wwPDB NMR Structure Validation Summary Report (i)

Jun 4, 2023 – 08:48 PM EDT

PDB ID	:	2LW1
BMRB ID	:	17989
Title	:	The C-terminal domain of the Uup protein is a DNA-binding coiled coil motif
Authors	:	Carlier, L.; Haase, A.S.; Burgos Zepeda, M.Y.; Dassa, E.; Lequin, O.
Deposited on	:	2012-07-19

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 (i) 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 (1)) were used in the production of this report:

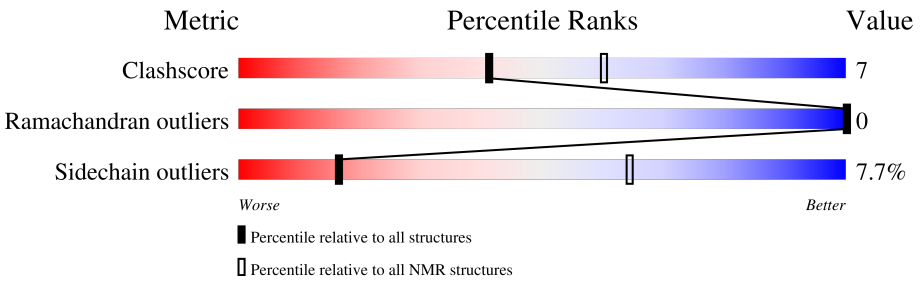
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 94%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	108	55% 10% 14% 21%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:563-A:632 (70)	0.51	18

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 6 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1358 atoms, of which 674 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ABC transporter ATP-binding protein uup.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	85	1358	428	674	115	140	1	0

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: ABC transporter ATP-binding protein uup

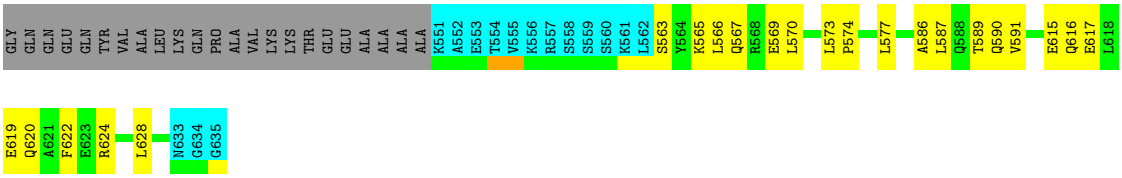
Chain A: 55% 10% 14% 21%

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

The representative model is number 18. Colouring as in section 4.1 above.

• Molecule 1: ABC transporter ATP-binding protein uup

Chain A: 44% 20% 14% 21%



5 Refinement protocol and experimental data overview (i)

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

Of the 400 calculated structures, 20 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
TopSpin	geometry optimization	2.0
ARIA	structure solution	2.2
CNS	structure solution	1.1
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	1362
Number of shifts mapped to atoms	1096
Number of unparsed shifts	0
Number of shifts with mapping errors	266
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

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	575	557	556	8±2
All	All	11500	11140	11120	167

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 7.

5 of 65 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:563:SER:HB2	1:A:566:LEU:HD13	0.70	1.64	3	1
1:A:590:GLN:HE21	1:A:590:GLN:HA	0.69	1.47	6	1
1:A:600:PRO:HD2	1:A:603:GLN:HG2	0.67	1.63	10	2
1:A:565:LYS:O	1:A:569:GLU:HB2	0.67	1.90	2	12
1:A:624:ARG:O	1:A:628:LEU:HG	0.66	1.91	7	19

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	70/108 (65%)	70±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	1400/2160 (65%)	1398 (100%)	2 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	60/88 (68%)	55±1 (92±2%)	5±1 (8±2%)	16	64
All	All	1200/1760 (68%)	1108 (92%)	92 (8%)	16	64

5 of 23 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	577	LEU	20
1	A	622	PHE	20
1	A	568	ARG	13
1	A	603	GLN	7
1	A	570	LEU	6

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 94% for the well-defined parts and 93% 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 (i)

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

Total number of shifts	1362
Number of shifts mapped to atoms	1096
Number of unparsed shifts	0
Number of shifts with mapping errors	266
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 266) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	528	GLY	H	8.44	0.02	1
1	A	528	GLY	HA2	3.97	0.02	1
1	A	528	GLY	HA3	3.97	0.02	1
1	A	528	GLY	C	174.19	0.1	1
1	A	528	GLY	CA	45.39	0.1	1
1	A	528	GLY	N	110.14	0.1	1
1	A	529	GLN	H	8.25	0.02	1
1	A	529	GLN	HA	4.33	0.02	1
1	A	529	GLN	HB2	2.12	0.02	2
1	A	529	GLN	HB3	1.99	0.02	2
1	A	529	GLN	HG2	2.35	0.02	1
1	A	529	GLN	HG3	2.35	0.02	1
1	A	529	GLN	C	176.22	0.1	1
1	A	529	GLN	CA	56.17	0.1	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	529	GLN	CB	29.41	0.1	1
1	A	529	GLN	CG	33.82	0.1	1
1	A	529	GLN	N	119.93	0.1	1
1	A	530	GLN	H	8.46	0.02	1
1	A	530	GLN	HA	4.3	0.02	1
1	A	530	GLN	HB2	2.11	0.02	2
1	A	530	GLN	HB3	1.99	0.02	2
1	A	530	GLN	HG2	2.37	0.02	1
1	A	530	GLN	HG3	2.37	0.02	1
1	A	530	GLN	C	176.21	0.1	1
1	A	530	GLN	CA	56.37	0.1	1
1	A	530	GLN	CB	29.38	0.1	1
1	A	530	GLN	CG	33.86	0.1	1
1	A	530	GLN	N	121.27	0.1	1
1	A	531	GLU	H	8.47	0.02	1
1	A	531	GLU	HA	4.21	0.02	1
1	A	531	GLU	HB2	2.02	0.02	2
1	A	531	GLU	HB3	1.92	0.02	2
1	A	531	GLU	HG2	2.24	0.02	1
1	A	531	GLU	HG3	2.24	0.02	1
1	A	531	GLU	C	176.51	0.1	1
1	A	531	GLU	CA	57.1	0.1	1
1	A	531	GLU	CB	30.09	0.1	1
1	A	531	GLU	CG	36.32	0.1	1
1	A	531	GLU	N	121.99	0.1	1
1	A	532	GLN	H	8.31	0.02	1
1	A	532	GLN	HA	4.24	0.02	1
1	A	532	GLN	HB2	1.91	0.02	2
1	A	532	GLN	HB3	1.99	0.02	2
1	A	532	GLN	HG2	2.23	0.02	1
1	A	532	GLN	HG3	2.23	0.02	1
1	A	532	GLN	C	175.66	0.1	1
1	A	532	GLN	CA	56.07	0.1	1
1	A	532	GLN	CB	29.45	0.1	1
1	A	532	GLN	CG	33.68	0.1	1
1	A	532	GLN	N	120.57	0.1	1
1	A	533	TYR	H	8.16	0.02	1
1	A	533	TYR	HA	4.55	0.02	1
1	A	533	TYR	HB2	2.96	0.02	2
1	A	533	TYR	HB3	3.04	0.02	2
1	A	533	TYR	C	175.66	0.1	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	533	TYR	CA	58.19	0.1	1
1	A	533	TYR	CB	38.64	0.1	1
1	A	533	TYR	N	121.34	0.1	1
1	A	534	VAL	H	7.85	0.02	1
1	A	534	VAL	HA	3.98	0.02	1
1	A	534	VAL	HB	1.97	0.02	1
1	A	534	VAL	HG11	0.89	0.02	1
1	A	534	VAL	HG12	0.89	0.02	1
1	A	534	VAL	HG13	0.89	0.02	1
1	A	534	VAL	HG21	0.89	0.02	1
1	A	534	VAL	HG22	0.89	0.02	1
1	A	534	VAL	HG23	0.89	0.02	1
1	A	534	VAL	C	175.36	0.1	1
1	A	534	VAL	CA	62.35	0.1	1
1	A	534	VAL	CB	32.89	0.1	1
1	A	534	VAL	CG1	20.53	0.1	2
1	A	534	VAL	CG2	20.94	0.1	2
1	A	534	VAL	N	122.84	0.1	1
1	A	535	ALA	H	8.17	0.02	1
1	A	535	ALA	HA	4.23	0.02	1
1	A	535	ALA	HB1	1.37	0.02	1
1	A	535	ALA	HB2	1.37	0.02	1
1	A	535	ALA	HB3	1.37	0.02	1
1	A	535	ALA	C	177.54	0.1	1
1	A	535	ALA	CA	52.48	0.1	1
1	A	535	ALA	CB	19.1	0.1	1
1	A	535	ALA	N	127.19	0.1	1
1	A	536	LEU	H	8.03	0.02	1
1	A	536	LEU	HA	4.29	0.02	1
1	A	536	LEU	HB2	1.56	0.02	2
1	A	536	LEU	HB3	1.62	0.02	2
1	A	536	LEU	HG	1.58	0.02	1
1	A	536	LEU	HD11	0.89	0.02	1
1	A	536	LEU	HD12	0.89	0.02	1
1	A	536	LEU	HD13	0.89	0.02	1
1	A	536	LEU	HD21	0.89	0.02	1
1	A	536	LEU	HD22	0.89	0.02	1
1	A	536	LEU	HD23	0.89	0.02	1
1	A	536	LEU	C	177.25	0.1	1
1	A	536	LEU	CA	55.16	0.1	1
1	A	536	LEU	CB	42.46	0.1	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	536	LEU	CG	26.92	0.1	1
1	A	536	LEU	CD1	24.84	0.1	2
1	A	536	LEU	CD2	23.55	0.1	2
1	A	536	LEU	N	121.27	0.1	1
1	A	537	LYS	H	8.19	0.02	1
1	A	537	LYS	HA	4.29	0.02	1
1	A	537	LYS	HB2	1.79	0.02	2
1	A	537	LYS	HB3	1.74	0.02	2
1	A	537	LYS	HG2	1.39	0.02	1
1	A	537	LYS	HG3	1.39	0.02	1
1	A	537	LYS	HD2	1.69	0.02	1
1	A	537	LYS	HD3	1.69	0.02	1
1	A	537	LYS	HE2	2.98	0.02	1
1	A	537	LYS	HE3	2.98	0.02	1
1	A	537	LYS	C	176.18	0.1	1
1	A	537	LYS	CA	56.11	0.1	1
1	A	537	LYS	CB	32.96	0.1	1
1	A	537	LYS	CG	24.71	0.1	1
1	A	537	LYS	CD	29.01	0.1	1
1	A	537	LYS	CE	42.24	0.1	1
1	A	537	LYS	N	122.14	0.1	1
1	A	538	GLN	H	8.3	0.02	1
1	A	538	GLN	HA	4.33	0.02	1
1	A	538	GLN	HB2	1.92	0.02	2
1	A	538	GLN	HB3	2.12	0.02	2
1	A	538	GLN	HG2	2.37	0.02	1
1	A	538	GLN	HG3	2.37	0.02	1
1	A	538	GLN	C	173.86	0.1	1
1	A	538	GLN	CA	53.69	0.1	1
1	A	538	GLN	CB	28.96	0.1	1
1	A	538	GLN	N	122.55	0.1	1
1	A	539	PRO	HA	4.39	0.02	1
1	A	539	PRO	HB2	2.29	0.02	2
1	A	539	PRO	HB3	1.89	0.02	2
1	A	539	PRO	HG2	1.97	0.02	2
1	A	539	PRO	HG3	2.04	0.02	2
1	A	539	PRO	HD2	3.66	0.02	2
1	A	539	PRO	HD3	3.73	0.02	2
1	A	539	PRO	C	176.49	0.1	1
1	A	539	PRO	CA	63.17	0.1	1
1	A	539	PRO	CB	32.03	0.1	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	539	PRO	CG	27.29	0.1	1
1	A	539	PRO	CD	50.77	0.1	1
1	A	540	ALA	H	8.37	0.02	1
1	A	540	ALA	HA	4.31	0.02	1
1	A	540	ALA	HB1	1.37	0.02	1
1	A	540	ALA	HB2	1.37	0.02	1
1	A	540	ALA	HB3	1.37	0.02	1
1	A	540	ALA	C	177.76	0.1	1
1	A	540	ALA	CA	52.48	0.1	1
1	A	540	ALA	CB	19.25	0.1	1
1	A	540	ALA	N	124.44	0.1	1
1	A	541	VAL	H	8.05	0.02	1
1	A	541	VAL	HA	4.07	0.02	1
1	A	541	VAL	HB	2.03	0.02	1
1	A	541	VAL	HG11	0.93	0.02	1
1	A	541	VAL	HG12	0.93	0.02	1
1	A	541	VAL	HG13	0.93	0.02	1
1	A	541	VAL	HG21	0.93	0.02	1
1	A	541	VAL	HG22	0.93	0.02	1
1	A	541	VAL	HG23	0.93	0.02	1
1	A	541	VAL	C	176.06	0.1	1
1	A	541	VAL	CA	62.25	0.1	1
1	A	541	VAL	CB	32.83	0.1	1
1	A	541	VAL	CG1	20.84	0.1	2
1	A	541	VAL	CG2	21.08	0.1	2
1	A	541	VAL	N	119.72	0.1	1
1	A	542	LYS	H	8.36	0.02	1
1	A	542	LYS	HA	4.32	0.02	1
1	A	542	LYS	HB2	1.81	0.02	2
1	A	542	LYS	HB3	1.77	0.02	2
1	A	542	LYS	HG2	1.42	0.02	1
1	A	542	LYS	HG3	1.42	0.02	1
1	A	542	LYS	HD2	1.72	0.02	1
1	A	542	LYS	HD3	1.72	0.02	1
1	A	542	LYS	HE2	2.99	0.02	1
1	A	542	LYS	HE3	2.99	0.02	1
1	A	542	LYS	C	176.47	0.1	1
1	A	542	LYS	CA	56.29	0.1	1
1	A	542	LYS	CB	33.06	0.1	1
1	A	542	LYS	CG	24.7	0.1	1
1	A	542	LYS	CD	29.05	0.1	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	542	LYS	CE	42.17	0.1	1
1	A	542	LYS	N	125.63	0.1	1
1	A	543	LYS	H	8.44	0.02	1
1	A	543	LYS	HA	4.36	0.02	1
1	A	543	LYS	HB2	1.85	0.02	2
1	A	543	LYS	HB3	1.71	0.02	2
1	A	543	LYS	HG2	1.44	0.02	2
1	A	543	LYS	HG3	1.41	0.02	2
1	A	543	LYS	HD2	1.71	0.02	1
1	A	543	LYS	HD3	1.71	0.02	1
1	A	543	LYS	HE2	3.0	0.02	1
1	A	543	LYS	HE3	3.0	0.02	1
1	A	543	LYS	C	176.96	0.1	1
1	A	543	LYS	CA	56.44	0.1	1
1	A	543	LYS	CB	33.07	0.1	1
1	A	543	LYS	CG	24.7	0.1	1
1	A	543	LYS	CD	29.07	0.1	1
1	A	543	LYS	CE	42.19	0.1	1
1	A	543	LYS	N	123.73	0.1	1
1	A	544	THR	H	8.18	0.02	1
1	A	544	THR	HA	4.25	0.02	1
1	A	544	THR	HB	4.21	0.02	1
1	A	544	THR	HG21	1.2	0.02	1
1	A	544	THR	HG22	1.2	0.02	1
1	A	544	THR	HG23	1.2	0.02	1
1	A	544	THR	C	174.78	0.1	1
1	A	544	THR	CA	62.36	0.1	1
1	A	544	THR	CB	69.77	0.1	1
1	A	544	THR	CG2	21.69	0.1	1
1	A	544	THR	N	115.9	0.1	1
1	A	545	GLU	H	8.48	0.02	1
1	A	545	GLU	HA	4.31	0.02	1
1	A	545	GLU	HB2	1.97	0.02	2
1	A	545	GLU	HB3	2.03	0.02	2
1	A	545	GLU	HG2	2.27	0.02	1
1	A	545	GLU	HG3	2.27	0.02	1
1	A	545	GLU	C	176.79	0.1	1
1	A	545	GLU	CA	56.89	0.1	1
1	A	545	GLU	CB	30.23	0.1	1
1	A	545	GLU	CG	36.29	0.1	1
1	A	545	GLU	N	123.17	0.1	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	546	GLU	H	8.39	0.02	1
1	A	546	GLU	HA	4.22	0.02	1
1	A	546	GLU	HB2	2.03	0.02	2
1	A	546	GLU	HB3	1.97	0.02	2
1	A	546	GLU	HG2	2.28	0.02	1
1	A	546	GLU	HG3	2.28	0.02	1
1	A	546	GLU	C	176.75	0.1	1
1	A	546	GLU	CA	57.05	0.1	1
1	A	546	GLU	CB	30.25	0.1	1
1	A	546	GLU	CG	36.34	0.1	1
1	A	546	GLU	N	122.22	0.1	1
1	A	547	ALA	H	8.3	0.02	1
1	A	547	ALA	HA	4.27	0.02	1
1	A	547	ALA	HB1	1.41	0.02	1
1	A	547	ALA	HB2	1.41	0.02	1
1	A	547	ALA	HB3	1.41	0.02	1
1	A	547	ALA	C	178.02	0.1	1
1	A	547	ALA	CA	52.94	0.1	1
1	A	547	ALA	CB	19.0	0.1	1
1	A	547	ALA	N	124.9	0.1	1
1	A	548	ALA	H	8.17	0.02	1
1	A	548	ALA	HA	4.21	0.02	1
1	A	548	ALA	HB1	1.41	0.02	1
1	A	548	ALA	HB2	1.41	0.02	1
1	A	548	ALA	HB3	1.41	0.02	1
1	A	548	ALA	C	178.09	0.1	1
1	A	548	ALA	CA	52.83	0.1	1
1	A	548	ALA	CB	19.12	0.1	1
1	A	548	ALA	N	122.82	0.1	1
1	A	549	ALA	H	8.1	0.02	1
1	A	549	ALA	HA	4.28	0.02	1
1	A	549	ALA	HB1	1.41	0.02	1
1	A	549	ALA	HB2	1.41	0.02	1
1	A	549	ALA	HB3	1.41	0.02	1
1	A	549	ALA	C	177.91	0.1	1
1	A	549	ALA	CA	52.84	0.1	1
1	A	549	ALA	CB	18.97	0.1	1
1	A	549	ALA	N	122.68	0.1	1
1	A	550	ALA	H	8.08	0.02	1
1	A	550	ALA	HA	4.27	0.02	1
1	A	550	ALA	HB1	1.4	0.02	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	550	ALA	HB2	1.4	0.02	1
1	A	550	ALA	HB3	1.4	0.02	1
1	A	550	ALA	C	178.1	0.1	1
1	A	550	ALA	CA	52.75	0.1	1
1	A	550	ALA	CB	19.09	0.1	1
1	A	550	ALA	N	122.67	0.1	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	108	-0.59 ± 0.11	Should be checked
$^{13}C_{\beta}$	105	0.14 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	106	-0.64 ± 0.11	Should be applied
^{15}N	102	-0.63 ± 0.22	Should be applied

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 94%, i.e. 925 atoms were assigned a chemical shift out of a possible 984. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	343/346 (99%)	137/138 (99%)	139/140 (99%)	67/68 (99%)
Sidechain	520/570 (91%)	355/367 (97%)	156/183 (85%)	9/20 (45%)
Aromatic	62/68 (91%)	31/33 (94%)	30/32 (94%)	1/3 (33%)
Overall	925/984 (94%)	523/538 (97%)	325/355 (92%)	77/91 (85%)

7.1.4 Statistically unusual chemical shifts (i)

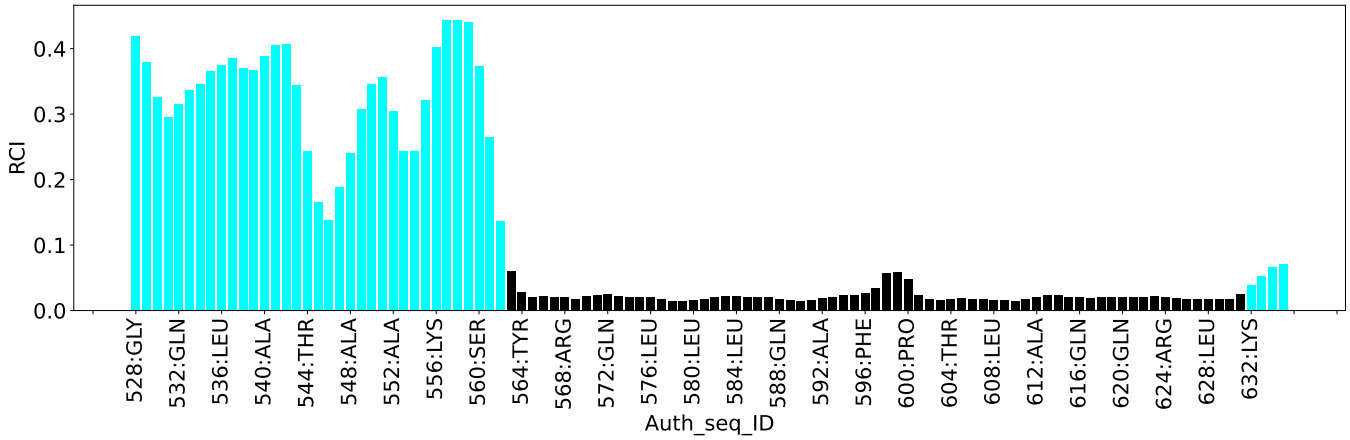
There are no statistically unusual chemical shifts.

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 (i)

8.1 Conformationally restricting restraints (i)

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	2215
Intra-residue (|i-j|=0)	802
Sequential (|i-j|=1)	424
Medium range (|i-j|>1 and |i-j|<5)	594
Long range (|i-j|≥5)	355
Inter-chain	0
Hydrogen bond restraints	40
Disulfide bond restraints	0
Total dihedral-angle restraints	158
Number of unmapped restraints	0
Number of restraints per residue	22.0
Number of long range restraints per residue[1]	3.3

[1]Long 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 (i)

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 (i)

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)	35.5	0.2
0.2-0.5 (Medium)	35.8	0.5
>0.5 (Large)	40.5	2.59

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)	4.3	4.6
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

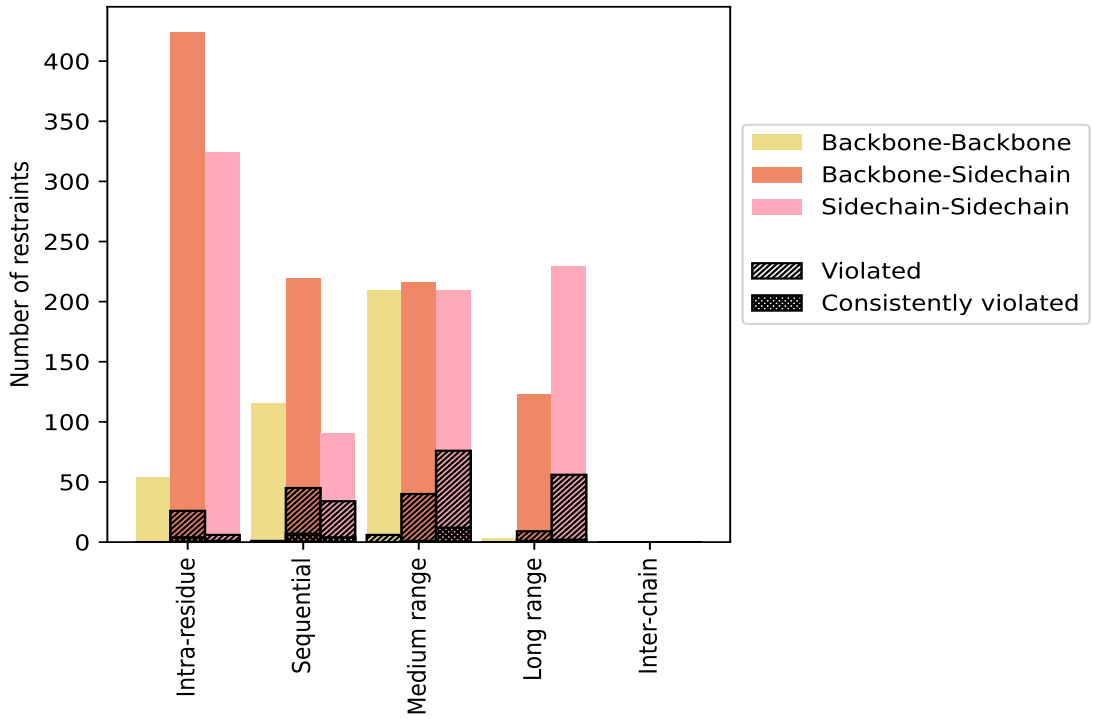
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	802	36.2	32	4.0	1.4	5	0.6	0.2
Backbone-Backbone	54	2.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	424	19.1	26	6.1	1.2	4	0.9	0.2
Sidechain-Sidechain	324	14.6	6	1.9	0.3	1	0.3	0.0
Sequential (|i-j|=1)	424	19.1	80	18.9	3.6	11	2.6	0.5
Backbone-Backbone	115	5.2	1	0.9	0.0	0	0.0	0.0
Backbone-Sidechain	219	9.9	45	20.5	2.0	7	3.2	0.3
Sidechain-Sidechain	90	4.1	34	37.8	1.5	4	4.4	0.2
Medium range (|i-j|>1 & |i-j|<5)	594	26.8	120	20.2	5.4	13	2.2	0.6
Backbone-Backbone	169	7.6	4	2.4	0.2	0	0.0	0.0
Backbone-Sidechain	216	9.8	40	18.5	1.8	1	0.5	0.0
Sidechain-Sidechain	209	9.4	76	36.4	3.4	12	5.7	0.5
Long range (|i-j|≥5)	355	16.0	65	18.3	2.9	3	0.8	0.1
Backbone-Backbone	3	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	123	5.6	9	7.3	0.4	1	0.8	0.0
Sidechain-Sidechain	229	10.3	56	24.5	2.5	2	0.9	0.1
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	40	1.8	2	5.0	0.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2215	100.0	299	13.5	13.5	32	1.4	1.4
Backbone-Backbone	381	17.2	7	1.8	0.3	0	0.0	0.0
Backbone-Sidechain	982	44.3	120	12.2	5.4	13	1.3	0.6
Sidechain-Sidechain	852	38.5	172	20.2	7.8	19	2.2	0.9

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

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



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and 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	16	34	56	24	0	130	0.51	1.82	0.43	0.34
2	13	34	45	22	0	114	0.52	2.05	0.44	0.37
3	13	32	45	17	0	107	0.47	1.68	0.38	0.35
4	16	27	36	20	0	99	0.44	1.71	0.37	0.3
5	10	37	45	24	0	116	0.6	2.43	0.49	0.44
6	13	33	51	17	0	114	0.47	1.63	0.38	0.32
7	12	30	46	25	0	113	0.54	2.21	0.45	0.4
8	11	34	42	22	0	109	0.45	1.93	0.39	0.28
9	18	32	47	19	0	116	0.44	1.74	0.36	0.31
10	11	37	54	28	0	130	0.6	2.39	0.5	0.45
11	12	36	43	21	0	112	0.51	2.16	0.43	0.36

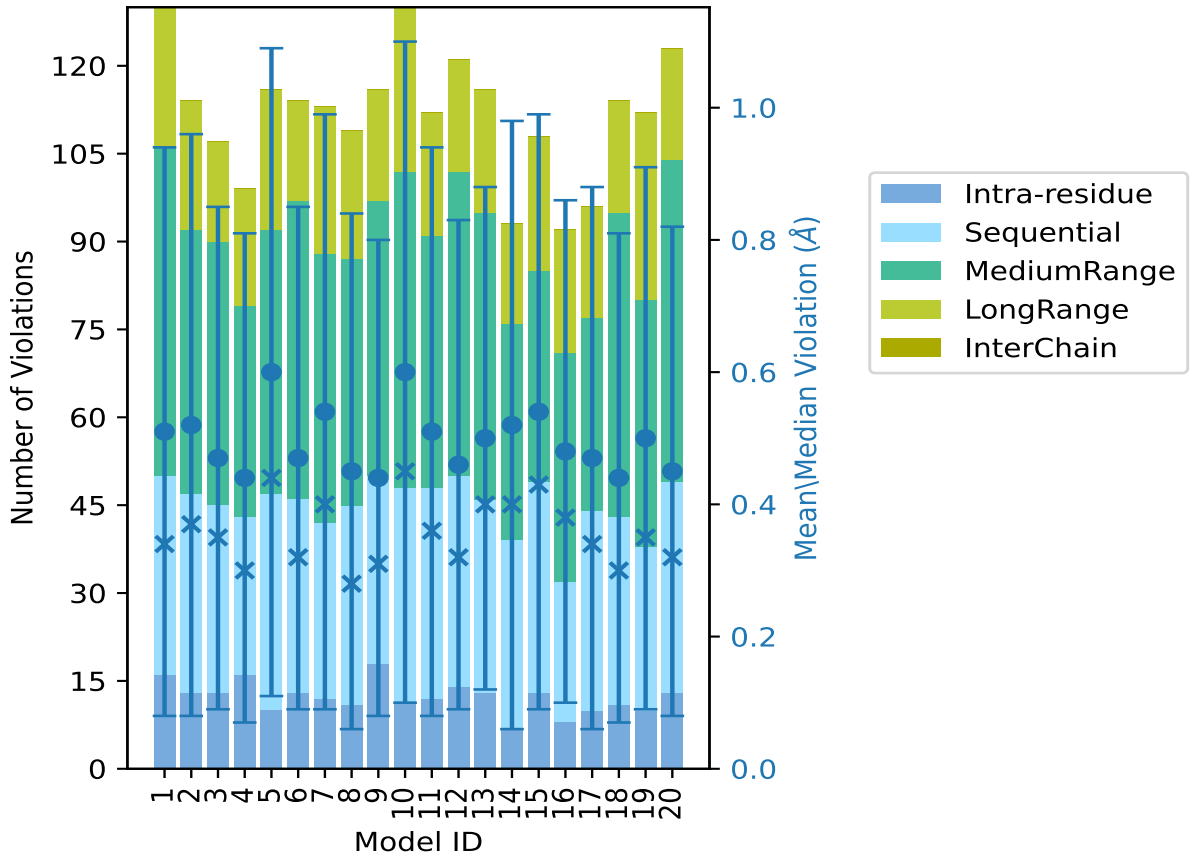
Continued on next page...

Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	14	36	52	19	0	121	0.46	1.7	0.37	0.32
13	13	33	49	21	0	116	0.5	1.86	0.38	0.4
14	7	32	37	17	0	93	0.52	2.59	0.46	0.4
15	13	36	36	23	0	108	0.54	2.17	0.45	0.43
16	8	24	39	21	0	92	0.48	1.62	0.38	0.38
17	10	34	33	19	0	96	0.47	2.02	0.41	0.34
18	11	32	52	19	0	114	0.44	1.61	0.37	0.3
19	10	28	42	32	0	112	0.5	1.96	0.41	0.35
20	13	36	55	19	0	123	0.45	1.71	0.37	0.32

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard 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

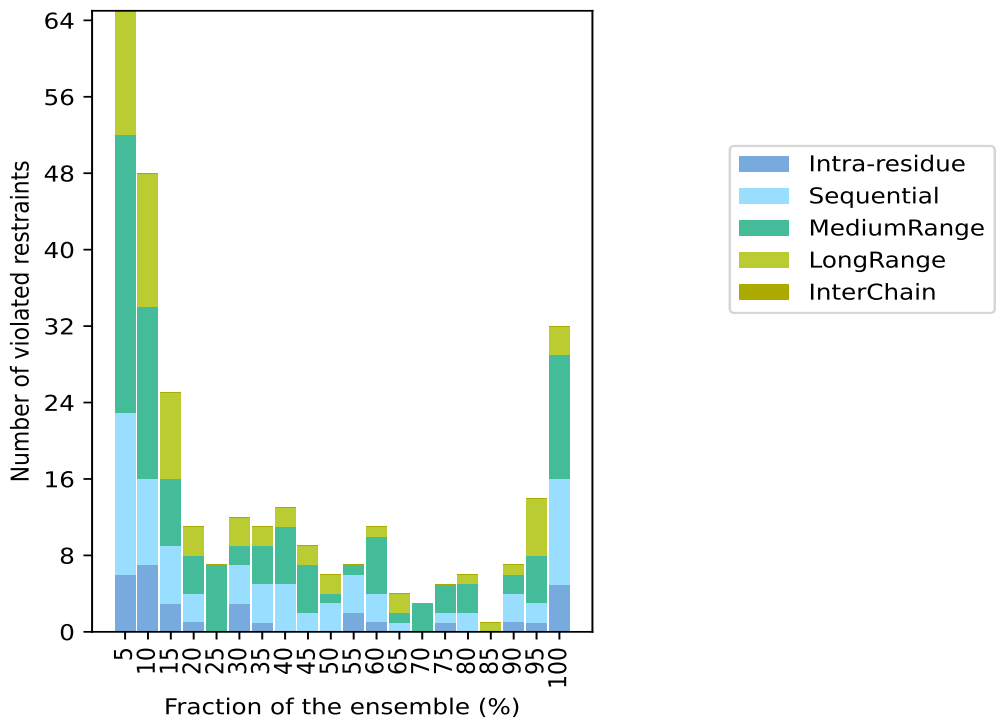
9.3 Distance violation statistics for the ensemble (i)

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, 1878(IR:770, SQ:344, MR:474, LR:290, 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]	%
6	17	29	13	0	65	1	5.0
7	9	18	14	0	48	2	10.0
3	6	7	9	0	25	3	15.0
1	3	4	3	0	11	4	20.0
0	0	7	0	0	7	5	25.0
3	4	2	3	0	12	6	30.0
1	4	4	2	0	11	7	35.0
0	5	6	2	0	13	8	40.0
0	2	5	2	0	9	9	45.0
0	3	1	2	0	6	10	50.0
2	4	1	0	0	7	11	55.0
1	3	6	1	0	11	12	60.0
0	1	1	2	0	4	13	65.0
0	0	3	0	0	3	14	70.0
1	1	3	0	0	5	15	75.0
0	2	3	1	0	6	16	80.0
0	0	0	1	0	1	17	85.0
1	3	2	1	0	7	18	90.0
1	2	5	6	0	14	19	95.0
5	11	13	3	0	32	20	100.0

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

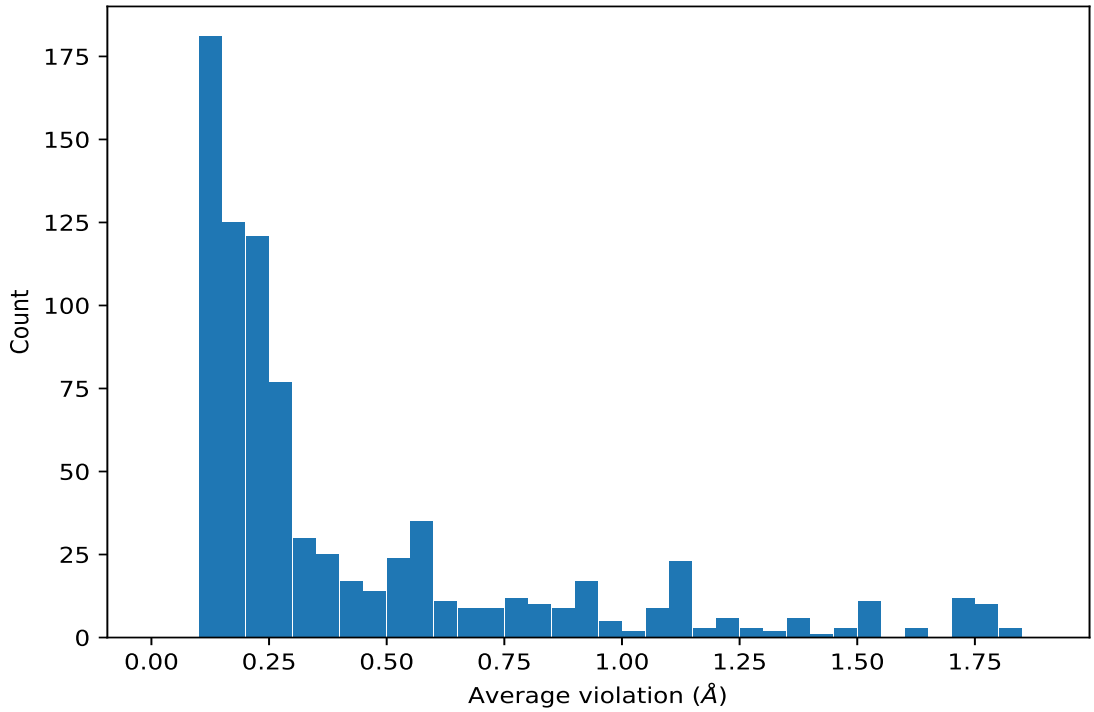
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,1385)	1:A:622:PHE:HB2	1:A:625:TRP:HB2	20	1.51	0.11	1.52
(1,611)	1:A:625:TRP:HH2	1:A:626:GLU:HG3	20	1.4	0.13	1.41
(1,1969)	1:A:579:ASP:HB3	1:A:575:GLN:HB2	20	1.38	0.1	1.38
(1,1969)	1:A:579:ASP:HB3	1:A:578:GLU:HB2	20	1.38	0.1	1.38
(1,1969)	1:A:579:ASP:HB3	1:A:578:GLU:HB3	20	1.38	0.1	1.38
(1,1069)	1:A:579:ASP:HB2	1:A:583:LYS:HB2	20	1.34	0.06	1.33
(1,1069)	1:A:579:ASP:HB2	1:A:583:LYS:HB3	20	1.34	0.06	1.33
(1,1930)	1:A:556:LYS:HB3	1:A:555:VAL:HB	20	1.25	0.44	1.17
(1,1930)	1:A:565:LYS:HB3	1:A:569:GLU:HG3	20	1.25	0.44	1.17
(1,1930)	1:A:565:LYS:HB3	1:A:569:GLU:HB3	20	1.25	0.44	1.17
(1,1936)	1:A:588:GLN:HG3	1:A:591:VAL:HG22	20	1.11	0.07	1.12
(1,1936)	1:A:588:GLN:HG3	1:A:591:VAL:HG21	20	1.11	0.07	1.12
(1,1936)	1:A:588:GLN:HG3	1:A:591:VAL:HG23	20	1.11	0.07	1.12
(1,1936)	1:A:588:GLN:HG3	1:A:591:VAL:HG12	20	1.11	0.07	1.12
(1,1936)	1:A:588:GLN:HG3	1:A:591:VAL:HG11	20	1.11	0.07	1.12
(1,1936)	1:A:588:GLN:HG3	1:A:591:VAL:HG13	20	1.11	0.07	1.12

Continued on next page...

Continued from previous page...

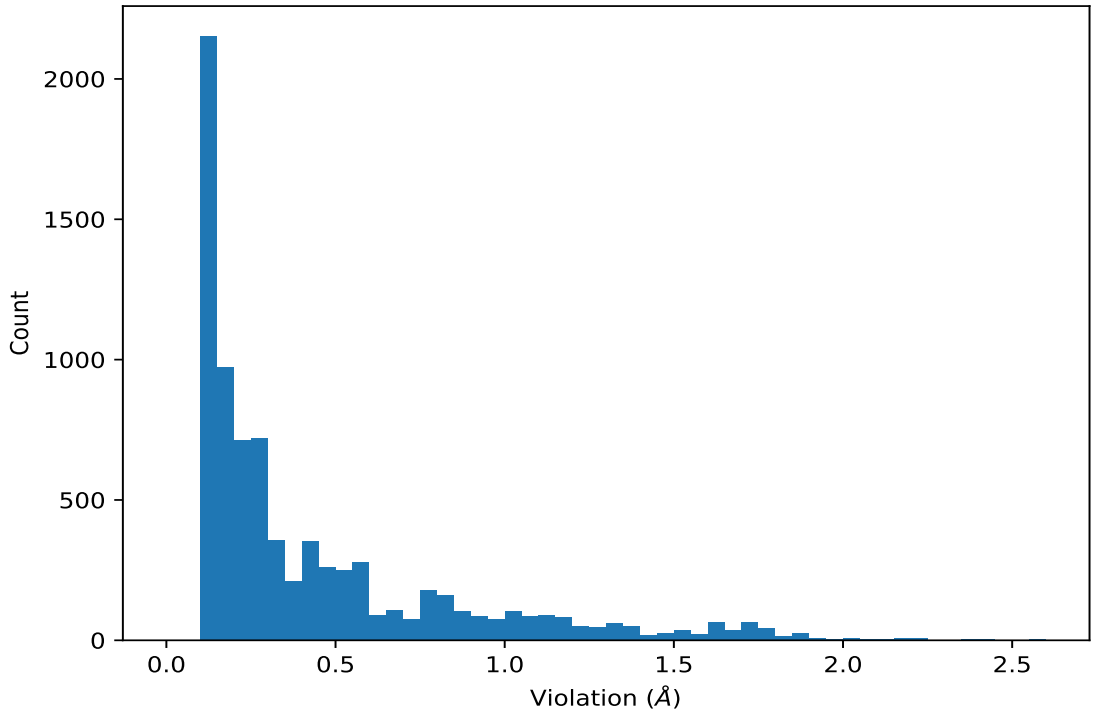
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1252)	1:A:580:LEU:HA	1:A:579:ASP:HB2	20	1.03	0.03	1.03
(1,43)	1:A:597:PHE:H	1:A:596:PHE:HB2	20	0.89	0.05	0.9
(1,2074)	1:A:574:PRO:HD3	1:A:576:LEU:HB2	20	0.86	0.07	0.85
(1,2074)	1:A:576:LEU:HB2	1:A:574:PRO:HA	20	0.86	0.07	0.85
(1,1393)	1:A:630:ALA:HB2	1:A:626:GLU:HB2	20	0.76	0.12	0.71

[1]Number of violated models, [2]Standard 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)
(1,1363)	1:A:562:LEU:HD22	1:A:631:LEU:HB2	14	2.59
(1,1363)	1:A:562:LEU:HD21	1:A:631:LEU:HB2	14	2.59
(1,1363)	1:A:562:LEU:HD23	1:A:631:LEU:HB2	14	2.59
(1,1363)	1:A:562:LEU:HD22	1:A:631:LEU:HB2	5	2.43
(1,1363)	1:A:562:LEU:HD21	1:A:631:LEU:HB2	5	2.43
(1,1363)	1:A:562:LEU:HD23	1:A:631:LEU:HB2	5	2.43
(1,929)	1:A:565:LYS:HG2	1:A:566:LEU:HD12	10	2.39
(1,929)	1:A:565:LYS:HG2	1:A:566:LEU:HD11	10	2.39
(1,929)	1:A:565:LYS:HG2	1:A:566:LEU:HD13	10	2.39
(1,1307)	1:A:566:LEU:HD12	1:A:565:LYS:HA	5	2.21
(1,1307)	1:A:566:LEU:HD11	1:A:565:LYS:HA	5	2.21
(1,1307)	1:A:566:LEU:HD13	1:A:565:LYS:HA	5	2.21
(1,1307)	1:A:566:LEU:HD12	1:A:565:LYS:HA	7	2.21
(1,1307)	1:A:566:LEU:HD11	1:A:565:LYS:HA	7	2.21
(1,1307)	1:A:566:LEU:HD13	1:A:565:LYS:HA	7	2.21
(1,1307)	1:A:566:LEU:HD12	1:A:565:LYS:HA	15	2.17
(1,1307)	1:A:566:LEU:HD11	1:A:565:LYS:HA	15	2.17
(1,1307)	1:A:566:LEU:HD13	1:A:565:LYS:HA	15	2.17
(1,1307)	1:A:566:LEU:HD12	1:A:565:LYS:HA	11	2.16
(1,1307)	1:A:566:LEU:HD11	1:A:565:LYS:HA	11	2.16
(1,1307)	1:A:566:LEU:HD13	1:A:565:LYS:HA	11	2.16
(1,938)	1:A:631:LEU:HG	1:A:562:LEU:HD22	5	2.14
(1,938)	1:A:631:LEU:HG	1:A:562:LEU:HD21	5	2.14
(1,938)	1:A:631:LEU:HG	1:A:562:LEU:HD23	5	2.14
(1,1309)	1:A:573:LEU:HD22	1:A:576:LEU:HB2	10	2.09
(1,1309)	1:A:573:LEU:HD21	1:A:576:LEU:HB2	10	2.09
(1,1309)	1:A:573:LEU:HD23	1:A:576:LEU:HB2	10	2.09
(1,1307)	1:A:566:LEU:HD12	1:A:565:LYS:HA	2	2.05

10 Dihedral-angle violation analysis (i)

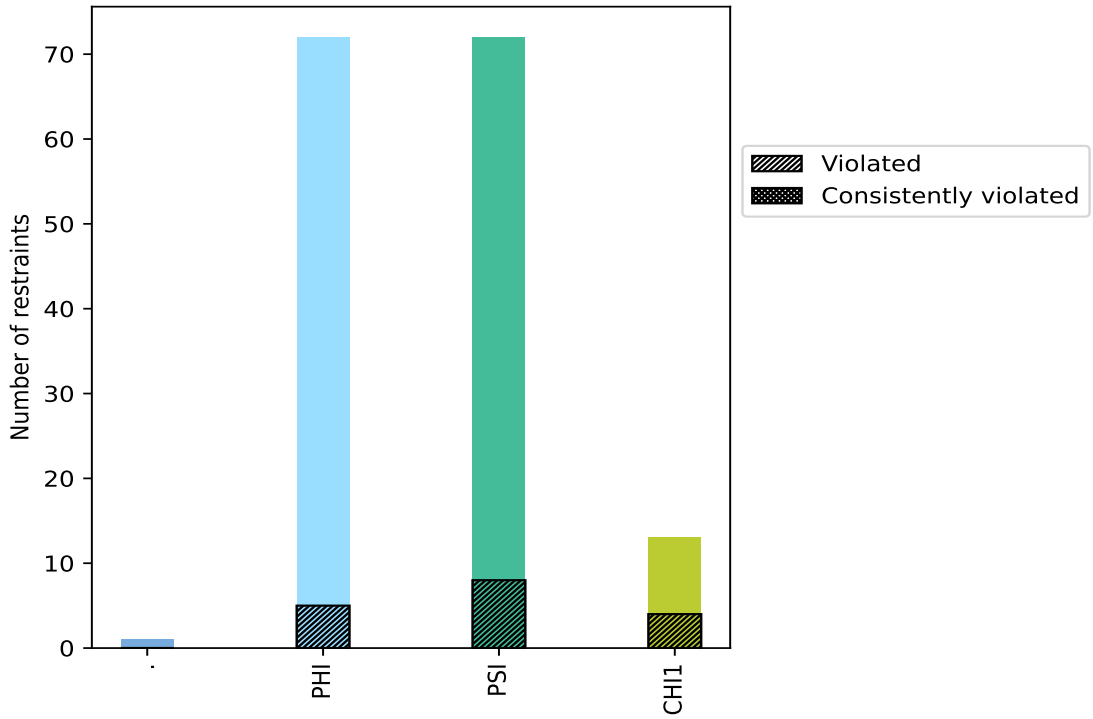
10.1 Summary of dihedral-angle violations (i)

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]
.	1	0.6	0	0.0	0.0	0	0.0	0.0
PHI	72	45.6	5	6.9	3.2	0	0.0	0.0
PSI	72	45.6	8	11.1	5.1	0	0.0	0.0
CHI1	13	8.2	4	30.8	2.5	0	0.0	0.0
Total	158	100.0	17	10.8	10.8	0	0.0	0.0

[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)



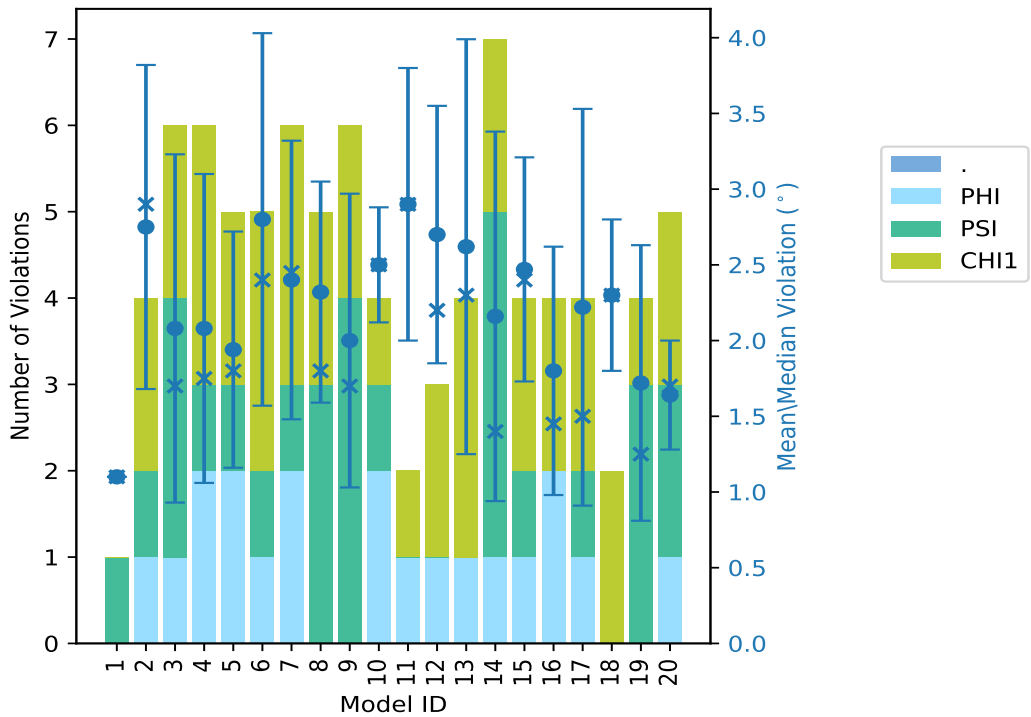
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	.	PHI	PSI	CHI1	Total				
1	0	0	1	0	1	1.1	1.1	0.0	1.1
2	0	1	1	2	4	2.75	4.1	1.07	2.9
3	0	1	3	2	6	2.08	4.6	1.15	1.7
4	0	2	1	3	6	2.08	3.8	1.02	1.75
5	0	2	1	2	5	1.94	3.4	0.78	1.8
6	0	1	1	3	5	2.8	4.4	1.23	2.4
7	0	2	1	3	6	2.4	4.0	0.92	2.45
8	0	0	3	2	5	2.32	3.4	0.73	1.8
9	0	0	4	2	6	2.0	4.0	0.97	1.7
10	0	2	1	1	4	2.5	3.0	0.38	2.5
11	0	1	0	1	2	2.9	3.8	0.9	2.9
12	0	1	0	2	3	2.7	3.9	0.85	2.2
13	0	1	0	3	4	2.62	4.6	1.37	2.3
14	0	1	4	2	7	2.16	4.3	1.22	1.4
15	0	1	1	2	4	2.47	3.4	0.74	2.4
16	0	2	0	2	4	1.8	3.2	0.82	1.45
17	0	1	1	2	4	2.22	4.5	1.31	1.5
18	0	0	0	2	2	2.3	2.8	0.5	2.3
19	0	0	3	1	4	1.72	3.3	0.91	1.25
20	0	1	2	2	5	1.64	2.2	0.36	1.7

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	CHI1	Total	Count[1]	%
0	1	3	1	5	1	5.0
0	0	2	0	2	2	10.0
0	1	0	0	1	3	15.0
0	2	0	0	2	4	20.0
0	0	0	0	0	5	25.0
0	0	1	1	2	6	30.0
0	0	1	0	1	7	35.0
0	1	1	0	2	8	40.0
0	0	0	0	0	9	45.0
0	0	0	0	0	10	50.0
0	0	0	0	0	11	55.0

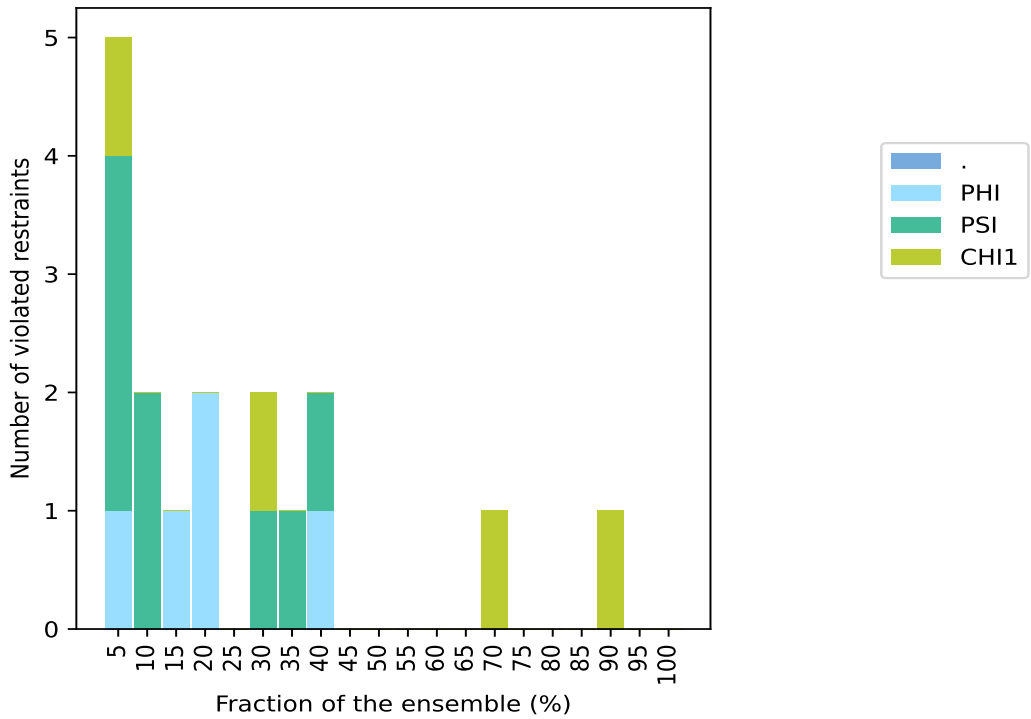
Continued on next page...

Continued from previous page...

Number of violated restraints					Fraction of the ensemble	
.	PHI	PSI	CHI1	Total	Count[1]	%
0	0	0	0	0	12	60.0
0	0	0	0	0	13	65.0
0	0	0	1	1	14	70.0
0	0	0	0	0	15	75.0
0	0	0	0	0	16	80.0
0	0	0	0	0	17	85.0
0	0	0	1	1	18	90.0
0	0	0	0	0	19	95.0
0	0	0	0	0	20	100.0

[1] Number of models with violations

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

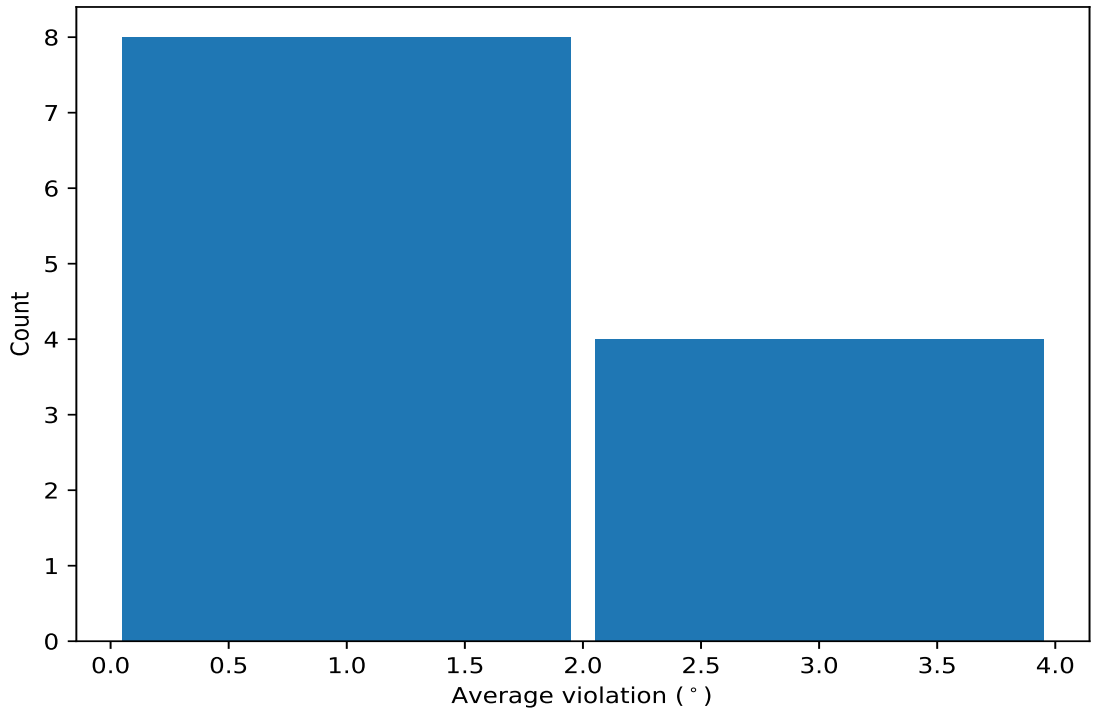


10.4 Most violated dihedral-angle restraints in the ensemble (i)

10.4.1 Histogram : Distribution of mean dihedral-angle violations (i)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints (i)

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

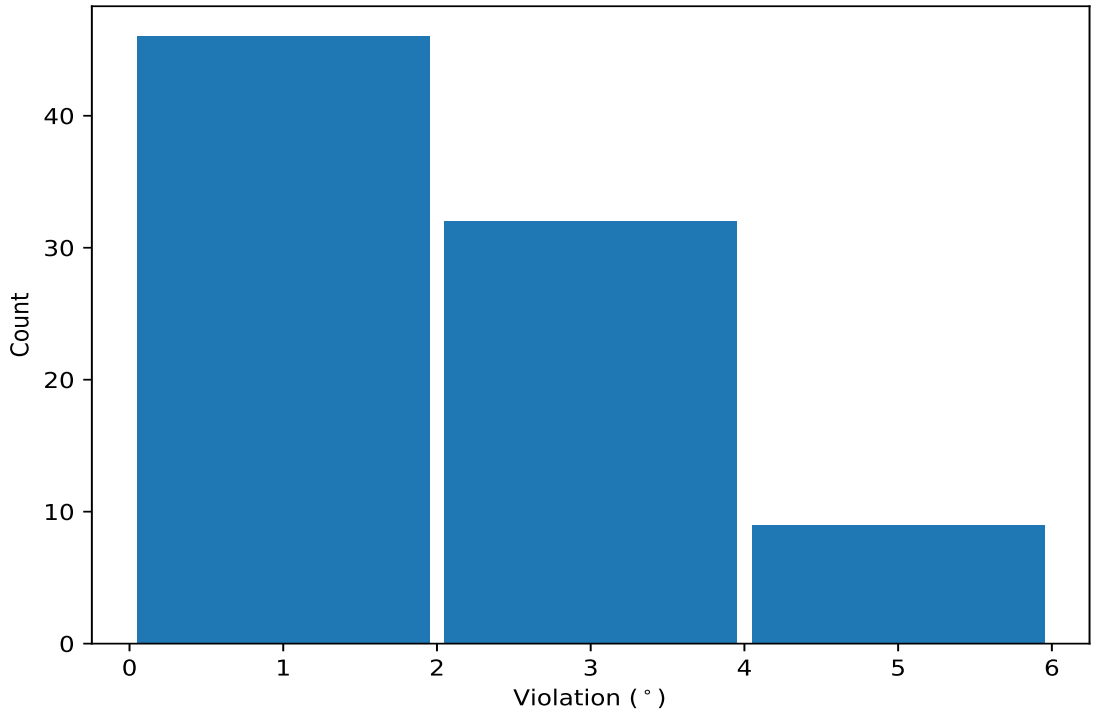
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,4)	1:A:573:LEU:N	1:A:573:LEU:CA	1:A:573:LEU:CB	1:A:573:LEU:CG	18	3.54	0.84	3.6
(1,5)	1:A:577:LEU:N	1:A:577:LEU:CA	1:A:577:LEU:CB	1:A:577:LEU:CG	14	2.15	0.55	2.2
(1,30)	1:A:570:LEU:N	1:A:570:LEU:CA	1:A:570:LEU:C	1:A:571:GLU:N	8	1.84	0.7	1.6
(1,95)	1:A:602:GLU:C	1:A:603:GLN:N	1:A:603:GLN:CA	1:A:603:GLN:C	8	1.65	0.42	1.65
(1,26)	1:A:568:ARG:N	1:A:568:ARG:CA	1:A:568:ARG:C	1:A:569:GLU:N	7	1.29	0.24	1.2
(1,7)	1:A:603:GLN:N	1:A:603:GLN:CA	1:A:603:GLN:CB	1:A:603:GLN:CG	6	3.2	0.89	3.5
(1,156)	1:A:633:ASN:N	1:A:633:ASN:CA	1:A:633:ASN:C	1:A:634:GLY:N	6	1.7	0.27	1.8
(1,21)	1:A:565:LYS:C	1:A:566:LEU:N	1:A:566:LEU:CA	1:A:566:LEU:C	4	2.7	0.97	2.6
(1,25)	1:A:567:GLN:C	1:A:568:ARG:N	1:A:568:ARG:CA	1:A:568:ARG:C	4	1.62	0.38	1.65
(1,157)	1:A:633:ASN:C	1:A:634:GLY:N	1:A:634:GLY:CA	1:A:634:GLY:C	3	1.33	0.17	1.4

[1] Number of violated models, [2]Standard 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 violationsfor 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 (°)
(1,4)	1:A:573:LEU:N	1:A:573:LEU:CA	1:A:573:LEU:CB	1:A:573:LEU:CG	3	4.6
(1,4)	1:A:573:LEU:N	1:A:573:LEU:CA	1:A:573:LEU:CB	1:A:573:LEU:CG	13	4.6
(1,4)	1:A:573:LEU:N	1:A:573:LEU:CA	1:A:573:LEU:CB	1:A:573:LEU:CG	17	4.5
(1,4)	1:A:573:LEU:N	1:A:573:LEU:CA	1:A:573:LEU:CB	1:A:573:LEU:CG	6	4.4
(1,4)	1:A:573:LEU:N	1:A:573:LEU:CA	1:A:573:LEU:CB	1:A:573:LEU:CG	14	4.3
(1,21)	1:A:565:LYS:C	1:A:566:LEU:N	1:A:566:LEU:CA	1:A:566:LEU:C	2	4.1
(1,7)	1:A:603:GLN:N	1:A:603:GLN:CA	1:A:603:GLN:CB	1:A:603:GLN:CG	6	4.0
(1,7)	1:A:603:GLN:N	1:A:603:GLN:CA	1:A:603:GLN:CB	1:A:603:GLN:CG	7	4.0
(1,4)	1:A:573:LEU:N	1:A:573:LEU:CA	1:A:573:LEU:CB	1:A:573:LEU:CG	9	4.0
(1,4)	1:A:573:LEU:N	1:A:573:LEU:CA	1:A:573:LEU:CB	1:A:573:LEU:CG	12	3.9