	0.000	.
1	B	150	SER	HB3	4.012	0.000	.
1	B	150	SER	CA	58.384	0.000	1
1	B	150	SER	CB	63.838	0.000	1
1	B	150	SER	N	115.218	0.000	1
1	B	151	ARG	H	8.027	0.000	1
1	B	151	ARG	HA	4.277	0.000	1
1	B	151	ARG	HB2	1.488	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	151	ARG	HB3	1.815	0.000	.
1	B	151	ARG	HD2	3.003	0.000	.
1	B	151	ARG	HD3	3.116	0.000	.
1	B	151	ARG	HG2	1.46	0.000	.
1	B	151	ARG	HG3	1.824	0.000	.
1	B	151	ARG	CA	56.442	0.000	1
1	B	151	ARG	CB	32.502	0.007	1
1	B	151	ARG	CD	44.233	0.002	1
1	B	151	ARG	CG	28.035	0.007	1
1	B	151	ARG	N	122.71	0.000	1
1	B	152	SER	H	8.486	0.000	1
1	B	152	SER	HA	4.548	0.000	1
1	B	152	SER	HB2	3.874	0.000	.
1	B	152	SER	HB3	3.874	0.000	.
1	B	152	SER	CA	57.317	0.000	1
1	B	152	SER	CB	64.677	0.000	1
1	B	152	SER	N	115.998	0.000	1
1	B	153	TYR	H	8.503	0.000	1
1	B	153	TYR	HA	4.46	0.000	1
1	B	153	TYR	HB2	2.199	0.000	.
1	B	153	TYR	HB3	3.179	0.000	.
1	B	153	TYR	HD1	6.109	0.000	.
1	B	153	TYR	HD2	6.109	0.000	.
1	B	153	TYR	CA	58.351	0.000	1
1	B	153	TYR	CB	38.404	0.009	1
1	B	153	TYR	CD1	131.952	0.000	.
1	B	153	TYR	N	120.362	0.000	1
1	B	190	PRO	HA	4.505	0.000	1
1	B	190	PRO	HB2	1.986	0.000	.
1	B	190	PRO	HB3	2.366	0.000	.
1	B	190	PRO	HD2	3.755	0.000	.
1	B	190	PRO	HD3	3.915	0.000	.
1	B	190	PRO	HG2	2.12	0.000	.
1	B	190	PRO	HG3	2.12	0.000	.
1	B	190	PRO	CA	62.893	0.000	1
1	B	190	PRO	CB	32.204	0.015	1
1	B	190	PRO	CD	50.546	0.004	1
1	B	190	PRO	CG	27.527	0.000	1
1	B	191	ALA	H	8.502	0.000	1
1	B	191	ALA	HA	4.346	0.000	1
1	B	191	ALA	HB1	1.443	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	191	ALA	HB2	1.443	0.000	1
1	B	191	ALA	HB3	1.443	0.000	1
1	B	191	ALA	CA	52.533	0.000	1
1	B	191	ALA	CB	19.293	0.000	1
1	B	191	ALA	N	124.726	0.000	1
1	B	192	ILE	H	8.117	0.000	1
1	B	192	ILE	HA	4.548	0.000	1
1	B	192	ILE	HB	1.934	0.000	1
1	B	192	ILE	HD11	0.934	0.000	1
1	B	192	ILE	HD12	0.934	0.000	1
1	B	192	ILE	HD13	0.934	0.000	1
1	B	192	ILE	HG12	1.241	0.000	.
1	B	192	ILE	HG13	1.577	0.000	.
1	B	192	ILE	HG21	1.021	0.000	1
1	B	192	ILE	HG22	1.021	0.000	1
1	B	192	ILE	HG23	1.021	0.000	1
1	B	192	ILE	CA	58.348	0.000	1
1	B	192	ILE	CB	38.877	0.000	1
1	B	192	ILE	CD1	13.064	0.000	1
1	B	192	ILE	CG1	27.066	0.018	1
1	B	192	ILE	CG2	17.359	0.000	1
1	B	192	ILE	N	120.679	0.000	1
1	B	193	PRO	HA	4.483	0.000	1
1	B	193	PRO	HB2	2.016	0.000	.
1	B	193	PRO	HB3	2.374	0.000	.
1	B	193	PRO	HD2	3.764	0.000	.
1	B	193	PRO	HD3	3.924	0.000	.
1	B	193	PRO	HG2	2.117	0.000	.
1	B	193	PRO	HG3	2.117	0.000	.
1	B	193	PRO	CA	63.255	0.000	1
1	B	193	PRO	CB	32.255	0.007	1
1	B	193	PRO	CD	51.091	0.000	1
1	B	193	PRO	CG	27.527	0.000	1
1	B	194	GLU	H	8.556	0.000	1
1	B	194	GLU	HA	4.361	0.000	1
1	B	194	GLU	HB2	2.028	0.000	.
1	B	194	GLU	HB3	2.156	0.000	.
1	B	194	GLU	HG2	2.364	0.000	.
1	B	194	GLU	HG3	2.364	0.000	.
1	B	194	GLU	CA	56.688	0.000	1
1	B	194	GLU	CB	30.769	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	194	GLU	CG	36.49	0.000	1
1	B	194	GLU	N	121.708	0.000	1
1	B	195	GLY	H	8.059	0.000	1
1	B	195	GLY	HA2	3.839	0.000	.
1	B	195	GLY	HA3	3.839	0.000	.
1	B	195	GLY	CA	46.236	0.000	1
1	B	195	GLY	N	116.329	0.000	1

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
$^{13}\text{C}_\alpha$	223	-0.82 ± 0.12	Should be checked
$^{13}\text{C}_\beta$	200	0.25 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	211	0.04 ± 0.21	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 74%, i.e. 1918 atoms were assigned a chemical shift out of a possible 2600. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	730/932 (78%)	369/376 (98%)	184/376 (49%)	177/180 (98%)
Sidechain	1085/1466 (74%)	744/949 (78%)	327/463 (71%)	14/54 (26%)
Aromatic	103/202 (51%)	64/100 (64%)	38/94 (40%)	1/8 (12%)
Overall	1918/2600 (74%)	1177/1425 (83%)	549/933 (59%)	192/242 (79%)

7.1.4 Statistically unusual chemical shifts [i](#)

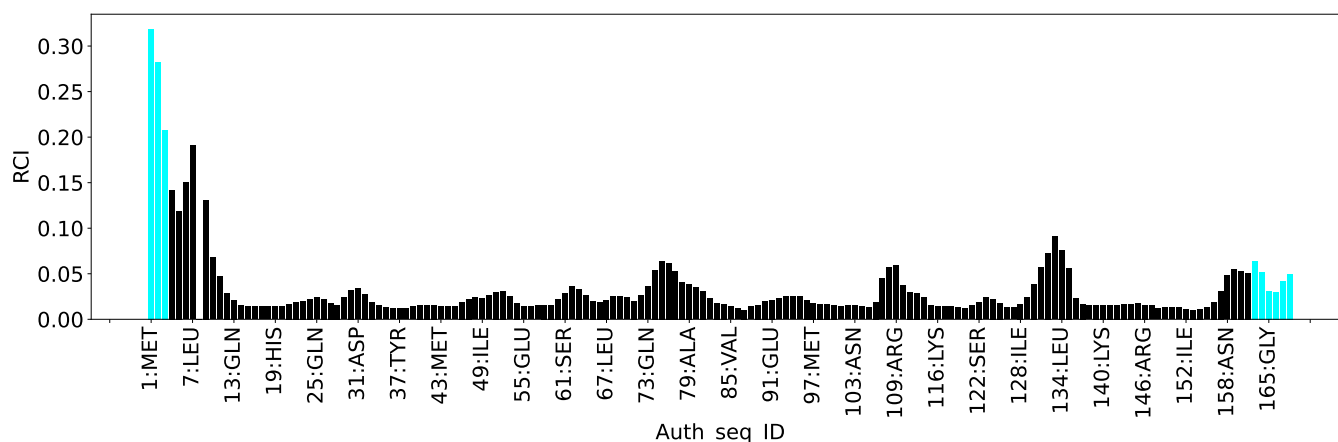
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	148	LYS	HB2	0.47	0.58 – 2.97	-5.5
1	A	148	LYS	HB3	0.45	0.46 – 3.04	-5.1

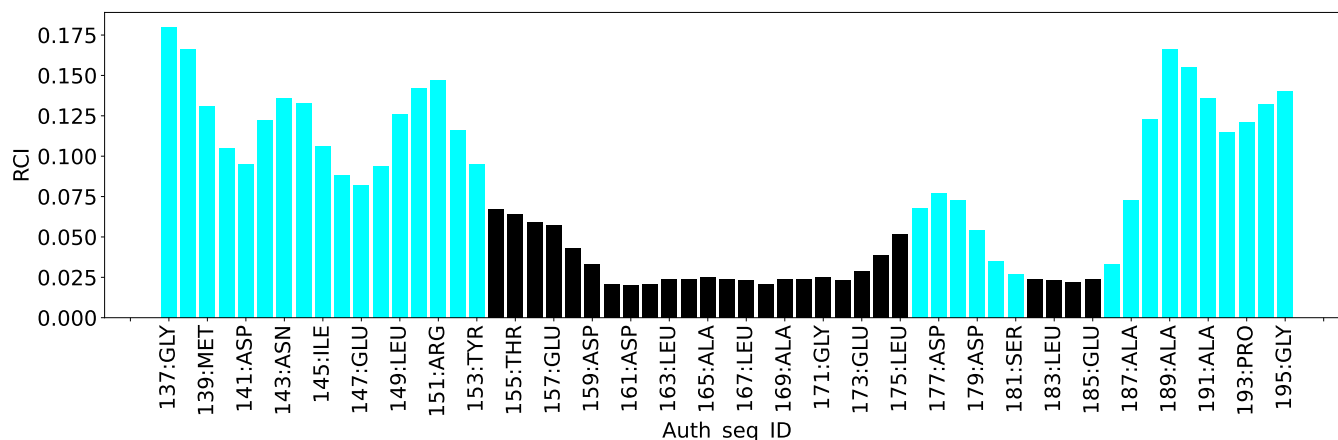
7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



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	2781
Intra-residue ($ i-j =0$)	669
Sequential ($ i-j =1$)	766
Medium range ($ i-j >1$ and $ i-j <5$)	670
Long range ($ i-j \geq 5$)	676
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	411
Number of unmapped restraints	104
Number of restraints per residue	14.1
Number of long range restraints per residue ¹	3.0

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)	23.9	0.2
0.2-0.5 (Medium)	14.9	0.5
>0.5 (Large)	0.5	0.79

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)	8.6	9.57
10.0-20.0 (Medium)	0.7	18.23
>20.0 (Large)	13.3	158.6

9 Distance violation analysis ⓘ

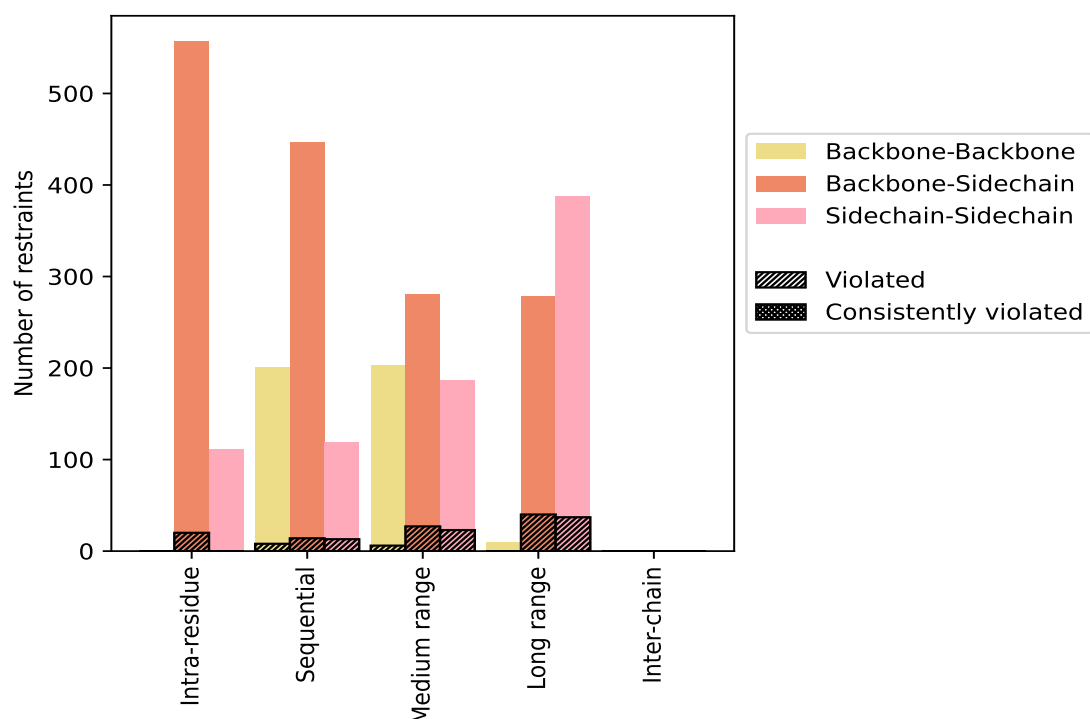
9.1 Summary of distance violations ⓘ

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)	669	24.1	20	3.0	0.7	0	0.0	0.0
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	557	20.0	20	3.6	0.7	0	0.0	0.0
Sidechain-Sidechain	111	4.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	766	27.5	35	4.6	1.3	0	0.0	0.0
Backbone-Backbone	201	7.2	8	4.0	0.3	0	0.0	0.0
Backbone-Sidechain	446	16.0	14	3.1	0.5	0	0.0	0.0
Sidechain-Sidechain	119	4.3	13	10.9	0.5	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	670	24.1	56	8.4	2.0	0	0.0	0.0
Backbone-Backbone	203	7.3	6	3.0	0.2	0	0.0	0.0
Backbone-Sidechain	281	10.1	27	9.6	1.0	0	0.0	0.0
Sidechain-Sidechain	186	6.7	23	12.4	0.8	0	0.0	0.0
Long range (i-j ≥5)	676	24.3	77	11.4	2.8	0	0.0	0.0
Backbone-Backbone	10	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	278	10.0	40	14.4	1.4	0	0.0	0.0
Sidechain-Sidechain	388	14.0	37	9.5	1.3	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2781	100.0	188	6.8	6.8	0	0.0	0.0
Backbone-Backbone	415	14.9	14	3.4	0.5	0	0.0	0.0
Backbone-Sidechain	1562	56.2	101	6.5	3.6	0	0.0	0.0
Sidechain-Sidechain	804	28.9	73	9.1	2.6	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

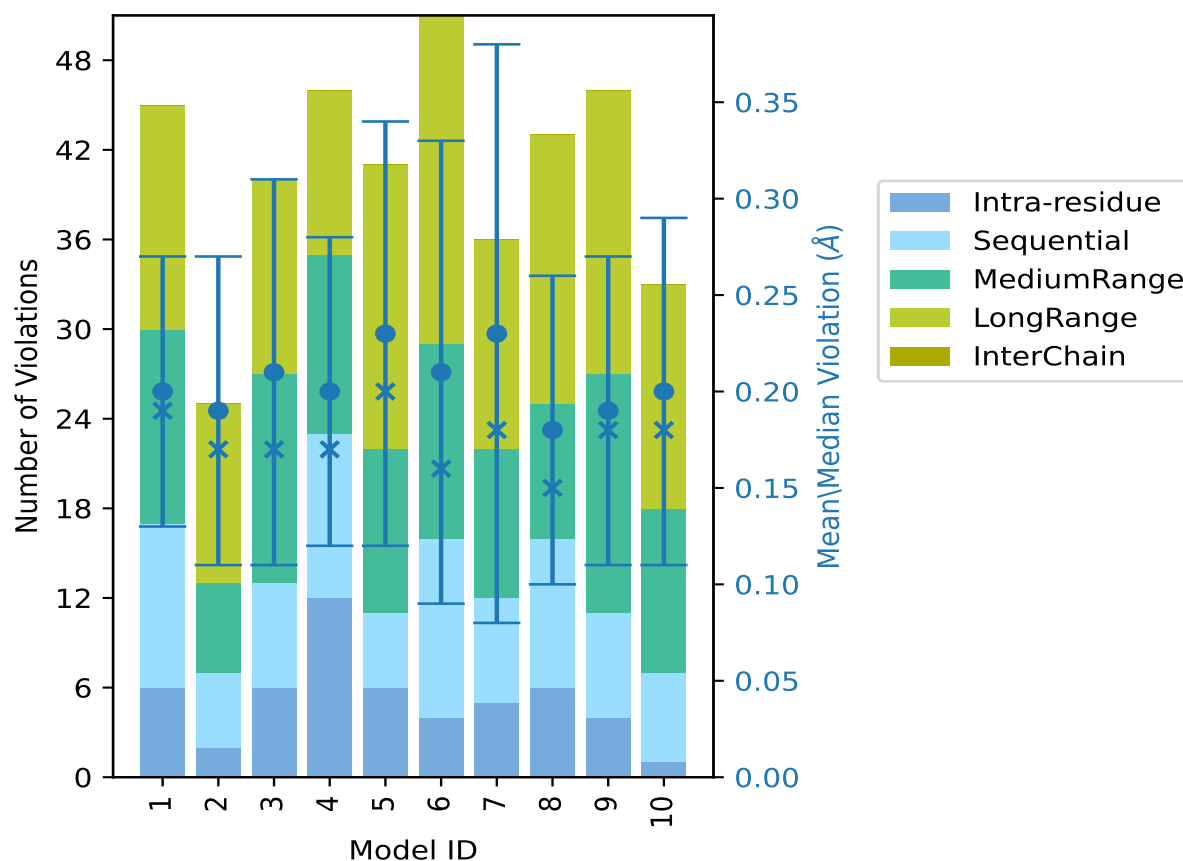
9.2 Distance violation statistics for each model [i](#)

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	6	11	13	15	0	45	0.2	0.4	0.07	0.19
2	2	5	6	12	0	25	0.19	0.44	0.08	0.17
3	6	7	14	13	0	40	0.21	0.49	0.1	0.17
4	12	11	12	11	0	46	0.2	0.47	0.08	0.17
5	6	5	11	19	0	41	0.23	0.5	0.11	0.2
6	4	12	13	22	0	51	0.21	0.68	0.12	0.16
7	5	7	10	14	0	36	0.23	0.79	0.15	0.18
8	6	10	9	18	0	43	0.18	0.51	0.08	0.15
9	4	7	16	19	0	46	0.19	0.38	0.08	0.18
10	1	6	11	15	0	33	0.2	0.45	0.09	0.18

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, 2593(IR:649, SQ:731, MR:614, LR:599, 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	%
9	15	28	49	0	101	1	10.0
5	8	15	11	0	39	2	20.0
3	5	4	5	0	17	3	30.0

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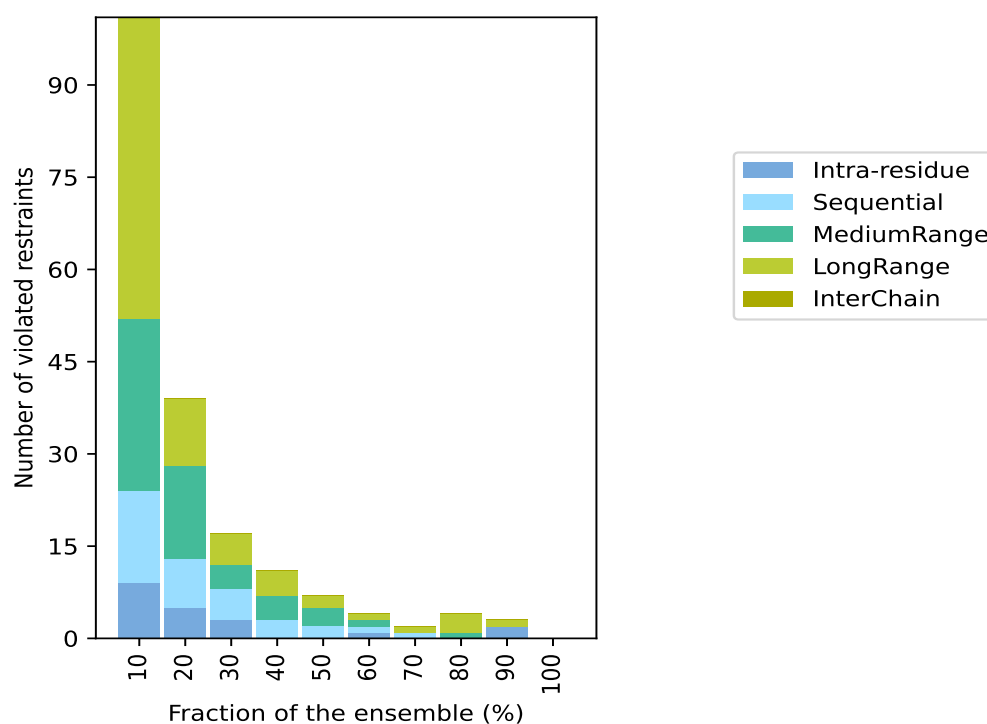
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	3	4	4	0	11	4	40.0
0	2	3	2	0	7	5	50.0
1	1	1	1	0	4	6	60.0
0	1	0	1	0	2	7	70.0
0	0	1	3	0	4	8	80.0
2	0	0	1	0	3	9	90.0
0	0	0	0	0	0	10	100.0

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](#)

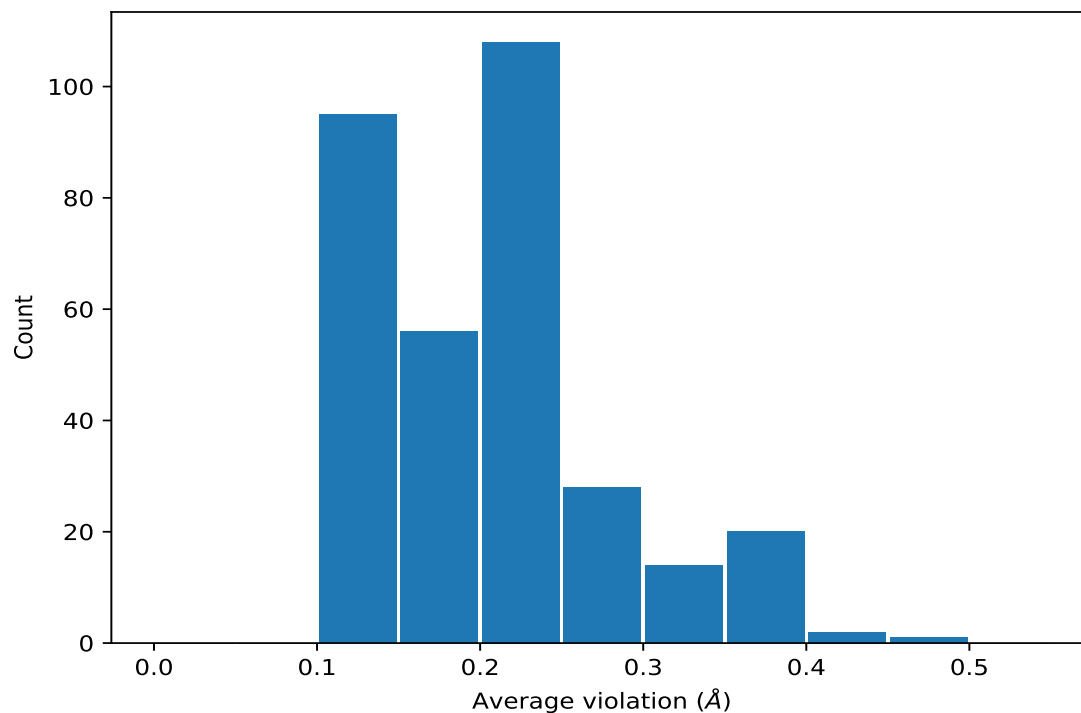


9.4 Most violated distance restraints in the ensemble [i](#)

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)
(1,2490)	1:43:A:MET:H	1:43:A:MET:HG2	9	0.42	0.05	0.42
(1,2490)	1:43:A:MET:H	1:43:A:MET:HG3	9	0.42	0.05	0.42
(1,891)	1:44:A:GLN:H	1:63:A:LEU:HG	9	0.29	0.04	0.27
(1,2533)	1:57:A:ARG:H	1:57:A:ARG:HG2	9	0.16	0.02	0.17
(1,2533)	1:57:A:ARG:H	1:57:A:ARG:HG3	9	0.16	0.02	0.17
(1,2614)	1:90:A:LEU:HD11	1:125:A:ILE:HA	8	0.24	0.06	0.25
(1,2614)	1:90:A:LEU:HD12	1:125:A:ILE:HA	8	0.24	0.06	0.25
(1,2614)	1:90:A:LEU:HD13	1:125:A:ILE:HA	8	0.24	0.06	0.25
(1,2614)	1:90:A:LEU:HD21	1:125:A:ILE:HA	8	0.24	0.06	0.25
(1,2614)	1:90:A:LEU:HD22	1:125:A:ILE:HA	8	0.24	0.06	0.25
(1,2614)	1:90:A:LEU:HD23	1:125:A:ILE:HA	8	0.24	0.06	0.25
(1,1660)	1:79:A:ALA:HB1	1:85:A:VAL:HB	8	0.23	0.06	0.24
(1,1660)	1:79:A:ALA:HB2	1:85:A:VAL:HB	8	0.23	0.06	0.24
(1,1660)	1:79:A:ALA:HB3	1:85:A:VAL:HB	8	0.23	0.06	0.24
(1,1534)	1:75:A:GLY:HA2	1:81:A:THR:HG21	8	0.22	0.18	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1534)	1:75:A:GLY:HA2	1:81:A:THR:HG22	8	0.22	0.18	0.12
(1,1534)	1:75:A:GLY:HA2	1:81:A:THR:HG23	8	0.22	0.18	0.12
(1,1269)	1:74:A:LEU:HD21	1:76:A:ASP:H	8	0.19	0.06	0.16
(1,1269)	1:74:A:LEU:HD22	1:76:A:ASP:H	8	0.19	0.06	0.16
(1,1269)	1:74:A:LEU:HD23	1:76:A:ASP:H	8	0.19	0.06	0.16
(1,2425)	1:33:A:VAL:HG11	1:90:A:LEU:HD11	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG11	1:90:A:LEU:HD12	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG11	1:90:A:LEU:HD13	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG11	1:90:A:LEU:HD21	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG11	1:90:A:LEU:HD22	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG11	1:90:A:LEU:HD23	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG12	1:90:A:LEU:HD11	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG12	1:90:A:LEU:HD12	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG12	1:90:A:LEU:HD13	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG12	1:90:A:LEU:HD21	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG12	1:90:A:LEU:HD22	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG12	1:90:A:LEU:HD23	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG13	1:90:A:LEU:HD11	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG13	1:90:A:LEU:HD12	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG13	1:90:A:LEU:HD13	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG13	1:90:A:LEU:HD21	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG13	1:90:A:LEU:HD22	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG13	1:90:A:LEU:HD23	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG21	1:90:A:LEU:HD11	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG21	1:90:A:LEU:HD12	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG21	1:90:A:LEU:HD13	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG21	1:90:A:LEU:HD21	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG21	1:90:A:LEU:HD22	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG21	1:90:A:LEU:HD23	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG22	1:90:A:LEU:HD11	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG22	1:90:A:LEU:HD12	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG22	1:90:A:LEU:HD13	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG22	1:90:A:LEU:HD21	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG22	1:90:A:LEU:HD22	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG22	1:90:A:LEU:HD23	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG23	1:90:A:LEU:HD11	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG23	1:90:A:LEU:HD12	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG23	1:90:A:LEU:HD13	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG23	1:90:A:LEU:HD21	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG23	1:90:A:LEU:HD22	7	0.21	0.07	0.19
(1,2425)	1:33:A:VAL:HG23	1:90:A:LEU:HD23	7	0.21	0.07	0.19
(1,2322)	1:17:A:ILE:H	1:18:A:GLN:HG2	7	0.2	0.04	0.22

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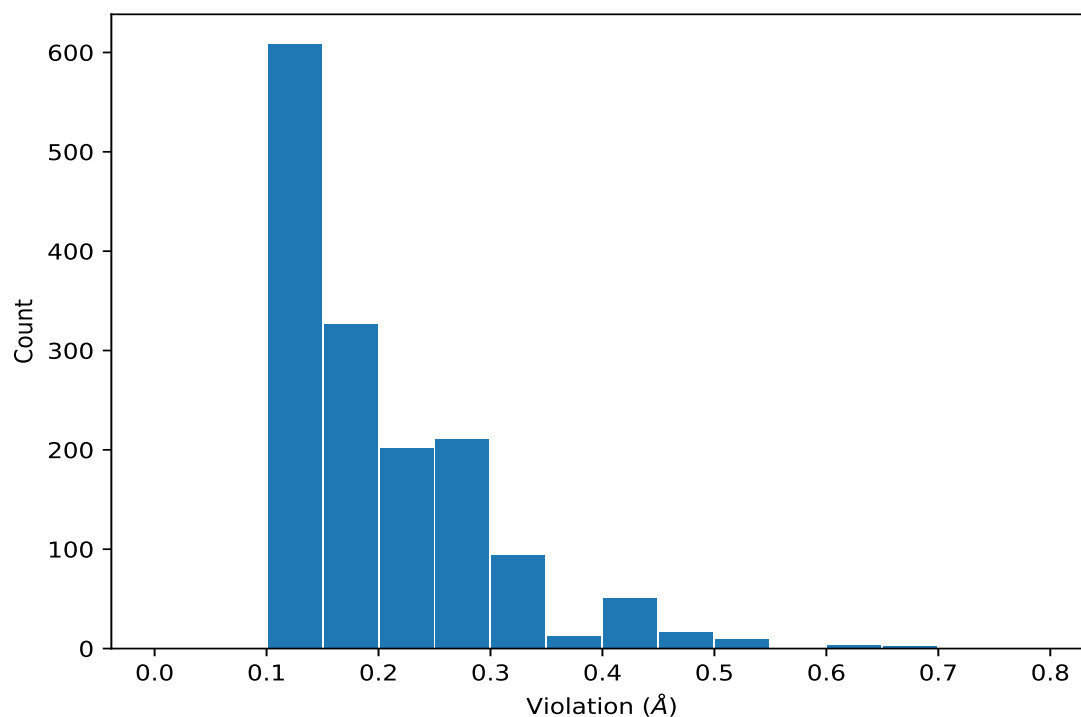
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2322)	1:17:A:ILE:H	1:18:A:GLN:HG3	7	0.2	0.04	0.22
(1,677)	1:156:A:LEU:H	1:156:A:LEU:HG	6	0.48	0.18	0.41

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)
(1,677)	1:156:A:LEU:H	1:156:A:LEU:HG	7	0.79
(1,1534)	1:75:A:GLY:HA2	1:81:A:THR:HG21	6	0.68
(1,1534)	1:75:A:GLY:HA2	1:81:A:THR:HG22	6	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1534)	1:75:A:GLY:HA2	1:81:A:THR:HG23	6	0.68
(1,2159)	1:45:A:THR:HA	1:47:A:MET:HE1	7	0.64
(1,2159)	1:45:A:THR:HA	1:47:A:MET:HE2	7	0.64
(1,2159)	1:45:A:THR:HA	1:47:A:MET:HE3	7	0.64
(1,677)	1:156:A:LEU:H	1:156:A:LEU:HG	6	0.64
(1,2490)	1:43:A:MET:H	1:43:A:MET:HG2	8	0.51
(1,2490)	1:43:A:MET:H	1:43:A:MET:HG3	8	0.51
(1,1121)	1:156:A:LEU:HD21	1:157:A:LYS:HE2	5	0.5
(1,1121)	1:156:A:LEU:HD21	1:157:A:LYS:HE3	5	0.5
(1,1121)	1:156:A:LEU:HD22	1:157:A:LYS:HE2	5	0.5
(1,1121)	1:156:A:LEU:HD22	1:157:A:LYS:HE3	5	0.5
(1,1121)	1:156:A:LEU:HD23	1:157:A:LYS:HE2	5	0.5
(1,1121)	1:156:A:LEU:HD23	1:157:A:LYS:HE3	5	0.5
(1,631)	1:133:A:GLU:H	1:133:A:GLU:HG2	5	0.5
(1,631)	1:133:A:GLU:H	1:133:A:GLU:HG3	5	0.5
(1,683)	1:155:A:CYS:H	1:156:A:LEU:HD21	3	0.49
(1,683)	1:155:A:CYS:H	1:156:A:LEU:HD22	3	0.49
(1,683)	1:155:A:CYS:H	1:156:A:LEU:HD23	3	0.49
(1,1225)	1:72:A:LYS:H	1:72:A:LYS:HD2	4	0.47
(1,1225)	1:72:A:LYS:H	1:72:A:LYS:HD3	4	0.47
(1,677)	1:156:A:LEU:H	1:156:A:LEU:HG	3	0.47

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

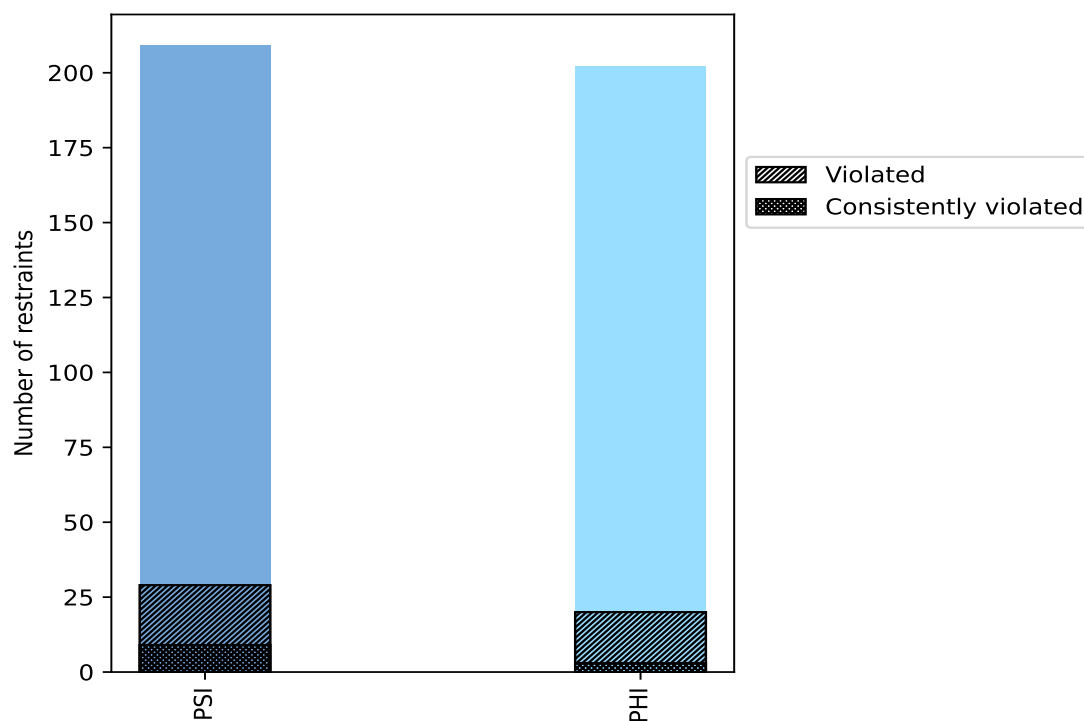
10.1 Summary of dihedral-angle violations [i](#)

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	209	50.9	29	13.9	7.1	9	4.3	2.2
PHI	202	49.1	20	9.9	4.9	3	1.5	0.7
Total	411	100.0	49	11.9	11.9	12	2.9	2.9

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 [i](#)



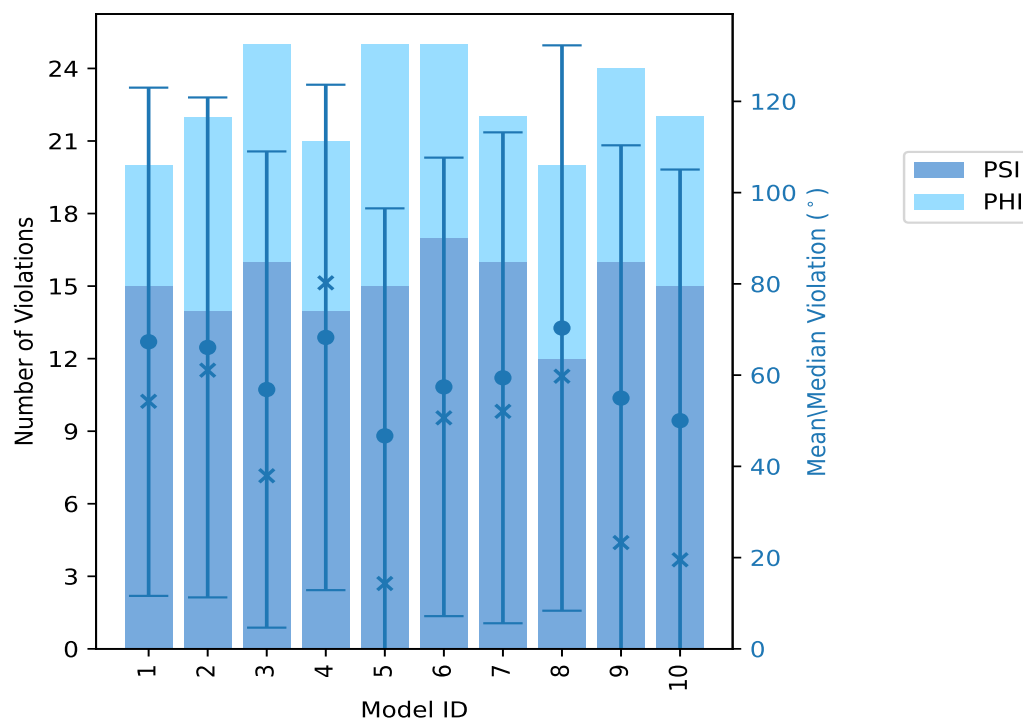
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	15	5	20	67.31	145.29	55.7	54.26
2	14	8	22	66.07	154.39	54.79	61.08
3	16	9	25	56.84	152.94	52.19	37.94
4	14	7	21	68.26	157.15	55.39	80.22
5	15	10	25	46.69	148.45	49.86	14.32
6	17	8	25	57.42	143.24	50.25	50.63
7	16	6	22	59.41	153.13	53.8	52.06
8	12	8	20	70.32	158.6	61.96	59.76
9	16	8	24	54.96	152.91	55.41	23.3
10	15	7	22	50.02	157.36	55.04	19.52

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

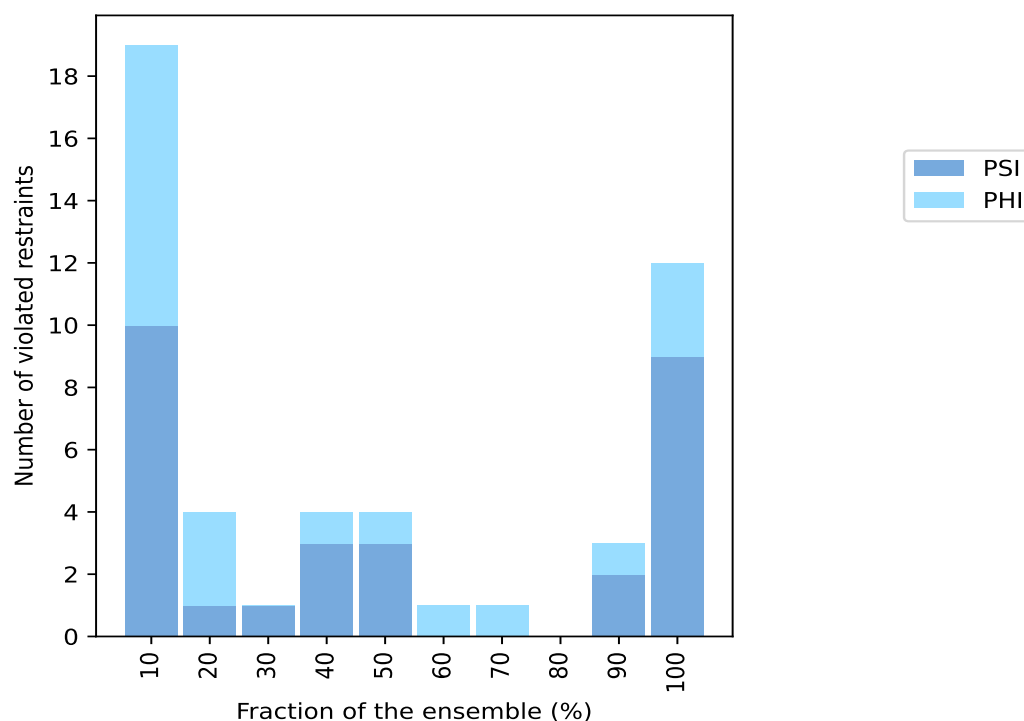
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
10	9	19	1	10.0
1	3	4	2	20.0
1	0	1	3	30.0
3	1	4	4	40.0
3	1	4	5	50.0
0	1	1	6	60.0
0	1	1	7	70.0
0	0	0	8	80.0
2	1	3	9	90.0
9	3	12	10	100.0

¹ Number of models with violations

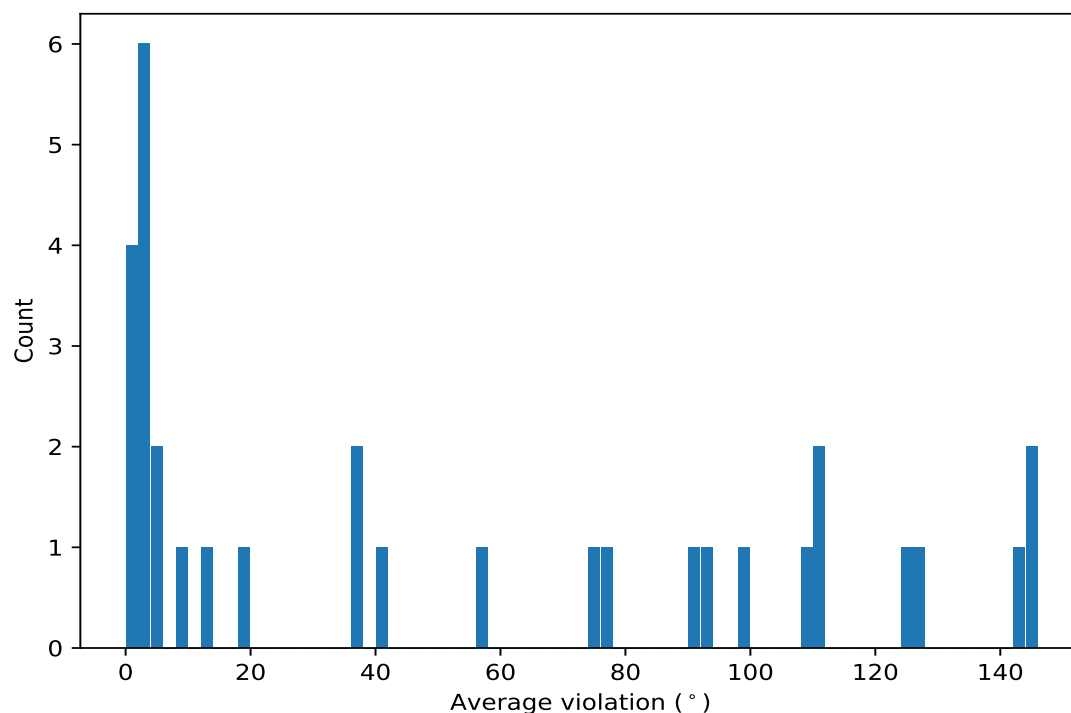
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

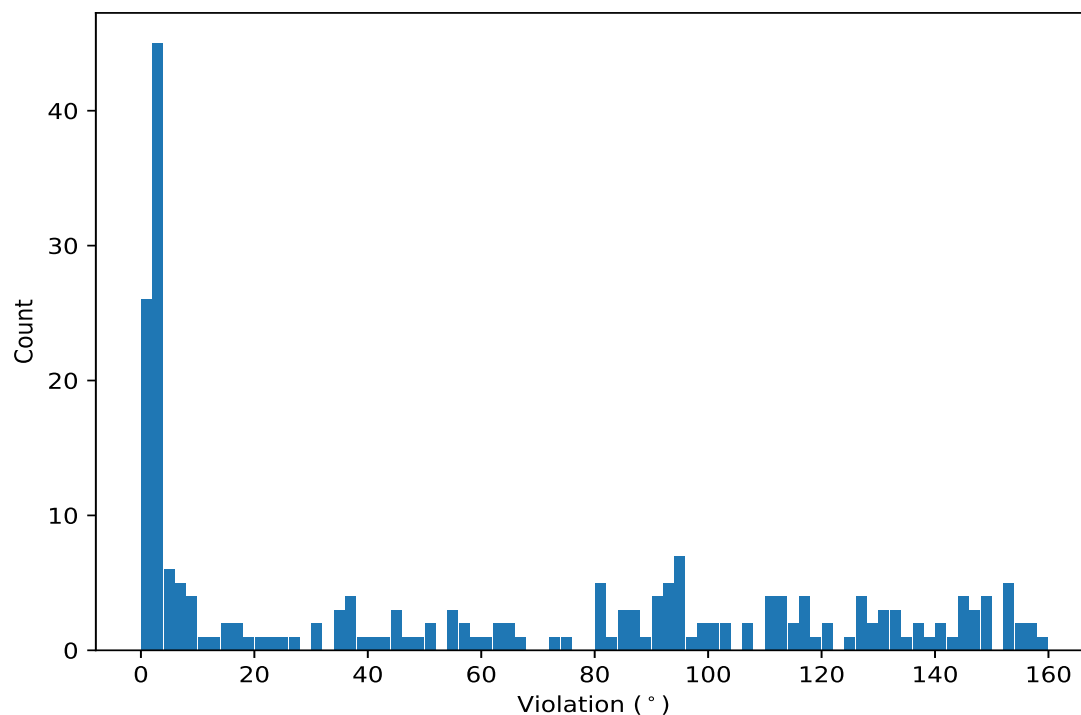
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,64)	2:155:B:THR:N	2:155:B:THR:CA	2:155:B:THR:C	2:156:B:PRO:N	10	145.18	4.26	146.26
(1,64)	2:155:B:THR:N	2:155:B:THR:CA	2:155:B:THR:C	2:156:B:PRO:N	10	145.18	4.26	146.26
(1,158)	2:179:B:ASP:N	2:179:B:ASP:CA	2:179:B:ASP:C	2:180:B:SER:N	10	142.66	12.94	146.67
(1,150)	2:177:B:ASP:N	2:177:B:ASP:CA	2:177:B:ASP:C	2:178:B:GLU:N	10	127.2	43.03	137.66
(1,72)	2:157:B:GLU:N	2:157:B:GLU:CA	2:157:B:GLU:C	2:158:B:LEU:N	10	124.05	13.36	122.54
(1,68)	2:156:B:PRO:N	2:156:B:PRO:CA	2:156:B:PRO:C	2:157:B:GLU:N	10	110.36	18.17	105.06
(1,68)	2:156:B:PRO:N	2:156:B:PRO:CA	2:156:B:PRO:C	2:157:B:GLU:N	10	110.36	18.17	105.06
(1,76)	2:158:B:LEU:N	2:158:B:LEU:CA	2:158:B:LEU:C	2:159:B:ASP:N	10	109.44	8.58	111.0
(1,60)	2:154:B:GLY:N	2:154:B:GLY:CA	2:154:B:GLY:C	2:155:B:THR:N	10	98.65	43.69	116.28
(1,112)	2:167:B:LEU:N	2:167:B:LEU:CA	2:167:B:LEU:C	2:168:B:ASP:N	10	93.36	2.76	93.98
(1,80)	2:159:B:ASP:N	2:159:B:ASP:CA	2:159:B:ASP:C	2:160:B:GLU:N	10	77.63	10.47	80.68
(1,160)	2:179:B:ASP:C	2:180:B:SER:N	2:180:B:SER:CA	2:180:B:SER:C	10	75.31	14.67	77.95

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 (°)
(1,150)	2:177:B:ASP:N	2:177:B:ASP:CA	2:177:B:ASP:C	2:178:B:GLU:N	8	158.6
(1,158)	2:179:B:ASP:N	2:179:B:ASP:CA	2:179:B:ASP:C	2:180:B:SER:N	10	157.36
(1,150)	2:177:B:ASP:N	2:177:B:ASP:CA	2:177:B:ASP:C	2:178:B:GLU:N	4	157.15
(1,158)	2:179:B:ASP:N	2:179:B:ASP:CA	2:179:B:ASP:C	2:180:B:SER:N	8	155.54
(1,162)	2:180:B:SER:N	2:180:B:SER:CA	2:180:B:SER:C	2:181:B:SER:N	2	154.39
(1,72)	2:157:B:GLU:N	2:157:B:GLU:CA	2:157:B:GLU:C	2:158:B:LEU:N	8	153.48
(1,150)	2:177:B:ASP:N	2:177:B:ASP:CA	2:177:B:ASP:C	2:178:B:GLU:N	10	153.29
(1,150)	2:177:B:ASP:N	2:177:B:ASP:CA	2:177:B:ASP:C	2:178:B:GLU:N	7	153.13
(1,158)	2:179:B:ASP:N	2:179:B:ASP:CA	2:179:B:ASP:C	2:180:B:SER:N	3	152.94
(1,158)	2:179:B:ASP:N	2:179:B:ASP:CA	2:179:B:ASP:C	2:180:B:SER:N	9	152.91