



wwPDB NMR Structure Validation Summary Report ⓘ

Dec 25, 2024 – 02:05 AM EST

PDB ID : 2NBV
BMRB ID : 25995
Title : Solution structure of the Rpn13 Pru domain engaging the hPLIC2 UBL domain
Authors : Chen, X.; Walters, K.J.
Deposited on : 2016-03-12

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 : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

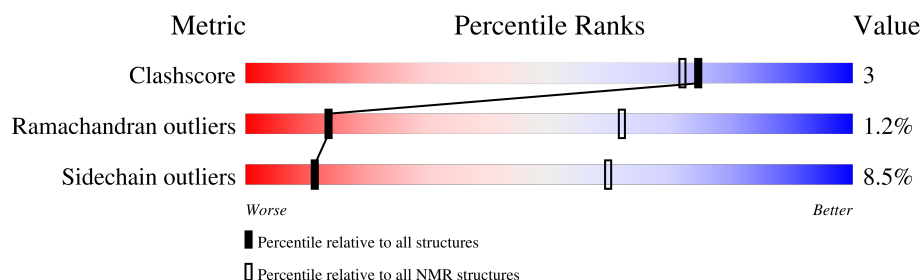
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 47%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	150	
2	B	78	

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:21-A:130, B:26-B:103 (188)	0.53	13

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 and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3087 atoms, of which 1558 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Proteasomal ubiquitin receptor ADRM1.

Mol	Chain	Residues	Atoms						Trace
1	A	110	Total	C	H	N	O	S	0
			1811	579	900	158	168	6	

- Molecule 2 is a protein called Ubiquilin-2.

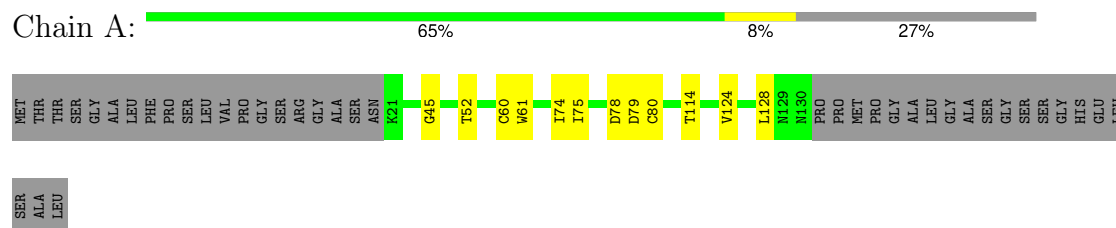
Mol	Chain	Residues	Atoms					Trace
2	B	78	Total	C	H	N	O	0
			1276	398	658	105	115	

4 Residue-property plots [i](#)

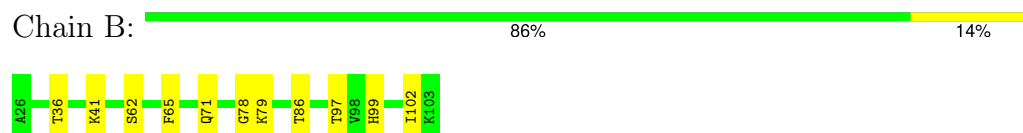
4.1 Average score per residue in the NMR ensemble

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: Proteasomal ubiquitin receptor ADRM1



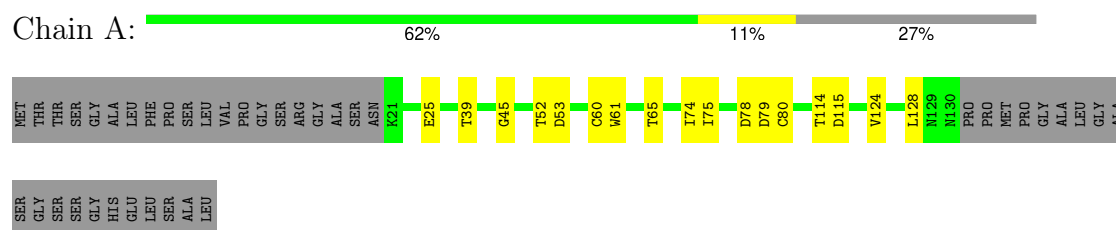
- Molecule 2: Ubiquitin-2



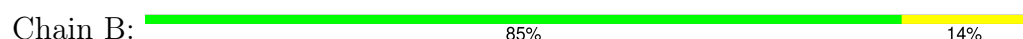
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 13. Colouring as in section 4.1 above.

- Molecule 1: Proteasomal ubiquitin receptor ADRM1



- Molecule 2: Ubiquitin-2





5 Refinement protocol and experimental data overview

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

Of the 200 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
HADDOCK	refinement	2.2
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	1640
Number of shifts mapped to atoms	1239
Number of unparsed shifts	0
Number of shifts with mapping errors	401
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	47%

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	911	900	897	5±2
2	B	618	658	652	6±2
All	All	30580	31160	30980	184

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 3.

5 of 59 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:79:LYS:HE3	2:B:79:LYS:HA	0.96	1.32	7	1
2:B:78:GLY:O	2:B:79:LYS:HD3	0.89	1.68	9	4
2:B:78:GLY:O	2:B:79:LYS:HD2	0.88	1.69	12	7
2:B:78:GLY:O	2:B:79:LYS:CD	0.79	2.29	12	7
1:A:73:LEU:HD23	2:B:79:LYS:NZ	0.69	2.02	10	4

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	108/150 (72%)	103±1 (96±1%)	5±1 (4±1%)	0±0 (0±0%)	50	84
2	B	76/78 (97%)	59±2 (78±2%)	15±2 (19±3%)	2±1 (3±1%)	6	40
All	All	3680/4560 (81%)	3247 (88%)	388 (11%)	45 (1%)	14	62

5 of 10 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	41	LYS	19
2	B	29	GLU	8
2	B	94	ASP	5
2	B	67	SER	4
2	B	66	LYS	3

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	102/130 (78%)	95±2 (93±2%)	7±2 (7±2%)	14	65
2	B	70/70 (100%)	63±2 (89±3%)	7±2 (11±3%)	8	53
All	All	3440/4000 (86%)	3146 (91%)	294 (9%)	11	60

5 of 57 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	52	THR	19
1	A	78	ASP	17
1	A	79	ASP	15
2	B	36	THR	15
2	B	65	PHE	14

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 47% for the well-defined parts and 47% 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	1640
Number of shifts mapped to atoms	1239
Number of unparsed shifts	0
Number of shifts with mapping errors	401
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

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 401) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	C	172.233	0.003	.
1	A	1	MET	CA	55.353	0.093	.
1	A	1	MET	CB	32.452	0.114	.
1	A	1	MET	CE	16.495	0	.
1	A	1	MET	CG	31.572	0.014	.
1	A	1	MET	H	8.486	0.003	.
1	A	1	MET	HA	4.581	0.002	.
1	A	1	MET	HB2	2.032	0.005	.
1	A	1	MET	HB3	2.125	0.003	.
1	A	1	MET	HE1	2.077	0	.
1	A	1	MET	HE2	2.077	0	.
1	A	1	MET	HE3	2.077	0	.
1	A	1	MET	HG2	2.606	0.006	.
1	A	1	MET	HG3	2.549	0.005	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	N	122.158	0.067	.
1	A	2	THR	C	173.871	0.003	.
1	A	2	THR	CA	61.475	0.189	.
1	A	2	THR	CB	69.536	0.108	.
1	A	2	THR	CG2	21.14	0.082	.
1	A	2	THR	H	8.222	0.002	.
1	A	2	THR	HA	4.431	0.006	.
1	A	2	THR	HB	4.253	0.005	.
1	A	2	THR	HG21	1.198	0	.
1	A	2	THR	HG22	1.198	0	.
1	A	2	THR	HG23	1.198	0	.
1	A	2	THR	N	115.148	0.082	.
1	A	3	THR	C	174.005	0.016	.
1	A	3	THR	CA	61.573	0.133	.
1	A	3	THR	CB	69.456	0.073	.
1	A	3	THR	CG2	21.141	0.065	.
1	A	3	THR	H	8.186	0.002	.
1	A	3	THR	HA	4.402	0.003	.
1	A	3	THR	HB	4.268	0.007	.
1	A	3	THR	HG21	1.195	0.001	.
1	A	3	THR	HG22	1.195	0.001	.
1	A	3	THR	HG23	1.195	0.001	.
1	A	3	THR	N	115.813	0.053	.
1	A	4	SER	C	173.695	0.004	.
1	A	4	SER	CA	58.346	0.104	.
1	A	4	SER	CB	63.576	0.131	.
1	A	4	SER	H	8.325	0.004	.
1	A	4	SER	HA	4.456	0.005	.
1	A	4	SER	HB2	3.882	0.006	.
1	A	4	SER	HB3	3.882	0.006	.
1	A	4	SER	N	117.789	0.044	.
1	A	5	GLY	C	175.042	0.029	.
1	A	5	GLY	CA	45.054	0.104	.
1	A	5	GLY	H	8.381	0.006	.
1	A	5	GLY	HA2	3.95	0.008	.
1	A	5	GLY	HA3	3.95	0.008	.
1	A	5	GLY	N	110.937	0.068	.
1	A	6	ALA	C	171.374	0.015	.
1	A	6	ALA	CA	52.025	0.093	.
1	A	6	ALA	CB	19.029	0.096	.
1	A	6	ALA	H	8.049	0.003	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	6	ALA	HA	4.257	0.015	.
1	A	6	ALA	HB1	1.293	0.001	.
1	A	6	ALA	HB2	1.293	0.001	.
1	A	6	ALA	HB3	1.293	0.001	.
1	A	6	ALA	N	123.36	0.057	.
1	A	7	LEU	C	172.091	0.002	.
1	A	7	LEU	CA	54.718	0.044	.
1	A	7	LEU	CB	42.129	0.033	.
1	A	7	LEU	CD1	24.289	0.018	.
1	A	7	LEU	CD2	23.024	0.028	.
1	A	7	LEU	CG	26.528	0.03	.
1	A	7	LEU	H	8.062	0.003	.
1	A	7	LEU	HA	4.225	0.004	.
1	A	7	LEU	HB2	1.347	0.006	.
1	A	7	LEU	HB3	1.485	0.004	.
1	A	7	LEU	HD11	0.858	0.001	.
1	A	7	LEU	HD12	0.858	0.001	.
1	A	7	LEU	HD13	0.858	0.001	.
1	A	7	LEU	HD21	0.792	0.002	.
1	A	7	LEU	HD22	0.792	0.002	.
1	A	7	LEU	HD23	0.792	0.002	.
1	A	7	LEU	HG	1.479	0.002	.
1	A	7	LEU	N	120.798	0.043	.
1	A	8	PHE	C	174.864	0	.
1	A	8	PHE	CA	55.081	0.055	.
1	A	8	PHE	CB	38.727	0.032	.
1	A	8	PHE	H	8.08	0.004	.
1	A	8	PHE	HA	4.874	0.001	.
1	A	8	PHE	HB2	2.903	0.003	.
1	A	8	PHE	HB3	3.144	0.005	.
1	A	8	PHE	N	120.71	0.053	.
1	A	9	PRO	C	171.923	0.003	.
1	A	9	PRO	CA	63.006	0.057	.
1	A	9	PRO	CB	31.631	0.058	.
1	A	9	PRO	CD	50.206	0.048	.
1	A	9	PRO	CG	26.911	0.024	.
1	A	9	PRO	HA	4.417	0.004	.
1	A	9	PRO	HB2	1.913	0.002	.
1	A	9	PRO	HB3	2.262	0.007	.
1	A	9	PRO	HD2	3.7	0.004	.
1	A	9	PRO	HD3	3.564	0.003	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	9	PRO	HG2	1.971	0.001	.
1	A	9	PRO	HG3	1.971	0.001	.
1	A	10	SER	C	174.284	0.003	.
1	A	10	SER	CA	58.052	0.025	.
1	A	10	SER	CB	63.605	0	.
1	A	10	SER	H	8.278	0.003	.
1	A	10	SER	HA	4.425	0.006	.
1	A	10	SER	HB2	3.848	0.002	.
1	A	10	SER	HB3	3.848	0.002	.
1	A	10	SER	N	115.408	0.057	.
1	A	11	LEU	C	171.699	0.002	.
1	A	11	LEU	CA	54.708	0.057	.
1	A	11	LEU	CB	41.986	0.093	.
1	A	11	LEU	CD1	24.449	0.051	.
1	A	11	LEU	CD2	23.02	0.001	.
1	A	11	LEU	CG	26.708	0.145	.
1	A	11	LEU	H	8.244	0.002	.
1	A	11	LEU	HA	4.382	0.002	.
1	A	11	LEU	HB2	1.585	0.01	.
1	A	11	LEU	HB3	1.585	0.01	.
1	A	11	LEU	HD11	0.887	0.002	.
1	A	11	LEU	HD12	0.887	0.002	.
1	A	11	LEU	HD13	0.887	0.002	.
1	A	11	LEU	HD21	0.835	0	.
1	A	11	LEU	HD22	0.835	0	.
1	A	11	LEU	HD23	0.835	0	.
1	A	11	LEU	HG	1.587	0	.
1	A	11	LEU	N	124.082	0.052	.
1	A	12	VAL	C	174.155	0	.
1	A	12	VAL	CA	59.551	0.046	.
1	A	12	VAL	CB	32.071	0.077	.
1	A	12	VAL	CG1	20.46	0.059	.
1	A	12	VAL	H	8.116	0.003	.
1	A	12	VAL	HA	4.366	0.002	.
1	A	12	VAL	HB	2.042	0.003	.
1	A	12	VAL	HG11	0.931	0.007	.
1	A	12	VAL	HG12	0.931	0.007	.
1	A	12	VAL	HG13	0.931	0.007	.
1	A	12	VAL	N	122.627	0.056	.
1	A	13	PRO	C	171.233	0.002	.
1	A	13	PRO	CA	63.112	0.07	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	13	PRO	CB	31.709	0.062	.
1	A	13	PRO	CD	49.22	0.039	.
1	A	13	PRO	CG	26.659	0.037	.
1	A	13	PRO	HA	4.478	0.002	.
1	A	13	PRO	HB2	2.004	0.008	.
1	A	13	PRO	HB3	2.305	0.005	.
1	A	13	PRO	HD2	3.601	0.002	.
1	A	13	PRO	HD3	3.569	0.003	.
1	A	13	PRO	HG2	2.037	0.003	.
1	A	13	PRO	HG3	2.037	0.003	.
1	A	14	GLY	C	174.369	0.092	.
1	A	14	GLY	CA	45.013	0.036	.
1	A	14	GLY	H	8.613	0.004	.
1	A	14	GLY	HA2	3.979	0.018	.
1	A	14	GLY	HA3	3.979	0.018	.
1	A	14	GLY	N	109.825	0.043	.
1	A	15	SER	C	173.885	0.008	.
1	A	15	SER	CA	58.234	0.034	.
1	A	15	SER	CB	63.803	0.011	.
1	A	15	SER	H	8.136	0.002	.
1	A	15	SER	HA	4.417	0.007	.
1	A	15	SER	HB2	3.86	0.002	.
1	A	15	SER	HB3	3.86	0.002	.
1	A	15	SER	N	115.443	0.073	.
1	A	16	ARG	C	171.905	0.007	.
1	A	16	ARG	CA	55.989	0.06	.
1	A	16	ARG	CB	30.165	0.044	.
1	A	16	ARG	CD	42.898	0.031	.
1	A	16	ARG	CG	26.645	0.042	.
1	A	16	ARG	H	8.455	0.003	.
1	A	16	ARG	HA	4.334	0.002	.
1	A	16	ARG	HB2	1.748	0.002	.
1	A	16	ARG	HB3	1.868	0.003	.
1	A	16	ARG	HD2	3.159	0.002	.
1	A	16	ARG	HD3	3.159	0.002	.
1	A	16	ARG	HG2	1.613	0.008	.
1	A	16	ARG	HG3	1.613	0.008	.
1	A	16	ARG	N	122.76	0.046	.
1	A	17	GLY	C	174.904	0.023	.
1	A	17	GLY	CA	44.957	0.069	.
1	A	17	GLY	H	8.353	0.004	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	17	GLY	HA2	3.905	0	.
1	A	17	GLY	HA3	3.905	0	.
1	A	17	GLY	N	109.771	0.057	.
1	A	18	ALA	C	170.856	0.028	.
1	A	18	ALA	CA	52.155	0.061	.
1	A	18	ALA	CB	19.008	0.033	.
1	A	18	ALA	H	8.151	0.004	.
1	A	18	ALA	HA	4.298	0.007	.
1	A	18	ALA	HB1	1.334	0.001	.
1	A	18	ALA	HB2	1.334	0.001	.
1	A	18	ALA	HB3	1.334	0.001	.
1	A	18	ALA	N	123.733	0.06	.
1	A	19	SER	C	174.568	0.003	.
1	A	19	SER	CA	58.011	0.055	.
1	A	19	SER	CB	63.499	0.129	.
1	A	19	SER	H	8.275	0.002	.
1	A	19	SER	HA	4.328	0.003	.
1	A	19	SER	HB2	3.773	0.004	.
1	A	19	SER	HB3	3.773	0.004	.
1	A	19	SER	N	114.784	0.057	.
1	A	20	ASN	C	174.38	0.004	.
1	A	20	ASN	CA	52.705	0.065	.
1	A	20	ASN	CB	38.392	0.039	.
1	A	20	ASN	H	8.173	0.002	.
1	A	20	ASN	HA	4.511	0.001	.
1	A	20	ASN	HB2	2.498	0.002	.
1	A	20	ASN	HB3	2.498	0.002	.
1	A	20	ASN	HD21	6.801	0.004	.
1	A	20	ASN	HD22	7.403	0.002	.
1	A	20	ASN	N	120.36	0.041	.
1	A	20	ASN	ND2	112.498	0.106	.
1	A	132	PRO	C	172.136	0.004	.
1	A	132	PRO	CA	62.364	0.047	.
1	A	132	PRO	CB	31.342	0.093	.
1	A	132	PRO	CD	50.083	0.082	.
1	A	132	PRO	CG	27.033	0.069	.
1	A	132	PRO	HA	4.477	0.009	.
1	A	132	PRO	HB2	2.043	0.005	.
1	A	132	PRO	HB3	2.301	0.006	.
1	A	132	PRO	HD2	3.825	0.005	.
1	A	132	PRO	HD3	3.524	0.002	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	132	PRO	HG2	2.099	0	.
1	A	132	PRO	HG3	2.099	0	.
1	A	133	MET	C	174.157	0	.
1	A	133	MET	CA	52.602	0.063	.
1	A	133	MET	CB	32.3	0.08	.
1	A	133	MET	CE	16.783	0	.
1	A	133	MET	CG	31.659	0.019	.
1	A	133	MET	H	8.414	0.002	.
1	A	133	MET	HA	4.863	0.004	.
1	A	133	MET	HB2	1.956	0.003	.
1	A	133	MET	HB3	2.072	0.005	.
1	A	133	MET	HE1	2.132	0	.
1	A	133	MET	HE2	2.132	0	.
1	A	133	MET	HE3	2.132	0	.
1	A	133	MET	HG2	2.69	0.004	.
1	A	133	MET	HG3	2.6	0.003	.
1	A	133	MET	N	121.509	0.053	.
1	A	134	PRO	C	171.134	0	.
1	A	134	PRO	CA	63.278	0.042	.
1	A	134	PRO	CB	31.591	0.042	.
1	A	134	PRO	CD	50.627	0.034	.
1	A	134	PRO	CG	27.038	0.065	.
1	A	134	PRO	HA	4.362	0.004	.
1	A	134	PRO	HB2	1.913	0.004	.
1	A	134	PRO	HB3	2.271	0.009	.
1	A	134	PRO	HD2	3.876	0.002	.
1	A	134	PRO	HD3	3.682	0.007	.
1	A	134	PRO	HG2	2.051	0.007	.
1	A	134	PRO	HG3	2.051	0.007	.
1	A	135	GLY	C	174.568	0.011	.
1	A	135	GLY	CA	45.026	0.047	.
1	A	135	GLY	H	8.504	0.005	.
1	A	135	GLY	HA2	3.923	0.004	.
1	A	135	GLY	HA3	3.923	0.004	.
1	A	135	GLY	N	109.582	0.043	.
1	A	136	ALA	C	170.727	0	.
1	A	136	ALA	CA	52.343	0.022	.
1	A	136	ALA	CB	18.975	0.031	.
1	A	136	ALA	H	8.086	0.003	.
1	A	136	ALA	HA	4.311	0.004	.
1	A	136	ALA	HB3	1.407	0.003	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	136	ALA	HB2	1.407	0.003	.
1	A	136	ALA	N	123.487	0.059	.
1	A	137	LEU	C	170.637	0.014	.
1	A	137	LEU	CA	55.102	0.042	.
1	A	137	LEU	CB	41.522	0.036	.
1	A	137	LEU	CD1	24.447	0	.
1	A	137	LEU	CD2	23.043	0	.
1	A	137	LEU	CG	26.63	0	.
1	A	137	LEU	H	8.268	0.002	.
1	A	137	LEU	HA	4.327	0	.
1	A	137	LEU	HB2	1.644	0	.
1	A	137	LEU	HB3	0.883	0	.
1	A	137	LEU	HD11	1.169	0	.
1	A	137	LEU	HD12	1.169	0	.
1	A	137	LEU	HD13	1.169	0	.
1	A	137	LEU	HD21	0.602	0	.
1	A	137	LEU	HD22	0.602	0	.
1	A	137	LEU	HD23	0.602	0	.
1	A	137	LEU	HG	0.891	0	.
1	A	137	LEU	N	120.911	0.05	.
1	A	138	GLY	C	174.661	0.001	.
1	A	138	GLY	CA	44.994	0.06	.
1	A	138	GLY	H	8.316	0.004	.
1	A	138	GLY	HA2	3.926	0.005	.
1	A	138	GLY	HA3	3.926	0.005	.
1	A	138	GLY	N	109.339	0.055	.
1	A	139	ALA	C	170.635	0.004	.
1	A	139	ALA	CA	52.338	0.08	.
1	A	139	ALA	CB	18.953	0.038	.
1	A	139	ALA	H	8.161	0.002	.
1	A	139	ALA	HA	4.349	0.008	.
1	A	139	ALA	HB3	1.385	0.006	.
1	A	139	ALA	HB2	1.385	0.006	.
1	A	139	ALA	N	123.78	0.077	.
1	A	140	SER	C	173.467	0.006	.
1	A	140	SER	CA	58.406	0.043	.
1	A	140	SER	CB	63.707	0.045	.
1	A	140	SER	H	8.366	0.002	.
1	A	140	SER	HA	4.435	0	.
1	A	140	SER	HB2	3.898	0	.
1	A	140	SER	HB3	3.898	0	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	140	SER	N	115.047	0.058	.
1	A	141	GLY	C	174.405	0.006	.
1	A	141	GLY	CA	45.168	0.061	.
1	A	141	GLY	H	8.388	0.004	.
1	A	141	GLY	HA2	4.005	0.001	.
1	A	141	GLY	HA3	4.005	0.001	.
1	A	141	GLY	N	110.701	0.071	.
1	A	142	SER	C	173.891	0	.
1	A	142	SER	CA	58.095	0.033	.
1	A	142	SER	CB	63.81	0.058	.
1	A	142	SER	H	8.231	0.002	.
1	A	142	SER	HA	4.511	0.003	.
1	A	142	SER	HB2	3.879	0.003	.
1	A	142	SER	HB3	3.879	0.003	.
1	A	142	SER	N	115.533	0.081	.
1	A	143	SER	C	173.661	0.01	.
1	A	143	SER	CA	58.448	0.085	.
1	A	143	SER	CB	63.769	0.017	.
1	A	143	SER	H	8.461	0.003	.
1	A	143	SER	HA	4.47	0.005	.
1	A	143	SER	HB2	3.882	0.001	.
1	A	143	SER	HB3	3.882	0.001	.
1	A	143	SER	N	117.83	0.054	.
1	A	144	GLY	C	174.643	0.002	.
1	A	144	GLY	CA	45.121	0.04	.
1	A	144	GLY	H	8.451	0.005	.
1	A	144	GLY	HA2	3.931	0	.
1	A	144	GLY	HA3	3.931	0	.
1	A	144	GLY	N	110.487	0.051	.
1	A	145	HIS	C	173.819	0.003	.
1	A	145	HIS	CA	55.506	0.079	.
1	A	145	HIS	CB	29.617	0.114	.
1	A	145	HIS	H	8.22	0.003	.
1	A	145	HIS	HA	4.665	0.003	.
1	A	145	HIS	HB2	3.192	0.012	.
1	A	145	HIS	HB3	3.068	0.002	.
1	A	145	HIS	N	118.579	0.094	.
1	A	146	GLU	C	172.144	0.004	.
1	A	146	GLU	CA	56.564	0.091	.
1	A	146	GLU	CB	29.544	0.069	.
1	A	146	GLU	CG	35.79	0.046	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	146	GLU	H	8.584	0.008	.
1	A	146	GLU	HA	4.244	0.001	.
1	A	146	GLU	HB2	1.922	0.002	.
1	A	146	GLU	HB3	2.018	0.003	.
1	A	146	GLU	HG2	2.23	0.003	.
1	A	146	GLU	HG3	2.23	0.003	.
1	A	146	GLU	N	121.988	0.031	.
1	A	147	LEU	C	171.298	0.003	.
1	A	147	LEU	CA	54.975	0.035	.
1	A	147	LEU	CB	41.75	0.171	.
1	A	147	LEU	CD1	24.491	0.034	.
1	A	147	LEU	CD2	23.033	0.013	.
1	A	147	LEU	CG	26.597	0.04	.
1	A	147	LEU	H	8.354	0.003	.
1	A	147	LEU	HA	4.342	0.005	.
1	A	147	LEU	HB2	1.624	0.007	.
1	A	147	LEU	HB3	1.624	0.007	.
1	A	147	LEU	HD11	0.915	0.002	.
1	A	147	LEU	HD12	0.915	0.002	.
1	A	147	LEU	HD13	0.915	0.002	.
1	A	147	LEU	HD21	0.864	0.001	.
1	A	147	LEU	HD22	0.864	0.001	.
1	A	147	LEU	HD23	0.864	0.001	.
1	A	147	LEU	HG	1.634	0.005	.
1	A	147	LEU	N	123.032	0.047	.
1	A	148	SER	C	174.769	0.004	.
1	A	148	SER	CA	58.035	0.02	.
1	A	148	SER	CB	63.699	0.058	.
1	A	148	SER	H	8.218	0.003	.
1	A	148	SER	HA	4.406	0.001	.
1	A	148	SER	HB2	3.845	0.001	.
1	A	148	SER	HB3	3.845	0.001	.
1	A	148	SER	N	116.267	0.072	.
1	A	149	ALA	C	172.225	0.001	.
1	A	149	ALA	CA	52.072	0.043	.
1	A	149	ALA	CB	18.934	0.042	.
1	A	149	ALA	H	8.25	0.003	.
1	A	149	ALA	HA	4.367	0.004	.
1	A	149	ALA	HB3	1.377	0.008	.
1	A	149	ALA	HB2	1.377	0.008	.
1	A	149	ALA	N	126.608	0.048	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	150	LEU	C	166.222	0	.
1	A	150	LEU	CA	56.351	0.082	.
1	A	150	LEU	CB	42.92	0.105	.
1	A	150	LEU	CD1	24.677	0.077	.
1	A	150	LEU	CD2	23.095	0.013	.
1	A	150	LEU	CG	26.776	0.046	.
1	A	150	LEU	H	7.761	0.003	.
1	A	150	LEU	HA	4.148	0.001	.
1	A	150	LEU	HB2	1.566	0.005	.
1	A	150	LEU	HB3	1.566	0.005	.
1	A	150	LEU	HD11	0.891	0.001	.
1	A	150	LEU	HD12	0.891	0.001	.
1	A	150	LEU	HD13	0.891	0.001	.
1	A	150	LEU	HD21	0.849	0.003	.
1	A	150	LEU	HD22	0.849	0.003	.
1	A	150	LEU	HD23	0.849	0.003	.
1	A	150	LEU	HG	1.591	0.004	.
1	A	150	LEU	N	126.935	0.046	.

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	148	-0.14 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	135	0.74 ± 0.23	Should be checked
$^{13}\text{C}'$	148	2.12 ± 0.19	Should be applied
^{15}N	138	-0.12 ± 0.53	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 47%, i.e. 1239 atoms were assigned a chemical shift out of a possible 2664. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	534/931 (57%)	213/376 (57%)	218/376 (58%)	103/179 (58%)
Sidechain	701/1523 (46%)	473/980 (48%)	220/480 (46%)	8/63 (13%)
Aromatic	4/210 (2%)	2/103 (2%)	0/95 (0%)	2/12 (17%)
Overall	1239/2664 (47%)	688/1459 (47%)	438/951 (46%)	113/254 (44%)

7.1.4 Statistically unusual chemical shifts [i](#)

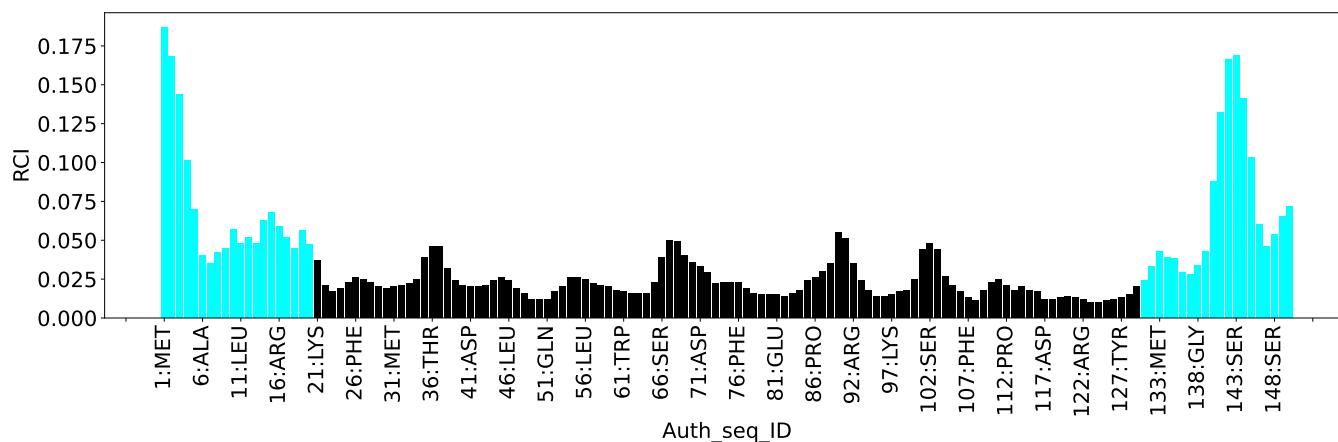
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	47	VAL	HB	0.02	0.43 – 3.54	-6.3
1	A	30	LYS	HG2	-0.10	0.13 – 2.61	-5.9
1	A	60	CYS	HB2	0.41	0.81 – 5.11	-5.9
1	A	150	LEU	C	166.22	167.56 – 186.66	-5.7
1	A	30	LYS	HE3	1.83	1.92 – 3.89	-5.5

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	105
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	103
Hydrogen bond restraints	2
Disulfide bond restraints	0
Total dihedral-angle restraints	200
Number of unmapped restraints	0
Number of restraints per residue	1.3
Number of long range restraints per residue ¹	0.0

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)	1.7	0.2
0.2-0.5 (Medium)	1.0	0.5
>0.5 (Large)	3.8	5.24

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	4.87
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

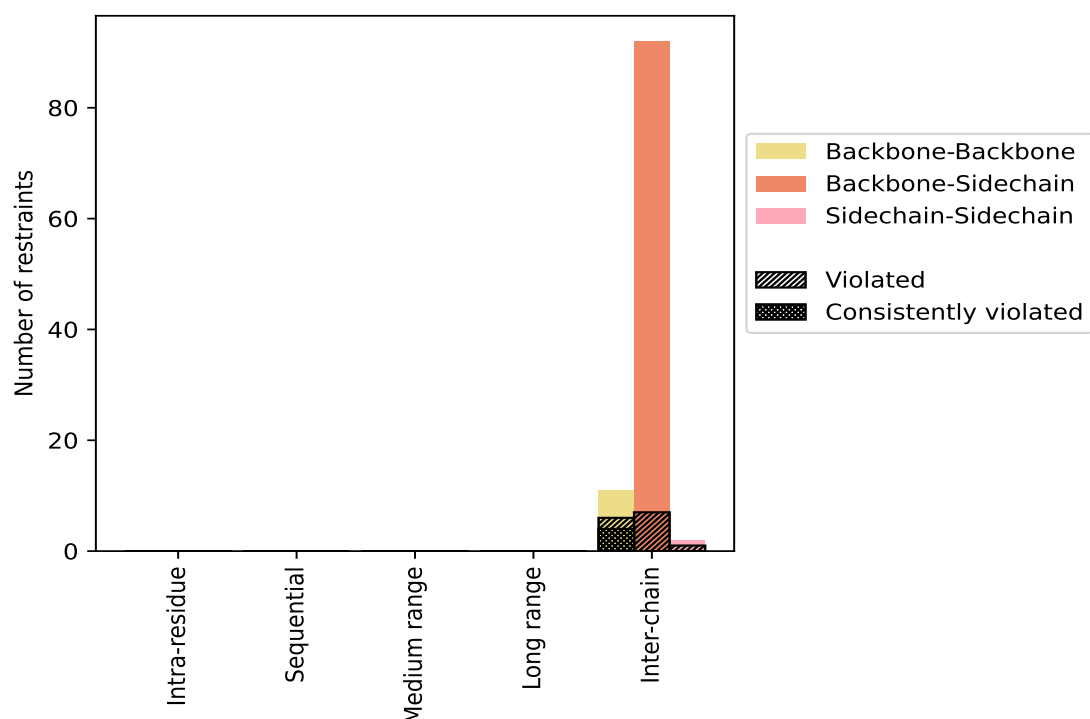
9.1 Summary of distance violations ⓘ

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)	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
Medium range (i-j >1 & i-j <5)	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
Long range (i-j ≥5)	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
Inter-chain	103	98.1	13	12.6	12.4	4	3.9	3.8
Backbone-Backbone	11	10.5	6	54.5	5.7	4	36.4	3.8
Backbone-Sidechain	92	87.6	7	7.6	6.7	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	2	1.9	1	50.0	1.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	105	100.0	14	13.3	13.3	4	3.8	3.8
Backbone-Backbone	11	10.5	6	54.5	5.7	4	36.4	3.8
Backbone-Sidechain	92	87.6	7	7.6	6.7	0	0.0	0.0
Sidechain-Sidechain	2	1.9	1	50.0	1.0	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	0	0	0	5	5	2.01	4.54	1.95	1.09
2	0	0	0	0	8	8	1.39	4.95	1.91	0.32
3	0	0	0	0	8	8	1.51	4.93	1.91	0.48
4	0	0	0	0	11	11	1.18	4.76	1.65	0.27
5	0	0	0	0	6	6	1.76	4.18	1.73	0.88
6	0	0	0	0	7	7	1.44	4.17	1.72	0.41
7	0	0	0	0	8	8	1.53	5.24	1.99	0.39
8	0	0	0	0	6	6	1.94	4.65	1.94	1.07
9	0	0	0	0	4	4	2.7	4.57	1.82	2.9
10	0	0	0	0	6	6	1.64	4.49	1.94	0.44

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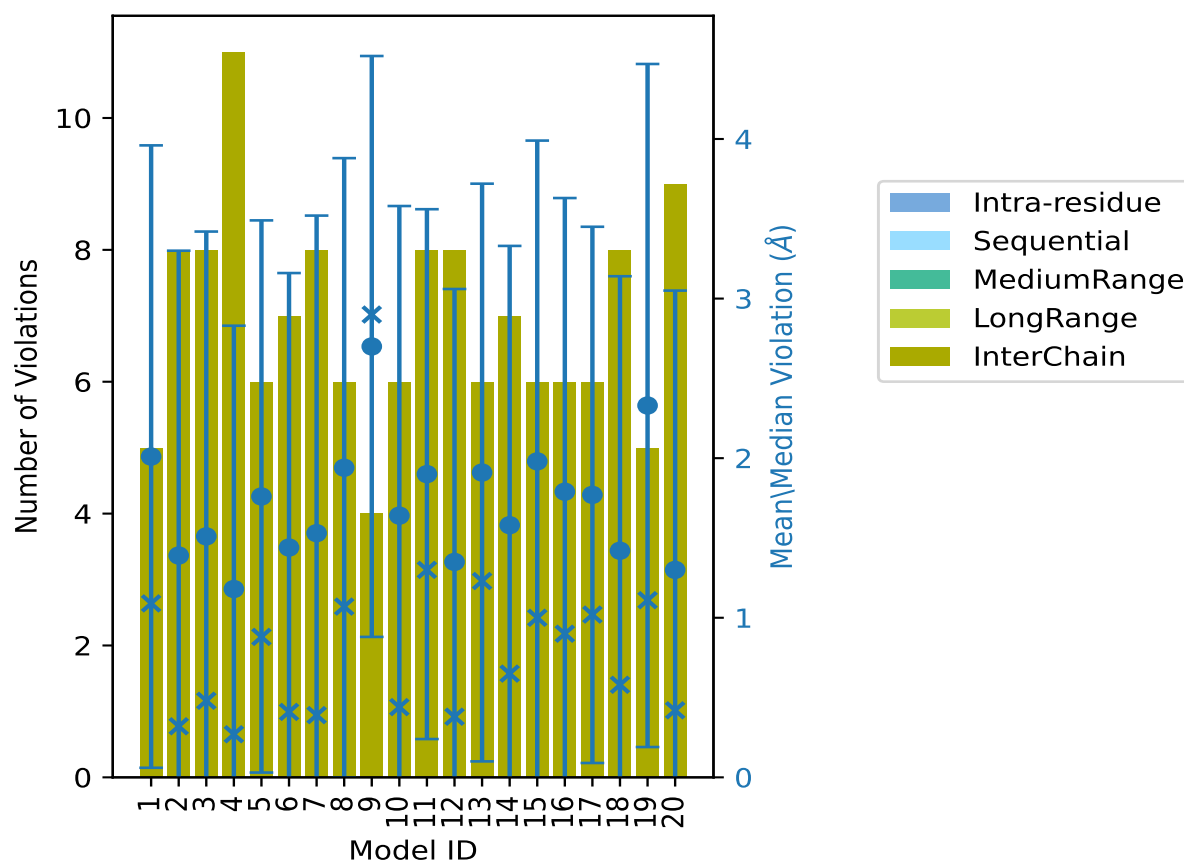
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	0	0	8	8	1.9	4.74	1.66	1.3
12	0	0	0	0	8	8	1.35	4.3	1.71	0.38
13	0	0	0	0	6	6	1.91	4.39	1.81	1.23
14	0	0	0	0	7	7	1.58	4.44	1.75	0.65
15	0	0	0	0	6	6	1.98	5.16	2.01	1.0
16	0	0	0	0	6	6	1.79	4.51	1.84	0.9
17	0	0	0	0	6	6	1.77	4.31	1.68	1.02
18	0	0	0	0	8	8	1.42	4.36	1.72	0.58
19	0	0	0	0	5	5	2.33	5.18	2.14	1.11
20	0	0	0	0	9	9	1.3	4.71	1.75	0.42

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

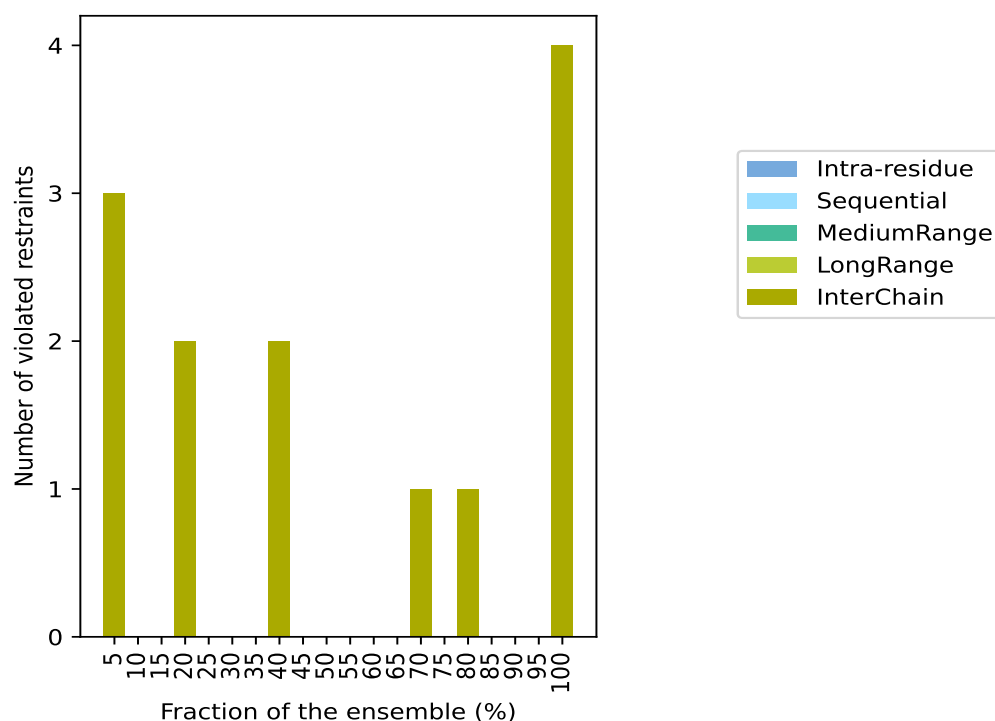
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 90(IR:0, SQ:0, MR:0, LR:0, IC:90) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	3	3	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	2	2	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	2	2	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	1	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	1	1	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	4	4	20	100.0

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

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

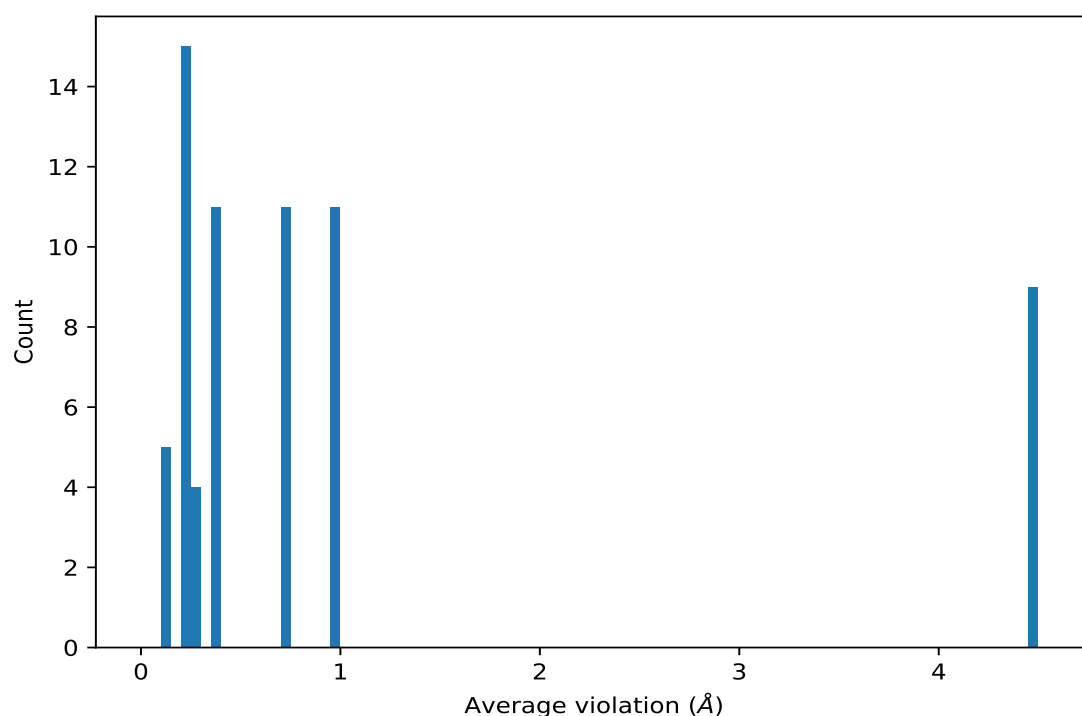
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG11	20	4.49	0.39	4.41
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG12	20	4.49	0.39	4.41
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG13	20	4.49	0.39	4.41
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG21	20	4.49	0.39	4.41
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG22	20	4.49	0.39	4.41
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG23	20	4.49	0.39	4.41
(1,37)	1:104:A:ARG:N	2:77:B:ALA:HB1	20	4.47	0.2	4.47
(1,37)	1:104:A:ARG:N	2:77:B:ALA:HB2	20	4.47	0.2	4.47
(1,37)	1:104:A:ARG:N	2:77:B:ALA:HB3	20	4.47	0.2	4.47
(1,39)	2:79:B:LYS:HA	1:74:A:ILE:HD11	20	0.98	0.3	1.06
(1,39)	2:79:B:LYS:HA	1:74:A:ILE:HD12	20	0.98	0.3	1.06
(1,39)	2:79:B:LYS:HA	1:74:A:ILE:HD13	20	0.98	0.3	1.06
(1,39)	2:79:B:LYS:HZ1	1:74:A:ILE:HG12	20	0.98	0.3	1.06
(1,39)	2:79:B:LYS:HZ1	1:74:A:ILE:HG13	20	0.98	0.3	1.06
(1,39)	2:79:B:LYS:HZ3	1:74:A:ILE:HG12	20	0.98	0.3	1.06
(1,39)	2:79:B:LYS:HZ3	1:74:A:ILE:HG13	20	0.98	0.3	1.06

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,39)	2:79:B:LYS:H	1:76:A:PHE:HE1	20	0.98	0.3	1.06
(1,39)	2:79:B:LYS:H	1:76:A:PHE:HE2	20	0.98	0.3	1.06
(1,39)	2:79:B:LYS:N	1:76:A:PHE:HE1	20	0.98	0.3	1.06
(1,39)	2:79:B:LYS:N	1:76:A:PHE:HE2	20	0.98	0.3	1.06
(1,36)	1:101:A:GLY:H	2:97:B:THR:OG1	20	0.71	0.43	0.62
(1,36)	1:101:A:GLY:H	2:97:B:THR:HG1	20	0.71	0.43	0.62
(1,36)	1:101:A:GLY:HA2	2:97:B:THR:H	20	0.71	0.43	0.62
(1,36)	1:101:A:GLY:N	2:97:B:THR:HG1	20	0.71	0.43	0.62
(1,36)	1:101:A:GLY:H	2:97:B:THR:HB	20	0.71	0.43	0.62
(1,36)	1:101:A:GLY:H	2:77:B:ALA:HB1	20	0.71	0.43	0.62
(1,36)	1:101:A:GLY:H	2:77:B:ALA:HB2	20	0.71	0.43	0.62
(1,36)	1:101:A:GLY:H	2:77:B:ALA:HB3	20	0.71	0.43	0.62
(1,36)	1:101:A:GLY:HA3	2:77:B:ALA:HB1	20	0.71	0.43	0.62
(1,36)	1:101:A:GLY:HA3	2:77:B:ALA:HB2	20	0.71	0.43	0.62
(1,36)	1:101:A:GLY:HA3	2:77:B:ALA:HB3	20	0.71	0.43	0.62
(1,40)	2:80:B:ILE:HG23	1:74:A:ILE:HD11	16	0.35	0.21	0.3
(1,40)	2:80:B:ILE:HG23	1:74:A:ILE:HD12	16	0.35	0.21	0.3
(1,40)	2:80:B:ILE:HG23	1:74:A:ILE:HD13	16	0.35	0.21	0.3
(1,40)	2:80:B:ILE:HG13	1:74:A:ILE:HD11	16	0.35	0.21	0.3
(1,40)	2:80:B:ILE:HG13	1:74:A:ILE:HD12	16	0.35	0.21	0.3
(1,40)	2:80:B:ILE:HG13	1:74:A:ILE:HD13	16	0.35	0.21	0.3
(1,40)	2:80:B:ILE:HG23	1:76:A:PHE:HZ	16	0.35	0.21	0.3
(1,40)	2:80:B:ILE:HG22	1:74:A:ILE:HD11	16	0.35	0.21	0.3
(1,40)	2:80:B:ILE:HG22	1:74:A:ILE:HD12	16	0.35	0.21	0.3
(1,40)	2:80:B:ILE:HG22	1:74:A:ILE:HD13	16	0.35	0.21	0.3
(1,40)	2:80:B:ILE:HG22	1:76:A:PHE:HZ	16	0.35	0.21	0.3
(1,2)	1:78:A:ASP:HB2	2:41:B:LYS:H	14	0.27	0.41	0.16
(1,2)	1:78:A:ASP:HB3	2:41:B:LYS:H	14	0.27	0.41	0.16
(1,1)	1:78:A:ASP:HB2	2:39:B:THR:H	8	0.28	0.43	0.12
(1,1)	1:78:A:ASP:HB3	2:39:B:THR:H	8	0.28	0.43	0.12
(1,34)	1:76:A:PHE:HD2	2:75:B:ILE:HG21	8	0.21	0.03	0.2
(1,34)	1:76:A:PHE:HD2	2:75:B:ILE:HG22	8	0.21	0.03	0.2
(1,34)	1:76:A:PHE:HD2	2:75:B:ILE:HG23	8	0.21	0.03	0.2
(1,34)	1:76:A:PHE:HE2	2:75:B:ILE:HG21	8	0.21	0.03	0.2
(1,34)	1:76:A:PHE:HE2	2:75:B:ILE:HG22	8	0.21	0.03	0.2
(1,34)	1:76:A:PHE:HE2	2:75:B:ILE:HG23	8	0.21	0.03	0.2
(1,34)	1:76:A:PHE:HE1	2:75:B:ILE:HG21	8	0.21	0.03	0.2
(1,34)	1:76:A:PHE:HE1	2:75:B:ILE:HG22	8	0.21	0.03	0.2
(1,34)	1:76:A:PHE:HE1	2:75:B:ILE:HG23	8	0.21	0.03	0.2
(1,34)	1:76:A:PHE:HD2	2:101:B:VAL:HG11	8	0.21	0.03	0.2
(1,34)	1:76:A:PHE:HD2	2:101:B:VAL:HG12	8	0.21	0.03	0.2
(1,34)	1:76:A:PHE:HD2	2:101:B:VAL:HG13	8	0.21	0.03	0.2

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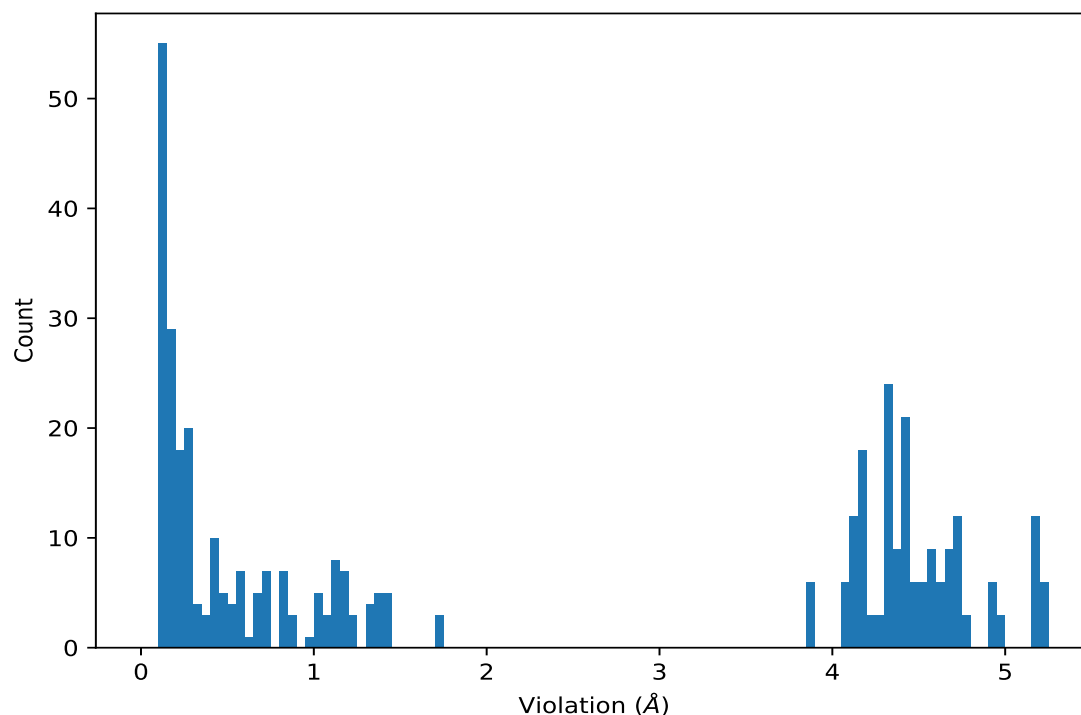
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,34)	1:76:A:PHE:HD2	2:101:B:VAL:HG21	8	0.21	0.03	0.2
(1,34)	1:76:A:PHE:HD2	2:101:B:VAL:HG22	8	0.21	0.03	0.2
(1,34)	1:76:A:PHE:HD2	2:101:B:VAL:HG23	8	0.21	0.03	0.2
(1,10)	1:75:A:ILE:HG21	2:78:B:GLY:H	4	0.11	0.01	0.11
(1,10)	1:75:A:ILE:HG22	2:78:B:GLY:H	4	0.11	0.01	0.11
(1,10)	1:75:A:ILE:HG23	2:78:B:GLY:H	4	0.11	0.01	0.11
(1,3)	1:76:A:PHE:HE1	2:77:B:ALA:H	4	0.1	0.0	0.1

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)
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG11	7	5.24
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG12	7	5.24
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG13	7	5.24
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG21	7	5.24
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG22	7	5.24
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG23	7	5.24
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG11	19	5.18
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG12	19	5.18
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG13	19	5.18
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG21	19	5.18
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG22	19	5.18
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG23	19	5.18
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG11	15	5.16
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG12	15	5.16
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG13	15	5.16
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG21	15	5.16
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG22	15	5.16
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG23	15	5.16
(1,37)	1:104:A:ARG:N	2:77:B:ALA:HB1	2	4.95
(1,37)	1:104:A:ARG:N	2:77:B:ALA:HB2	2	4.95
(1,37)	1:104:A:ARG:N	2:77:B:ALA:HB3	2	4.95
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG11	3	4.93
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG12	3	4.93
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG13	3	4.93
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG21	3	4.93
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG22	3	4.93
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG23	3	4.93
(1,37)	1:104:A:ARG:N	2:77:B:ALA:HB1	4	4.76
(1,37)	1:104:A:ARG:N	2:77:B:ALA:HB2	4	4.76
(1,37)	1:104:A:ARG:N	2:77:B:ALA:HB3	4	4.76
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG11	11	4.74
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG12	11	4.74
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG13	11	4.74
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG21	11	4.74
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG22	11	4.74
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG23	11	4.74
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG11	20	4.71
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG12	20	4.71
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG13	20	4.71
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG21	20	4.71
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG22	20	4.71
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG23	20	4.71
(1,37)	1:104:A:ARG:N	2:77:B:ALA:HB1	19	4.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,37)	1:104:A:ARG:N	2:77:B:ALA:HB2	19	4.65
(1,37)	1:104:A:ARG:N	2:77:B:ALA:HB3	19	4.65
(1,33)	1:55:A:SER:O	2:101:B:VAL:HG11	8	4.65

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

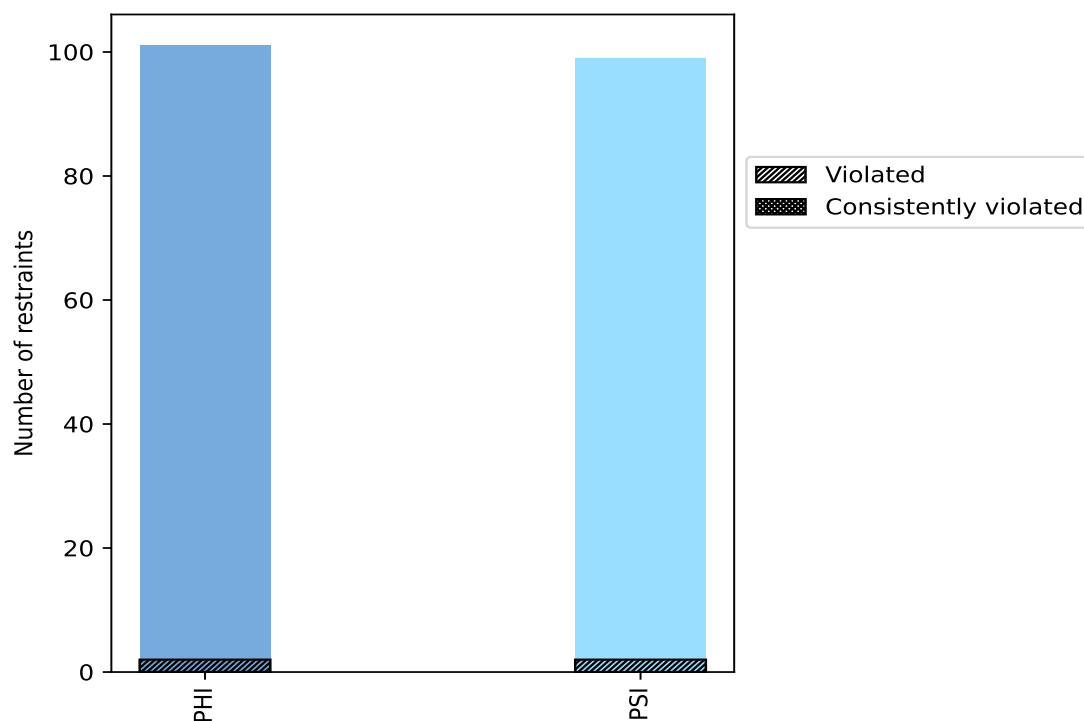
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	101	50.5	2	2.0	1.0	0	0.0	0.0
PSI	99	49.5	2	2.0	1.0	0	0.0	0.0
Total	200	100.0	4	2.0	2.0	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](#)



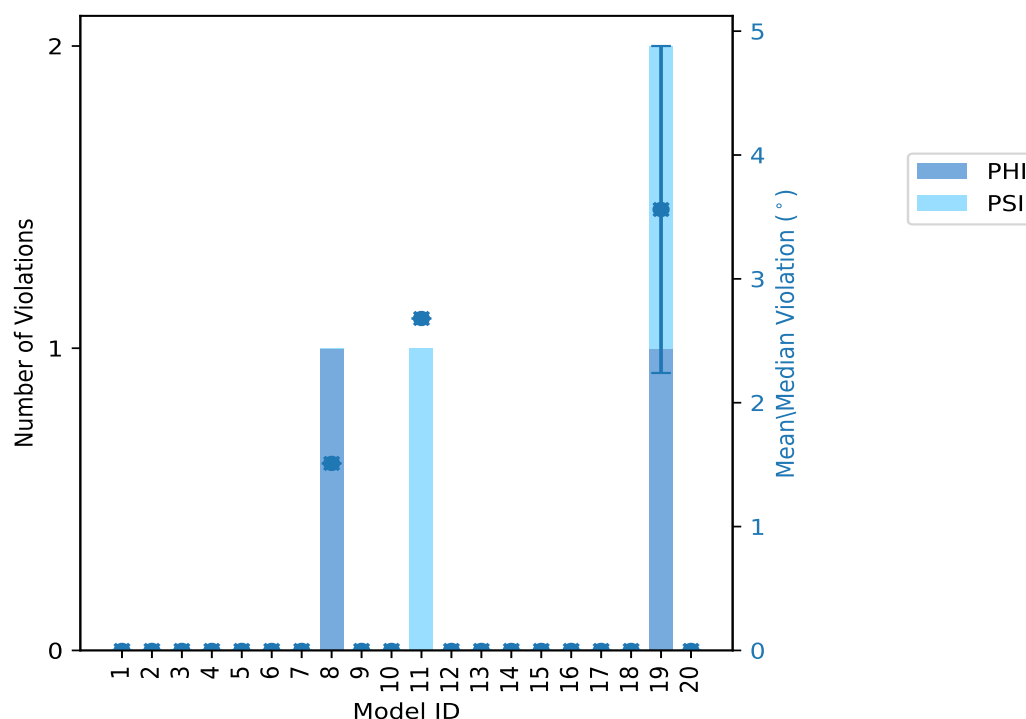
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0.0	0.0	0.0	0.0
8	1	0	1	1.51	1.51	0.0	1.51
9	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0.0	0.0	0.0	0.0
11	0	1	1	2.68	2.68	0.0	2.68
12	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0.0	0.0	0.0	0.0
19	1	1	2	3.56	4.87	1.32	3.56
20	0	0	0	0.0	0.0	0.0	0.0

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	Total	Count ¹	%
2	2	4	1	5.0
0	0	0	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

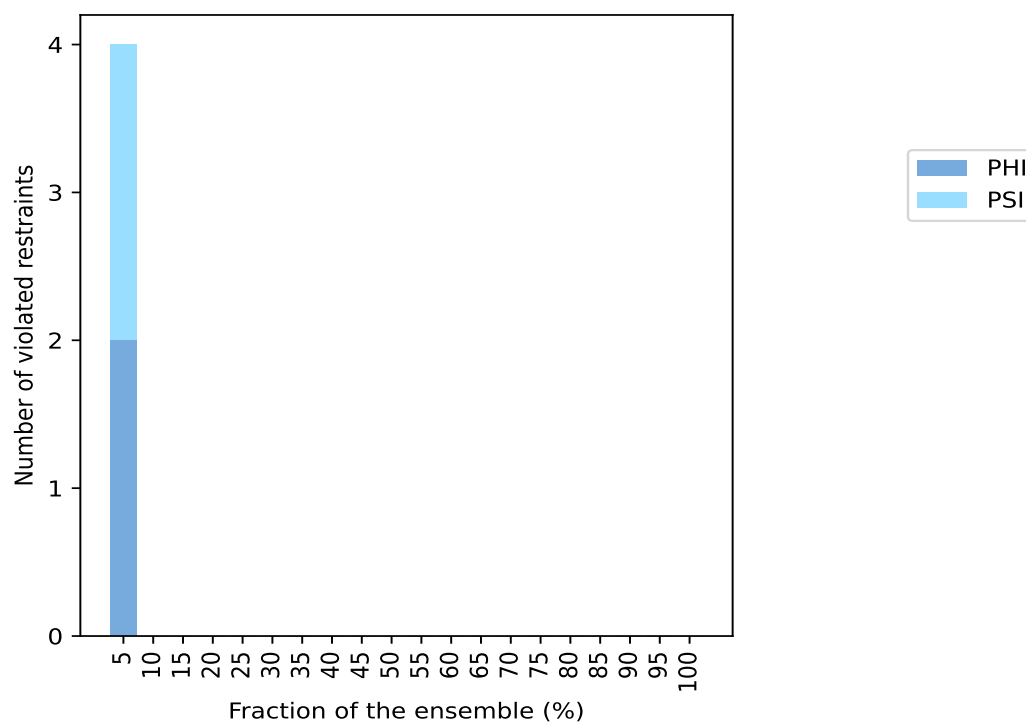
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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



10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

No violations found

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.

Data insufficient to plot histogram

10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its 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 (°)
(1,81)	1:81:A:GLU:C	1:82:A:PHE:N	1:82:A:PHE:CA	1:82:A:PHE:C	19	4.87
(1,200)	2:88:B:ILE:N	2:88:B:ILE:CA	2:88:B:ILE:C	2:89:B:GLN:N	11	2.68
(1,80)	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	1:82:A:PHE:N	19	2.24
(1,77)	1:75:A:ILE:C	1:76:A:PHE:N	1:76:A:PHE:CA	1:76:A:PHE:C	8	1.51