



wwPDB NMR Structure Validation Summary Report ⓘ

Sep 22, 2026 – 04:37 PM JST

PDB ID : 46AF / pdb_000046af
BMRB ID : 36877
Title : solution NMR structure of de novo lasso protein HF360
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Deposited on : 2026-09-16

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

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2.1
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

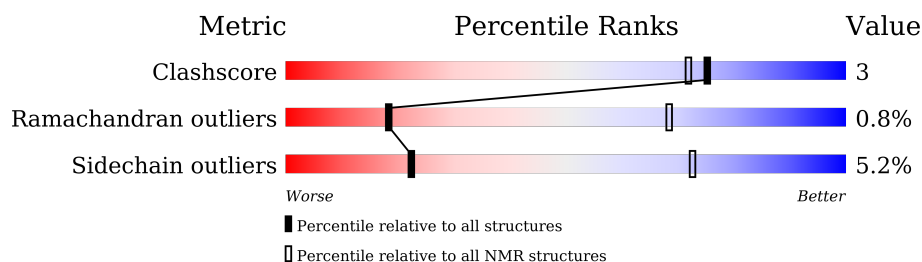
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 55%.

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	160	

2 Ensemble composition and analysis

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: *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:4-A:123, A:130-A:152 (143)	0.78	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 3 clusters and 5 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2552 atoms, of which 1294 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HF360.

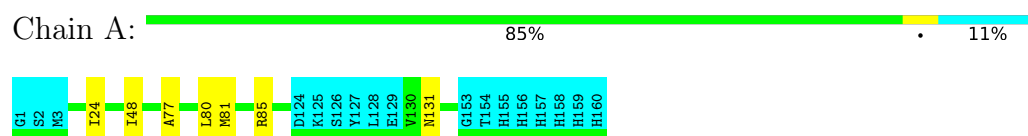
Mol	Chain	Residues	Atoms						Trace
1	A	160	Total	C	H	N	O	S	0
			2552	785	1294	216	252	5	

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.

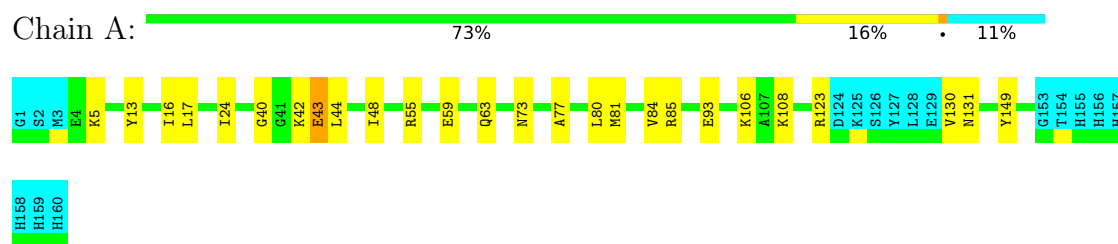
- Molecule 1: HF360



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: HF360



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CNS	refinement	
CYANA	structure calculation	

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	1533
Number of shifts mapped to atoms	1533
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	55%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.22±0.03	0±0/1122 (0.0± 0.0%)	1.13±0.02	0±0/1504 (0.0± 0.0%)
All	All	1.22	2/22440 (0.0%)	1.13	0/30080 (0.0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	24	ILE	CA-CB	5.14	1.60	1.54	2	2

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	1116	1169	1169	7±2
All	All	22320	23380	23380	141

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:LEU:HD23	1:A:92:ILE:HD13	0.67	1.66	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:ILE:HG13	1:A:57:ILE:HG13	0.62	1.72	16	1
1:A:24:ILE:HG21	1:A:85:ARG:HB2	0.62	1.70	8	19
1:A:61:VAL:HG23	1:A:80:LEU:HD23	0.60	1.72	20	1
1:A:77:ALA:O	1:A:81:MET:HG3	0.55	2.02	9	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	143/160 (89%)	139±1 (97±1%)	3±1 (2±1%)	1±1 (1±0%)	18	68
All	All	2860/3200 (89%)	2775 (97%)	63 (2%)	22 (1%)	18	68

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	131	ASN	17
1	A	123	ARG	4
1	A	40	GLY	1

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	117/132 (89%)	111±2 (95±2%)	6±2 (5±2%)	22	72
All	All	2340/2640 (89%)	2218 (95%)	122 (5%)	22	72

5 of 47 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	48	ILE	19
1	A	109	GLU	5
1	A	39	GLU	5
1	A	121	LYS	5
1	A	22	GLU	5

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 55% for the well-defined parts and 52% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *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	1533
Number of shifts mapped to atoms	1533
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

- Can not parse the chemical shift value. First 5 (of 390) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	GLY	HA2	4.117	0.01	.
1	A	1	GLY	HA3	4.046	0.00	.
1	A	2	SER	HB2	3.981	0.01	.
1	A	2	SER	HB3	3.921	0.00	.
1	A	3	MET	HB2	2.637	0.00	.
1	A	3	MET	HB3	2.095	0.00	.
1	A	4	GLU	HB2	2.075	0.00	.
1	A	4	GLU	HG2	2.328	0.01	.
1	A	5	LYS	HB2	1.850	0.00	.
1	A	5	LYS	HB3	1.776	0.01	.
1	A	6	LYS	HB2	1.913	0.00	.
1	A	7	LEU	HB2	1.751	0.00	.
1	A	7	LEU	HB3	1.593	0.00	.
1	A	7	LEU	HD11	0.903	0.00	.
1	A	7	LEU	HD12	0.903	0.00	.
1	A	7	LEU	HD13	0.903	0.00	.
1	A	7	LEU	HD21	0.797	0.00	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	LEU	HD22	0.797	0.00	.
1	A	7	LEU	HD23	0.797	0.00	.
1	A	7	LEU	CD1	25.092	0.07	.
1	A	7	LEU	CD2	23.859	0.12	.
1	A	8	GLU	HB2	2.038	0.00	.
1	A	8	GLU	HG2	2.303	0.01	.
1	A	10	ASN	HB2	2.743	0.00	.
1	A	10	ASN	HB3	2.257	0.00	.
1	A	10	ASN	HD21	6.626	0.00	.
1	A	10	ASN	HD22	6.313	0.00	.
1	A	11	LEU	HB2	1.838	0.00	.
1	A	11	LEU	HB3	1.606	0.00	.
1	A	11	LEU	HD11	0.784	0.00	.
1	A	11	LEU	HD12	0.784	0.00	.
1	A	11	LEU	HD13	0.784	0.00	.
1	A	11	LEU	HD21	0.879	0.00	.
1	A	11	LEU	HD22	0.879	0.00	.
1	A	11	LEU	HD23	0.879	0.00	.
1	A	11	LEU	CD1	23.501	0.08	.
1	A	13	TYR	HB2	3.083	0.00	.
1	A	13	TYR	HB3	3.034	0.00	.
1	A	13	TYR	HD1	6.894	0.00	.
1	A	14	LEU	HB2	2.045	0.00	.
1	A	14	LEU	HB3	1.950	0.01	.
1	A	14	LEU	HD11	0.897	0.00	.
1	A	14	LEU	HD12	0.897	0.00	.
1	A	14	LEU	HD13	0.897	0.00	.
1	A	14	LEU	HD21	0.875	0.00	.
1	A	14	LEU	HD22	0.875	0.00	.
1	A	14	LEU	HD23	0.875	0.00	.
1	A	14	LEU	CD1	25.688	0.07	.
1	A	15	GLY	HA2	3.643	0.01	.
1	A	15	GLY	HA3	3.507	0.01	.
1	A	16	ILE	HG12	1.877	0.01	.
1	A	16	ILE	HG13	1.381	0.01	.
1	A	17	LEU	HB2	1.194	0.00	.
1	A	17	LEU	HD21	0.806	0.00	.
1	A	17	LEU	HD22	0.806	0.00	.
1	A	17	LEU	HD23	0.806	0.00	.
1	A	17	LEU	CD2	23.489	0.06	.
1	A	18	LEU	HB2	1.934	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	18	LEU	HB3	1.493	0.01	.
1	A	18	LEU	HD21	0.872	0.00	.
1	A	18	LEU	HD22	0.872	0.00	.
1	A	18	LEU	HD23	0.872	0.00	.
1	A	18	LEU	CD2	22.444	0.14	.
1	A	19	GLU	HB2	2.120	0.01	.
1	A	19	GLU	HG2	2.374	0.00	.
1	A	20	SER	HB2	4.208	0.02	.
1	A	21	LEU	HB2	1.953	0.00	.
1	A	21	LEU	HB3	1.543	0.00	.
1	A	21	LEU	CD1	25.072	0.00	.
1	A	22	GLU	HB2	2.326	0.01	.
1	A	22	GLU	HB3	2.077	0.00	.
1	A	22	GLU	HG2	2.547	0.00	.
1	A	24	ILE	HG12	1.795	0.00	.
1	A	24	ILE	HG13	1.084	0.01	.
1	A	25	ASP	HB2	2.756	0.00	.
1	A	25	ASP	HB3	2.556	0.00	.
1	A	28	LEU	HB2	2.005	0.00	.
1	A	28	LEU	HB3	1.484	0.00	.
1	A	28	LEU	HD11	0.998	0.00	.
1	A	28	LEU	HD12	0.998	0.00	.
1	A	28	LEU	HD13	0.998	0.00	.
1	A	28	LEU	HD21	0.904	0.00	.
1	A	28	LEU	HD22	0.904	0.00	.
1	A	28	LEU	HD23	0.904	0.00	.
1	A	28	LEU	CD1	25.822	0.12	.
1	A	28	LEU	CD2	24.854	1.05	.
1	A	30	ARG	HB2	2.062	0.01	.
1	A	30	ARG	HB3	1.999	0.00	.
1	A	30	ARG	HD2	3.237	0.00	.
1	A	30	ARG	HD3	3.103	0.00	.
1	A	31	VAL	HG11	1.125	0.00	.
1	A	31	VAL	HG12	1.125	0.00	.
1	A	31	VAL	HG13	1.125	0.00	.
1	A	31	VAL	CG1	22.241	0.02	.
1	A	32	ASP	HB2	2.755	0.01	.
1	A	32	ASP	HB3	2.580	0.01	.
1	A	34	GLU	HB2	2.046	0.00	.
1	A	34	GLU	HB3	1.966	0.00	.
1	A	34	GLU	HG2	2.293	0.00	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	35	VAL	HG11	0.922	0.00	.
1	A	35	VAL	HG12	0.922	0.00	.
1	A	35	VAL	HG13	0.922	0.00	.
1	A	35	VAL	HG21	0.904	0.00	.
1	A	35	VAL	HG22	0.904	0.00	.
1	A	35	VAL	HG23	0.904	0.00	.
1	A	35	VAL	CG1	21.935	0.04	.
1	A	35	VAL	CG2	19.490	0.01	.
1	A	37	LYS	HB2	1.976	0.00	.
1	A	38	GLU	HB2	2.061	0.01	.
1	A	38	GLU	HB3	1.923	0.01	.
1	A	38	GLU	HG2	2.268	0.00	.
1	A	39	GLU	HB2	2.071	0.00	.
1	A	39	GLU	HB3	1.968	0.00	.
1	A	39	GLU	HG2	2.268	0.00	.
1	A	40	GLY	HA2	4.222	0.00	.
1	A	40	GLY	HA3	4.014	0.01	.
1	A	41	GLY	HA2	4.236	0.00	.
1	A	41	GLY	HA3	3.972	0.01	.
1	A	42	LYS	HB3	1.881	0.00	.
1	A	43	GLU	HB2	2.053	0.00	.
1	A	43	GLU	HG2	2.343	0.00	.
1	A	44	LEU	HB2	1.998	0.00	.
1	A	44	LEU	HB3	1.319	0.00	.
1	A	44	LEU	CD2	22.699	0.00	.
1	A	45	VAL	HG11	0.920	0.00	.
1	A	45	VAL	HG12	0.920	0.00	.
1	A	45	VAL	HG13	0.920	0.00	.
1	A	45	VAL	HG21	0.943	0.00	.
1	A	45	VAL	HG22	0.943	0.00	.
1	A	45	VAL	HG23	0.943	0.00	.
1	A	45	VAL	CG1	24.495	0.14	.
1	A	45	VAL	CG2	22.820	0.08	.
1	A	46	LYS	HB2	1.858	0.00	.
1	A	47	LYS	HB2	1.911	0.00	.
1	A	48	ILE	HG12	1.926	0.00	.
1	A	48	ILE	HG13	0.892	0.01	.
1	A	49	LEU	HB2	1.918	0.00	.
1	A	49	LEU	HB3	1.493	0.00	.
1	A	50	GLU	HB2	2.082	0.00	.
1	A	50	GLU	HB3	1.956	0.00	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	50	GLU	HG2	2.466	0.00	.
1	A	51	SER	HB2	3.955	0.00	.
1	A	51	SER	HB3	3.698	0.00	.
1	A	53	ASP	HB2	2.920	0.01	.
1	A	53	ASP	HB3	2.719	0.00	.
1	A	54	PRO	HB2	2.263	0.00	.
1	A	54	PRO	HB3	1.855	0.00	.
1	A	54	PRO	HD2	4.357	0.00	.
1	A	54	PRO	HD3	4.109	0.00	.
1	A	54	PRO	HG2	2.062	0.00	.
1	A	54	PRO	HG3	1.974	0.00	.
1	A	55	ARG	HB2	1.828	0.01	.
1	A	55	ARG	HB3	1.775	0.00	.
1	A	55	ARG	HD2	2.876	0.04	.
1	A	55	ARG	HD3	2.788	0.00	.
1	A	55	ARG	HG3	1.560	0.00	.
1	A	56	GLU	HB2	2.236	0.00	.
1	A	56	GLU	HB3	2.164	0.00	.
1	A	56	GLU	HG2	2.376	0.00	.
1	A	57	ILE	HG12	1.859	0.01	.
1	A	57	ILE	HG13	1.034	0.01	.
1	A	59	GLU	HB2	2.106	0.00	.
1	A	59	GLU	HB3	2.010	0.00	.
1	A	59	GLU	HG2	2.380	0.00	.
1	A	61	VAL	HG11	0.996	0.00	.
1	A	61	VAL	HG12	0.996	0.00	.
1	A	61	VAL	HG13	0.996	0.00	.
1	A	61	VAL	HG21	0.938	0.00	.
1	A	61	VAL	HG22	0.938	0.00	.
1	A	61	VAL	HG23	0.938	0.00	.
1	A	61	VAL	CG1	24.106	0.02	.
1	A	61	VAL	CG2	22.949	0.07	.
1	A	63	GLN	HB2	2.213	0.01	.
1	A	63	GLN	HB3	2.080	0.00	.
1	A	63	GLN	HG2	2.555	0.00	.
1	A	63	GLN	HG3	2.386	0.00	.
1	A	64	LEU	HB2	1.924	0.00	.
1	A	64	LEU	HB3	1.558	0.00	.
1	A	64	LEU	HD11	0.441	0.00	.
1	A	64	LEU	HD12	0.441	0.00	.
1	A	64	LEU	HD13	0.441	0.00	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	64	LEU	CD1	25.218	0.09	.
1	A	66	GLU	HB2	2.149	0.01	.
1	A	66	GLU	HB3	2.109	0.00	.
1	A	66	GLU	HG2	2.292	0.00	.
1	A	68	GLY	HA2	4.675	0.01	.
1	A	68	GLY	HA3	3.683	0.00	.
1	A	69	VAL	HG11	0.946	0.01	.
1	A	69	VAL	HG12	0.946	0.01	.
1	A	69	VAL	HG13	0.946	0.01	.
1	A	69	VAL	HG21	0.920	0.00	.
1	A	69	VAL	HG22	0.920	0.00	.
1	A	69	VAL	HG23	0.920	0.00	.
1	A	69	VAL	CG1	22.474	0.06	.
1	A	71	GLU	HB2	2.063	0.00	.
1	A	71	GLU	HG2	2.346	0.00	.
1	A	72	GLU	HB3	1.972	0.00	.
1	A	72	GLU	HG2	2.324	0.00	.
1	A	73	ASN	HB2	3.055	0.00	.
1	A	73	ASN	HB3	2.339	0.00	.
1	A	73	ASN	HD21	7.503	0.00	.
1	A	73	ASN	HD22	6.722	0.00	.
1	A	74	ARG	HB2	2.244	0.00	.
1	A	74	ARG	HB3	1.880	0.00	.
1	A	74	ARG	HD2	3.319	0.00	.
1	A	74	ARG	HD3	3.276	0.00	.
1	A	74	ARG	HG3	1.538	0.00	.
1	A	75	GLU	HB2	2.135	0.00	.
1	A	75	GLU	HB3	2.083	0.00	.
1	A	75	GLU	HG2	2.335	0.00	.
1	A	78	LYS	HB2	2.038	0.00	.
1	A	78	LYS	HB3	1.851	0.00	.
1	A	79	GLU	HB2	2.171	0.00	.
1	A	79	GLU	HG2	2.520	0.00	.
1	A	80	LEU	HB2	2.157	0.00	.
1	A	80	LEU	HB3	1.230	0.01	.
1	A	80	LEU	HD11	0.536	0.00	.
1	A	80	LEU	HD12	0.536	0.00	.
1	A	80	LEU	HD13	0.536	0.00	.
1	A	80	LEU	HD21	0.886	0.00	.
1	A	80	LEU	HD22	0.886	0.00	.
1	A	80	LEU	HD23	0.886	0.00	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	80	LEU	CD1	26.479	0.07	.
1	A	80	LEU	CD2	23.845	0.03	.
1	A	81	MET	HB2	2.295	0.00	.
1	A	81	MET	HB3	1.732	0.00	.
1	A	81	MET	HG2	2.940	0.00	.
1	A	81	MET	HG3	2.297	0.01	.
1	A	82	LYS	HB2	1.928	0.00	.
1	A	82	LYS	HB3	1.836	0.00	.
1	A	84	VAL	HG11	0.860	0.00	.
1	A	84	VAL	HG12	0.860	0.00	.
1	A	84	VAL	HG13	0.860	0.00	.
1	A	84	VAL	HG21	0.976	0.00	.
1	A	84	VAL	HG22	0.976	0.00	.
1	A	84	VAL	HG23	0.976	0.00	.
1	A	84	VAL	CG1	22.878	0.03	.
1	A	84	VAL	CG2	23.794	0.05	.
1	A	85	ARG	HB2	2.107	0.00	.
1	A	85	ARG	HB3	1.886	0.00	.
1	A	86	GLU	HB2	2.111	0.00	.
1	A	86	GLU	HG2	2.264	0.00	.
1	A	87	LEU	HB2	2.428	0.01	.
1	A	87	LEU	HB3	1.404	0.00	.
1	A	87	LEU	CD1	24.871	0.00	.
1	A	88	LEU	HB2	2.006	0.01	.
1	A	88	LEU	HB3	1.348	0.00	.
1	A	88	LEU	CD1	26.153	0.01	.
1	A	88	LEU	CD2	22.813	0.05	.
1	A	89	GLU	HB2	2.219	0.00	.
1	A	89	GLU	HB3	2.107	0.00	.
1	A	90	CYS	HB2	3.271	0.00	.
1	A	90	CYS	HB3	3.034	0.00	.
1	A	91	GLU	HB2	2.415	0.01	.
1	A	91	GLU	HB3	2.333	0.01	.
1	A	91	GLU	HG2	2.585	0.00	.
1	A	91	GLU	HG3	2.433	0.00	.
1	A	92	ILE	HG12	1.932	0.00	.
1	A	92	ILE	HG13	0.778	0.02	.
1	A	93	GLU	HB2	2.147	0.00	.
1	A	94	ASN	HB2	3.000	0.00	.
1	A	94	ASN	HB3	2.871	0.01	.
1	A	94	ASN	HD21	7.455	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	94	ASN	HD22	6.457	0.00	.
1	A	95	ILE	HG12	1.573	0.00	.
1	A	95	ILE	HG13	0.463	0.00	.
1	A	96	LEU	HB2	1.837	0.00	.
1	A	96	LEU	HB3	1.482	0.01	.
1	A	96	LEU	CD1	25.309	0.00	.
1	A	96	LEU	CD2	22.779	0.04	.
1	A	98	LYS	HB2	1.600	0.01	.
1	A	98	LYS	HB3	1.396	0.00	.
1	A	98	LYS	HD3	1.411	0.00	.
1	A	98	LYS	HE3	2.793	0.03	.
1	A	98	LYS	HG2	0.796	0.00	.
1	A	98	LYS	HG3	0.757	0.00	.
1	A	99	TYR	HB2	3.035	0.01	.
1	A	99	TYR	HE1	6.746	0.01	.
1	A	100	PRO	HB2	2.381	0.01	.
1	A	100	PRO	HB3	2.003	0.00	.
1	A	100	PRO	HD2	3.733	0.00	.
1	A	100	PRO	HD3	3.321	0.00	.
1	A	100	PRO	HG2	1.999	0.00	.
1	A	100	PRO	HG3	1.942	0.00	.
1	A	101	GLU	HB2	2.074	0.00	.
1	A	102	LEU	HB2	1.961	0.00	.
1	A	102	LEU	HB3	1.105	0.00	.
1	A	102	LEU	HD11	0.802	0.00	.
1	A	102	LEU	HD12	0.802	0.00	.
1	A	102	LEU	HD13	0.802	0.00	.
1	A	102	LEU	HD21	0.792	0.00	.
1	A	102	LEU	HD22	0.792	0.00	.
1	A	102	LEU	HD23	0.792	0.00	.
1	A	102	LEU	CD1	26.766	0.03	.
1	A	102	LEU	CD2	23.391	0.04	.
1	A	103	ASP	HB2	2.876	0.00	.
1	A	103	ASP	HB3	2.566	0.00	.
1	A	104	VAL	HG21	1.062	0.00	.
1	A	104	VAL	HG22	1.062	0.00	.
1	A	104	VAL	HG23	1.062	0.00	.
1	A	104	VAL	CG2	21.242	0.02	.
1	A	105	SER	HB2	4.005	0.03	.
1	A	105	SER	HB3	3.984	0.00	.
1	A	106	LYS	HB2	2.169	0.00	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	106	LYS	HB3	1.844	0.01	.
1	A	106	LYS	HD2	1.622	0.00	.
1	A	106	LYS	HG3	0.933	0.00	.
1	A	108	LYS	HB2	1.850	0.01	.
1	A	108	LYS	HG3	0.876	0.00	.
1	A	109	GLU	HB2	2.017	0.00	.
1	A	111	LEU	HB2	1.955	0.00	.
1	A	111	LEU	HB3	1.821	0.00	.
1	A	111	LEU	HD21	0.955	0.00	.
1	A	111	LEU	HD22	0.955	0.00	.
1	A	111	LEU	HD23	0.955	0.00	.
1	A	111	LEU	CD2	24.114	0.00	.
1	A	113	LYS	HB2	1.971	0.00	.
1	A	113	LYS	HB3	1.888	0.00	.
1	A	114	MET	HB2	1.957	0.00	.
1	A	114	MET	HB3	1.831	0.00	.
1	A	114	MET	HG2	2.520	0.00	.
1	A	115	SER	HB2	4.282	0.00	.
1	A	115	SER	HB3	4.028	0.00	.
1	A	116	TYR	HB2	3.216	0.00	.
1	A	116	TYR	HB3	2.980	0.01	.
1	A	116	TYR	HD1	7.067	0.00	.
1	A	116	TYR	HE1	6.858	0.01	.
1	A	117	GLU	HB2	2.085	0.00	.
1	A	117	GLU	HB3	1.952	0.00	.
1	A	118	GLU	HB2	2.044	0.00	.
1	A	118	GLU	HB3	2.210	0.00	.
1	A	119	ILE	HG12	1.937	0.00	.
1	A	119	ILE	HG13	1.001	0.00	.
1	A	120	LEU	HB2	1.656	0.00	.
1	A	120	LEU	HB3	1.413	0.00	.
1	A	120	LEU	HD11	0.701	0.00	.
1	A	120	LEU	HD12	0.701	0.00	.
1	A	120	LEU	HD13	0.701	0.00	.
1	A	120	LEU	HD21	0.775	0.00	.
1	A	120	LEU	HD22	0.775	0.00	.
1	A	120	LEU	HD23	0.775	0.00	.
1	A	120	LEU	CD1	25.020	0.08	.
1	A	120	LEU	CD2	22.040	0.04	.
1	A	121	LYS	HB2	1.831	0.00	.
1	A	121	LYS	HB3	1.751	0.00	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	122	ASN	HB2	2.556	0.00	.
1	A	122	ASN	HB3	2.497	0.01	.
1	A	122	ASN	HD21	7.863	0.00	.
1	A	122	ASN	HD22	7.252	0.00	.
1	A	124	ASP	HB2	2.914	0.00	.
1	A	124	ASP	HB3	2.689	0.01	.
1	A	125	LYS	HB3	1.605	0.00	.
1	A	125	LYS	HG2	1.416	0.00	.
1	A	125	LYS	HG3	1.212	0.00	.
1	A	130	VAL	HG21	0.981	0.02	.
1	A	130	VAL	HG22	0.981	0.02	.
1	A	130	VAL	HG23	0.981	0.02	.
1	A	130	VAL	CG2	21.060	0.03	.
1	A	131	ASN	HB2	3.057	0.00	.
1	A	131	ASN	HB3	2.752	0.00	.
1	A	132	LYS	HB2	1.869	0.00	.
1	A	133	GLU	HB2	2.083	0.00	.
1	A	134	CYS	HB2	3.050	0.00	.
1	A	134	CYS	HB3	3.028	0.01	.
1	A	135	LEU	HB2	1.718	0.00	.
1	A	136	GLU	HB2	2.129	0.00	.
1	A	137	LYS	HB2	1.943	0.00	.
1	A	139	ARG	HB2	1.995	0.00	.
1	A	139	ARG	HD2	3.220	0.00	.
1	A	140	GLU	HB2	2.223	0.00	.
1	A	141	LYS	HB2	2.042	0.00	.
1	A	142	VAL	HG11	0.984	0.01	.
1	A	142	VAL	HG12	0.984	0.01	.
1	A	142	VAL	HG13	0.984	0.01	.
1	A	142	VAL	HG21	0.803	0.00	.
1	A	142	VAL	HG22	0.803	0.00	.
1	A	142	VAL	HG23	0.803	0.00	.
1	A	142	VAL	CG1	23.840	0.03	.
1	A	142	VAL	CG2	21.454	0.04	.
1	A	143	LYS	HB2	1.997	0.00	.
1	A	144	GLU	HB2	2.119	0.00	.
1	A	148	LYS	HB2	1.969	0.00	.
1	A	149	TYR	HB2	3.251	0.01	.
1	A	149	TYR	HB3	2.834	0.01	.
1	A	149	TYR	HE1	6.806	0.00	.
1	A	150	LEU	HB2	1.917	0.00	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	150	LEU	HB3	1.490	0.00	.
1	A	150	LEU	CD1	25.461	0.00	.
1	A	150	LEU	CD2	22.699	0.00	.
1	A	153	GLY	HA2	3.946	0.00	.

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
$^{13}\text{C}_\alpha$	151	-0.61 ± 0.07	Should be checked
$^{13}\text{C}_\beta$	146	0.15 ± 0.04	None needed (< 0.5 ppm)
$^{13}\text{C}'$	150	-0.43 ± 0.05	None needed (< 0.5 ppm)
^{15}N	150	-0.04 ± 0.14	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 55%, i.e. 1089 atoms were assigned a chemical shift out of a possible 1977. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	704/715 (98%)	279/288 (97%)	284/286 (99%)	141/141 (100%)
Sidechain	385/1226 (31%)	147/793 (19%)	234/390 (60%)	4/43 (9%)
Aromatic	0/36 (0%)	0/16 (0%)	0/20 (0%)	0/0 (—%)
Overall	1089/1977 (55%)	426/1097 (39%)	518/696 (74%)	145/184 (79%)

7.1.4 Statistically unusual chemical shifts [i](#)

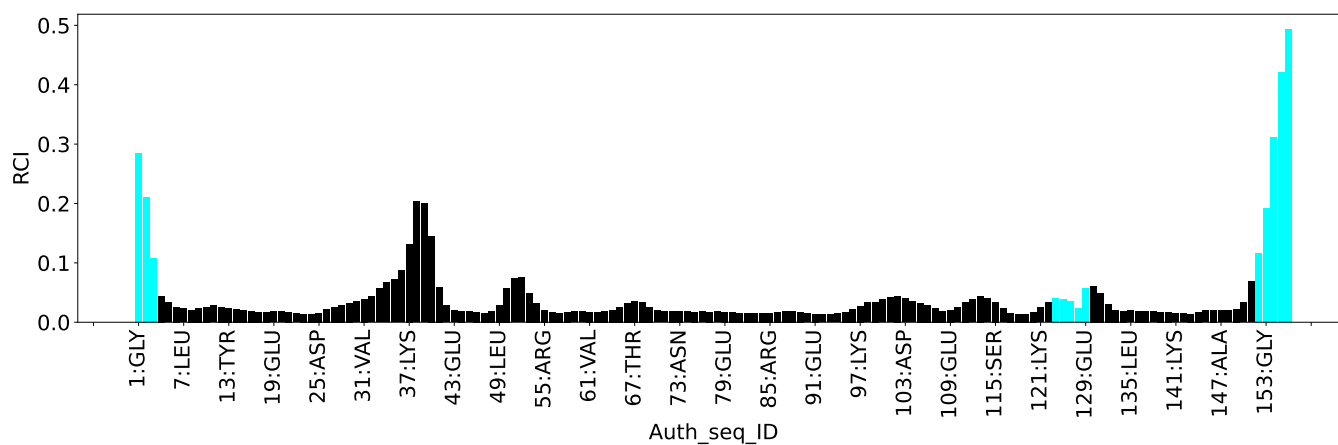
There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble

composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1370
Intra-residue ($ i-j =0$)	251
Sequential ($ i-j =1$)	370
Medium range ($ i-j >1$ and $ i-j <5$)	410
Long range ($ i-j \geq 5$)	165
Inter-chain	0
Hydrogen bond restraints	174
Disulfide bond restraints	0
Total dihedral-angle restraints	272
Number of unmapped restraints	0
Number of restraints per residue	10.3
Number of long range restraints per residue ¹	1.0

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)	15.5	0.2
0.2-0.5 (Medium)	3.5	0.46
>0.5 (Large)	0.1	0.78

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)	80.2	9.91
10.0-20.0 (Medium)	0.5	13.97
>20.0 (Large)	None	None

9 Distance violation analysis [i](#)

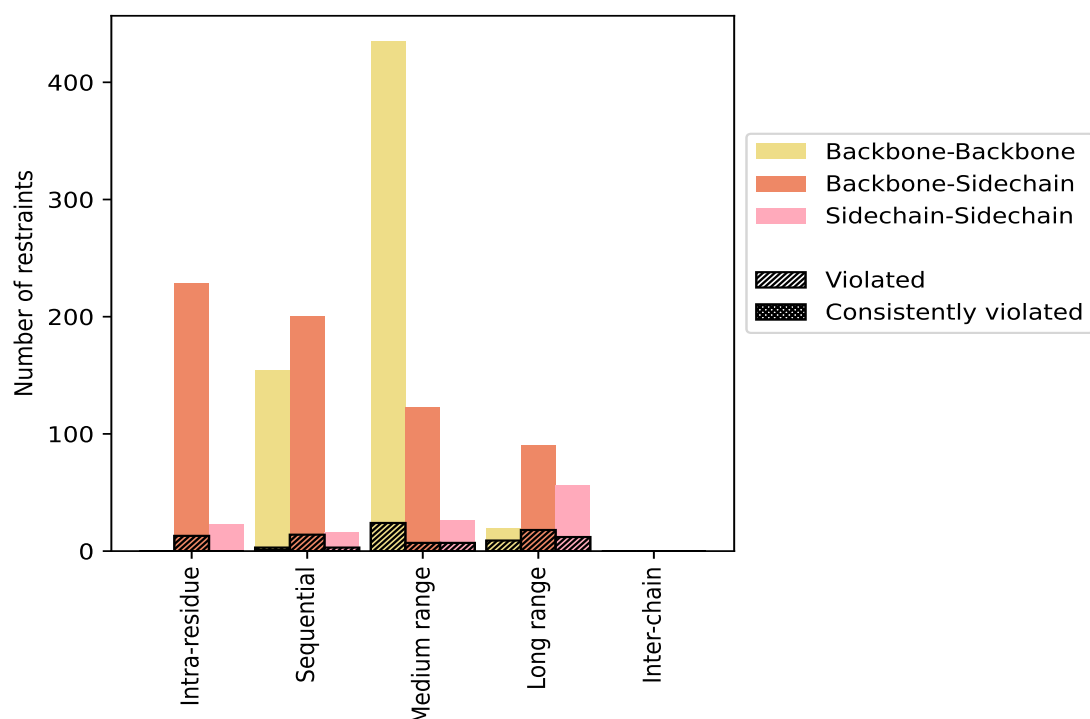
9.1 Summary of distance violations [i](#)

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	251	18.3	13	5.2	0.9	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	228	16.6	13	5.7	0.9	0	0.0	0.0
Sidechain-Sidechain	23	1.7	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	370	27.0	20	5.4	1.5	1	0.3	0.1
Backbone-Backbone	154	11.2	3	1.9	0.2	1	0.6	0.1
Backbone-Sidechain	200	14.6	14	7.0	1.0	0	0.0	0.0
Sidechain-Sidechain	16	1.2	3	18.8	0.2	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	410	29.9	21	5.1	1.5	0	0.0	0.0
Backbone-Backbone	261	19.1	7	2.7	0.5	0	0.0	0.0
Backbone-Sidechain	123	9.0	7	5.7	0.5	0	0.0	0.0
Sidechain-Sidechain	26	1.9	7	26.9	0.5	0	0.0	0.0
Long range (i-j ≥5)	165	12.0	39	23.6	2.8	0	0.0	0.0
Backbone-Backbone	19	1.4	9	47.4	0.7	0	0.0	0.0
Backbone-Sidechain	90	6.6	18	20.0	1.3	0	0.0	0.0
Sidechain-Sidechain	56	4.1	12	21.4	0.9	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	174	12.7	17	9.8	1.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1370	100.0	110	8.0	8.0	1	0.1	0.1
Backbone-Backbone	608	44.4	36	5.9	2.6	1	0.2	0.1
Backbone-Sidechain	641	46.8	52	8.1	3.8	0	0.0	0.0
Sidechain-Sidechain	121	8.8	22	18.2	1.6	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	1	5	3	7	0	16	0.16	0.3	0.05	0.17
2	3	7	3	4	0	17	0.15	0.36	0.06	0.14
3	2	10	4	8	0	24	0.16	0.36	0.06	0.14
4	3	6	4	5	0	18	0.17	0.28	0.06	0.16
5	3	4	8	4	0	19	0.21	0.78	0.17	0.13
6	4	8	5	8	0	25	0.18	0.29	0.05	0.16
7	4	7	7	5	0	23	0.17	0.46	0.09	0.14
8	2	4	6	9	0	21	0.15	0.25	0.04	0.14
9	1	7	9	8	0	25	0.15	0.24	0.03	0.15
10	2	5	4	6	0	17	0.15	0.24	0.04	0.14

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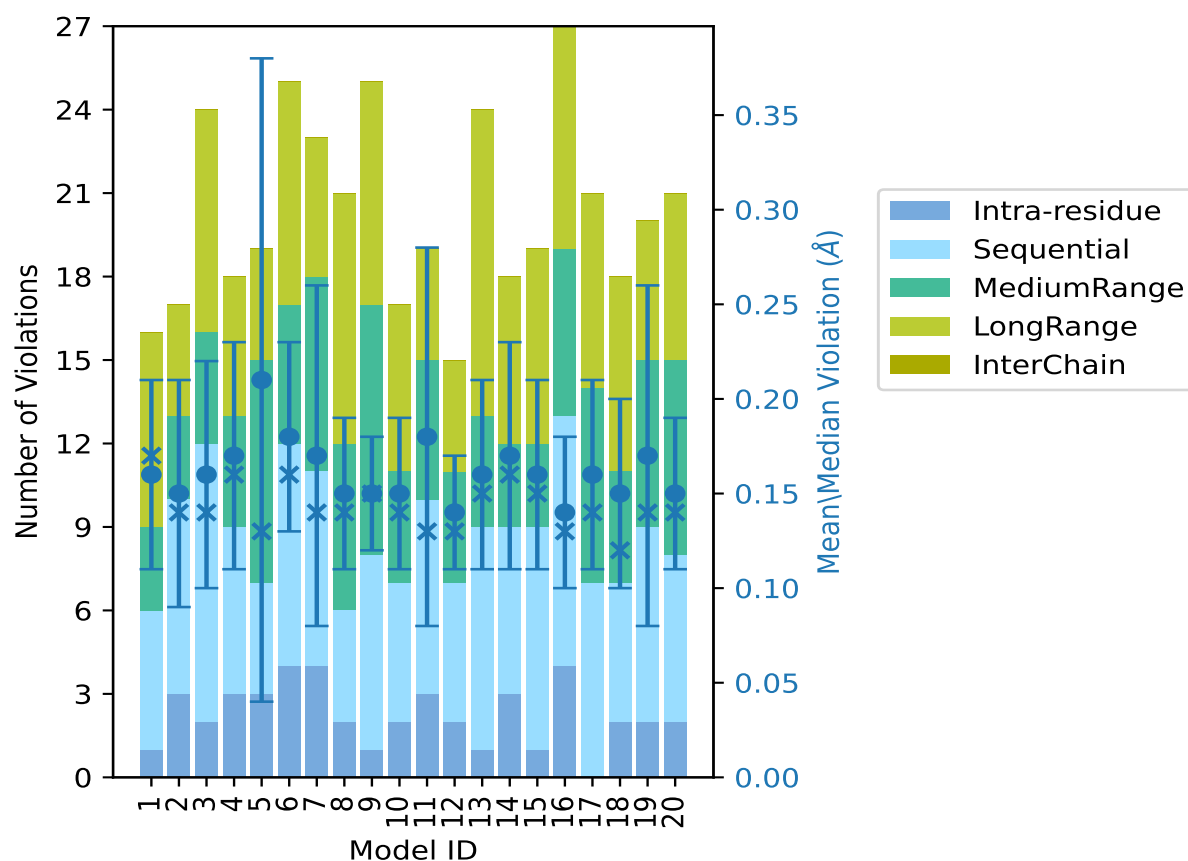
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	3	7	5	4	0	19	0.18	0.45	0.1	0.13
12	2	5	4	4	0	15	0.14	0.2	0.03	0.13
13	1	8	4	11	0	24	0.16	0.3	0.05	0.15
14	3	6	3	6	0	18	0.17	0.3	0.06	0.16
15	1	8	3	7	0	19	0.16	0.32	0.05	0.15
16	4	9	6	8	0	27	0.14	0.28	0.04	0.13
17	0	7	7	7	0	21	0.16	0.27	0.05	0.14
18	2	5	4	7	0	18	0.15	0.27	0.05	0.12
19	2	7	6	5	0	20	0.17	0.52	0.09	0.14
20	2	6	7	6	0	21	0.15	0.26	0.04	0.14

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

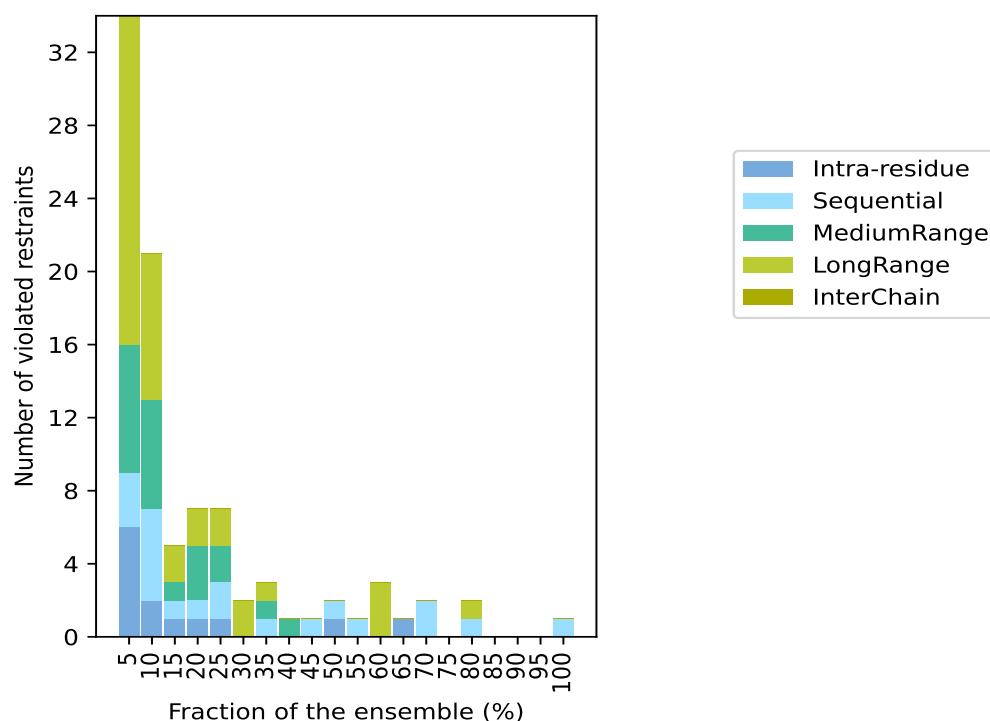
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1103(IR:238, SQ:350, MR:389, LR:126, IC:0) restraints are 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	3	7	18	0	34	1	5.0
2	5	6	8	0	21	2	10.0
1	1	1	2	0	5	3	15.0
1	1	3	2	0	7	4	20.0
1	2	2	2	0	7	5	25.0
0	0	0	2	0	2	6	30.0
0	1	1	1	0	3	7	35.0
0	0	1	0	0	1	8	40.0
0	1	0	0	0	1	9	45.0
1	1	0	0	0	2	10	50.0
0	1	0	0	0	1	11	55.0
0	0	0	3	0	3	12	60.0
1	0	0	0	0	1	13	65.0
0	2	0	0	0	2	14	70.0
0	0	0	0	0	0	15	75.0
0	1	0	1	0	2	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	1	0	0	0	1	20	100.0

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

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

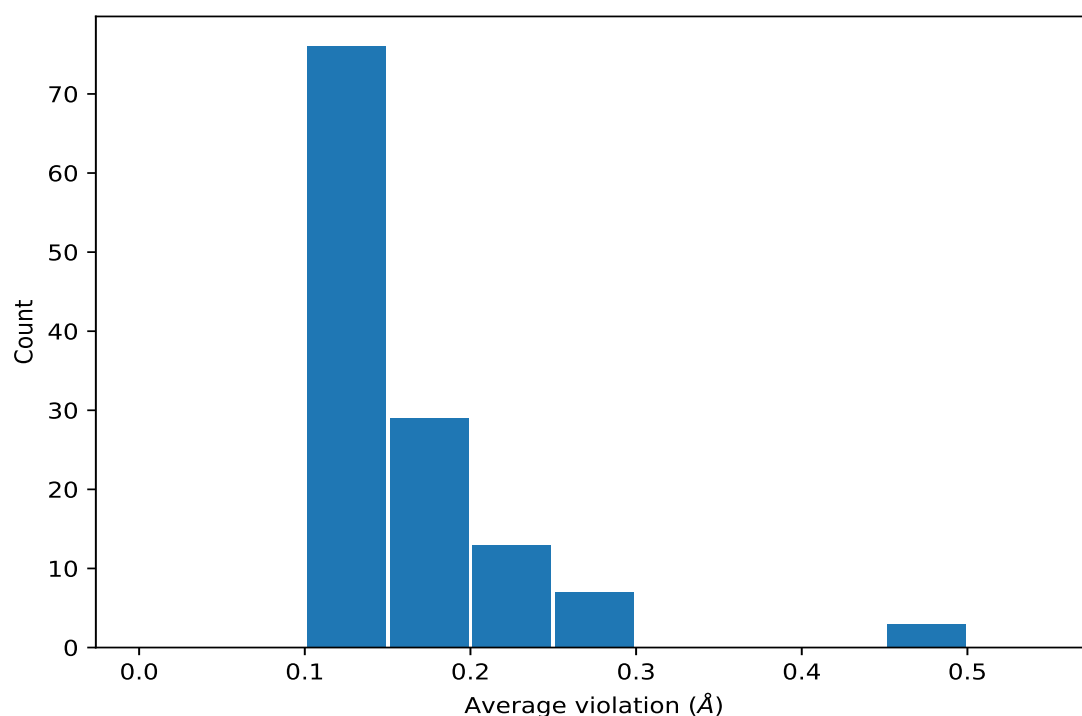
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

9.4.1 Histogram : Distribution of mean distance violations [i](#)

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



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1173)	1:67:A:THR:H	1:68:A:GLY:HA3	20	0.21	0.05	0.24
(2,1090)	1:116:A:TYR:HD1	1:117:A:GLU:H	16	0.18	0.09	0.15
(2,82)	1:24:A:ILE:HD11	1:85:A:ARG:HA	16	0.16	0.05	0.14
(2,82)	1:24:A:ILE:HD12	1:85:A:ARG:HA	16	0.16	0.05	0.14
(2,82)	1:24:A:ILE:HD13	1:85:A:ARG:HA	16	0.16	0.05	0.14
(2,903)	1:118:A:GLU:H	1:119:A:ILE:HD11	14	0.15	0.04	0.15
(2,903)	1:118:A:GLU:H	1:119:A:ILE:HD12	14	0.15	0.04	0.15
(2,903)	1:118:A:GLU:H	1:119:A:ILE:HD13	14	0.15	0.04	0.15
(2,559)	1:69:A:VAL:H	1:70:A:THR:HG21	14	0.15	0.04	0.14
(2,559)	1:69:A:VAL:H	1:70:A:THR:HG22	14	0.15	0.04	0.14
(2,559)	1:69:A:VAL:H	1:70:A:THR:HG23	14	0.15	0.04	0.14
(2,524)	1:24:A:ILE:H	1:24:A:ILE:HG13	13	0.12	0.02	0.12
(2,236)	1:31:A:VAL:HG11	1:74:A:ARG:HD3	12	0.16	0.03	0.15
(2,236)	1:31:A:VAL:HG12	1:74:A:ARG:HD3	12	0.16	0.03	0.15
(2,236)	1:31:A:VAL:HG13	1:74:A:ARG:HD3	12	0.16	0.03	0.15
(2,134)	1:36:A:THR:HG21	1:69:A:VAL:HA	12	0.15	0.04	0.15

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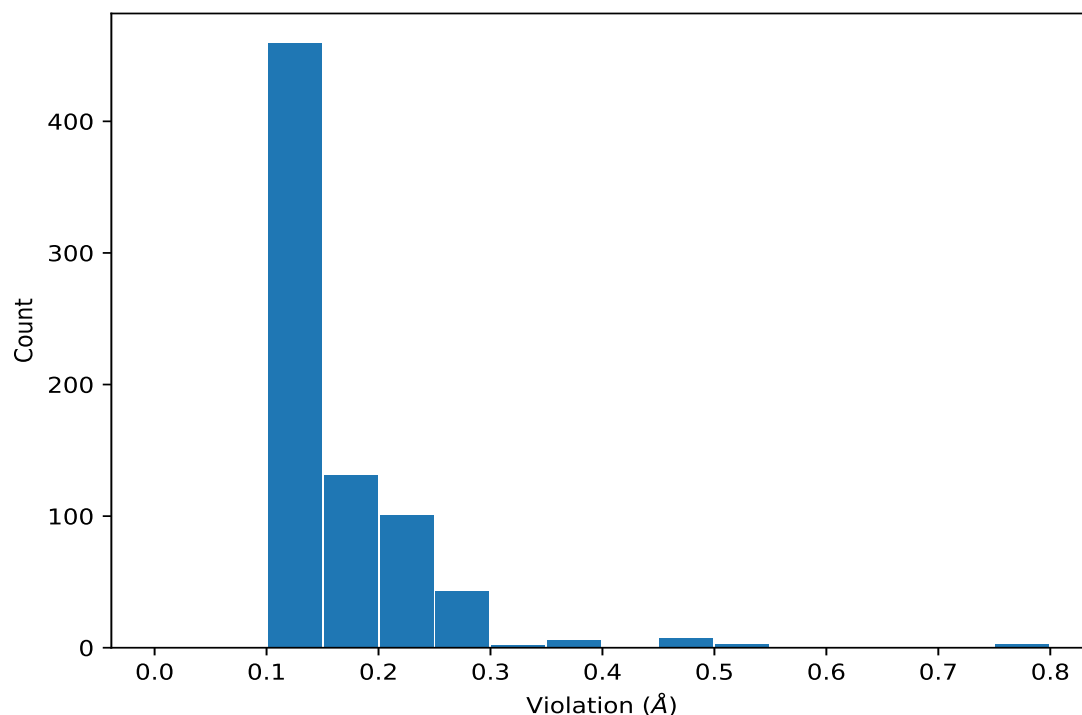
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,134)	1:36:A:THR:HG22	1:69:A:VAL:HA	12	0.15	0.04	0.15
(2,134)	1:36:A:THR:HG23	1:69:A:VAL:HA	12	0.15	0.04	0.15
(2,1153)	1:37:A:LYS:H	1:68:A:GLY:H	12	0.13	0.02	0.13
(2,718)	1:57:A:ILE:HG12	1:58:A:ALA:H	11	0.15	0.04	0.13

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)
(2,160)	1:116:A:TYR:HD1	1:120:A:LEU:HD11	5	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,160)	1:116:A:TYR:HD1	1:120:A:LEU:HD12	5	0.78
(2,160)	1:116:A:TYR:HD1	1:120:A:LEU:HD13	5	0.78
(2,172)	1:11:A:LEU:HA	1:11:A:LEU:HD11	19	0.52
(2,172)	1:11:A:LEU:HA	1:11:A:LEU:HD12	19	0.52
(2,172)	1:11:A:LEU:HA	1:11:A:LEU:HD13	19	0.52
(2,1090)	1:116:A:TYR:HD1	1:117:A:GLU:H	5	0.46
(2,172)	1:11:A:LEU:HA	1:11:A:LEU:HD11	7	0.46
(2,172)	1:11:A:LEU:HA	1:11:A:LEU:HD12	7	0.46
(2,172)	1:11:A:LEU:HA	1:11:A:LEU:HD13	7	0.46
(2,172)	1:11:A:LEU:HA	1:11:A:LEU:HD11	11	0.45
(2,172)	1:11:A:LEU:HA	1:11:A:LEU:HD12	11	0.45
(2,172)	1:11:A:LEU:HA	1:11:A:LEU:HD13	11	0.45
(2,1)	1:14:A:LEU:H	1:92:A:ILE:HD11	11	0.39
(2,1)	1:14:A:LEU:H	1:92:A:ILE:HD12	11	0.39
(2,1)	1:14:A:LEU:H	1:92:A:ILE:HD13	11	0.39
(2,1034)	1:94:A:ASN:H	1:94:A:ASN:HD22	2	0.36
(2,1034)	1:94:A:ASN:H	1:94:A:ASN:HD22	3	0.36
(2,282)	1:116:A:TYR:HA	1:116:A:TYR:HE1	5	0.36
(2,1034)	1:94:A:ASN:H	1:94:A:ASN:HD22	7	0.33

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

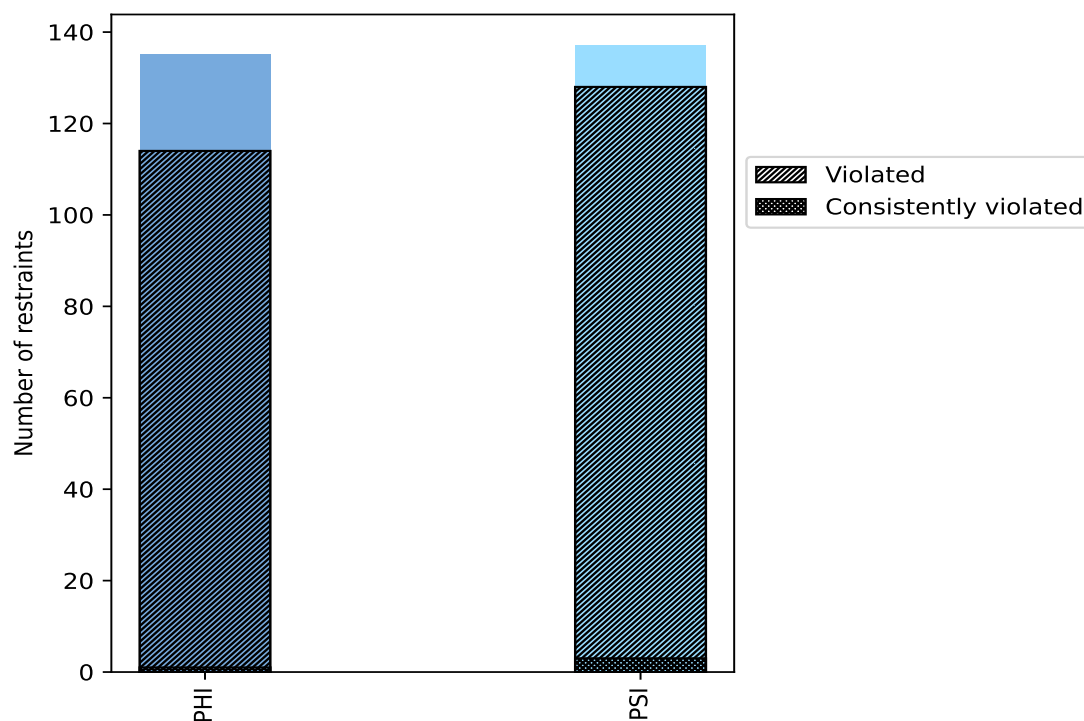
10.1 Summary of dihedral-angle violations [i](#)

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	135	49.6	114	84.4	41.9	1	0.7	0.4
PSI	137	50.4	128	93.4	47.1	3	2.2	1.1
Total	272	100.0	242	89.0	89.0	4	1.5	1.5

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](#)



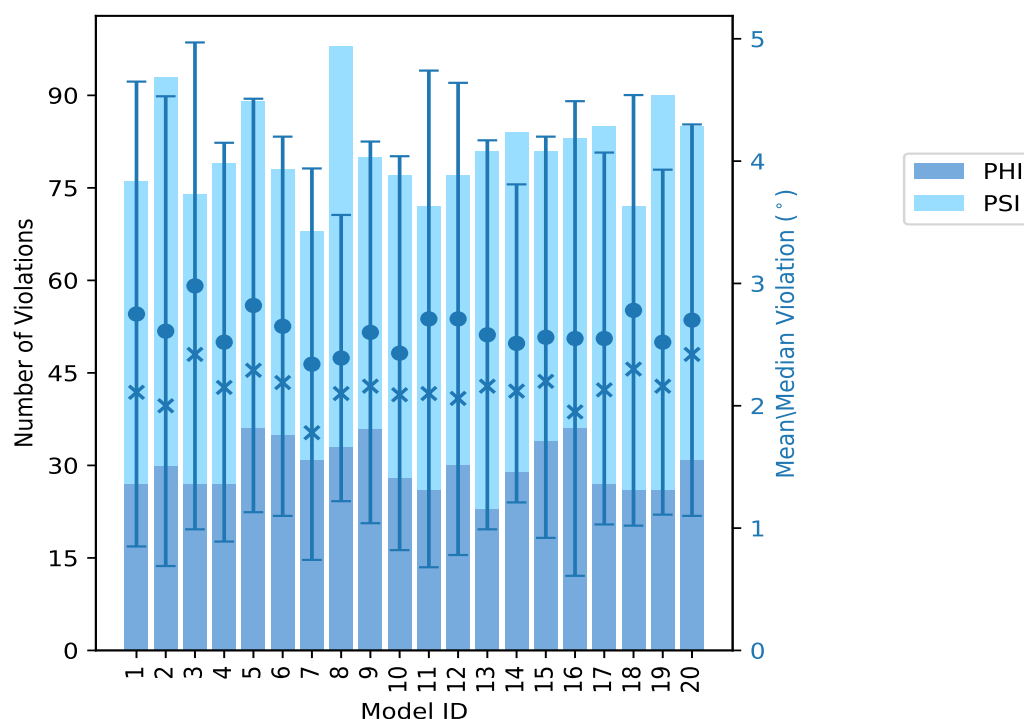
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	27	49	76	2.75	11.46	1.9	2.11
2	30	63	93	2.61	12.91	1.92	2.0
3	27	47	74	2.98	12.19	1.99	2.42
4	27	52	79	2.52	10.95	1.63	2.15
5	36	53	89	2.82	9.86	1.69	2.29
6	35	43	78	2.65	8.14	1.55	2.19
7	31	37	68	2.34	9.3	1.6	1.78
8	33	65	98	2.39	6.83	1.17	2.1
9	36	44	80	2.6	9.07	1.56	2.16
10	28	49	77	2.43	10.06	1.61	2.09
11	26	46	72	2.71	13.97	2.03	2.1
12	30	47	77	2.71	12.35	1.93	2.06
13	23	58	81	2.58	9.38	1.59	2.16
14	29	55	84	2.51	7.56	1.3	2.12
15	34	47	81	2.56	9.63	1.64	2.2
16	36	47	83	2.55	12.74	1.94	1.95
17	27	58	85	2.55	9.21	1.52	2.13
18	26	46	72	2.78	10.57	1.76	2.3
19	26	64	90	2.52	9.08	1.41	2.16
20	31	54	85	2.7	10.85	1.6	2.42

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	%
28	8	36	1	5.0
15	7	22	2	10.0
9	6	15	3	15.0
9	8	17	4	20.0
7	17	24	5	25.0
14	13	27	6	30.0
7	10	17	7	35.0
4	10	14	8	40.0
4	5	9	9	45.0
1	11	12	10	50.0
2	5	7	11	55.0

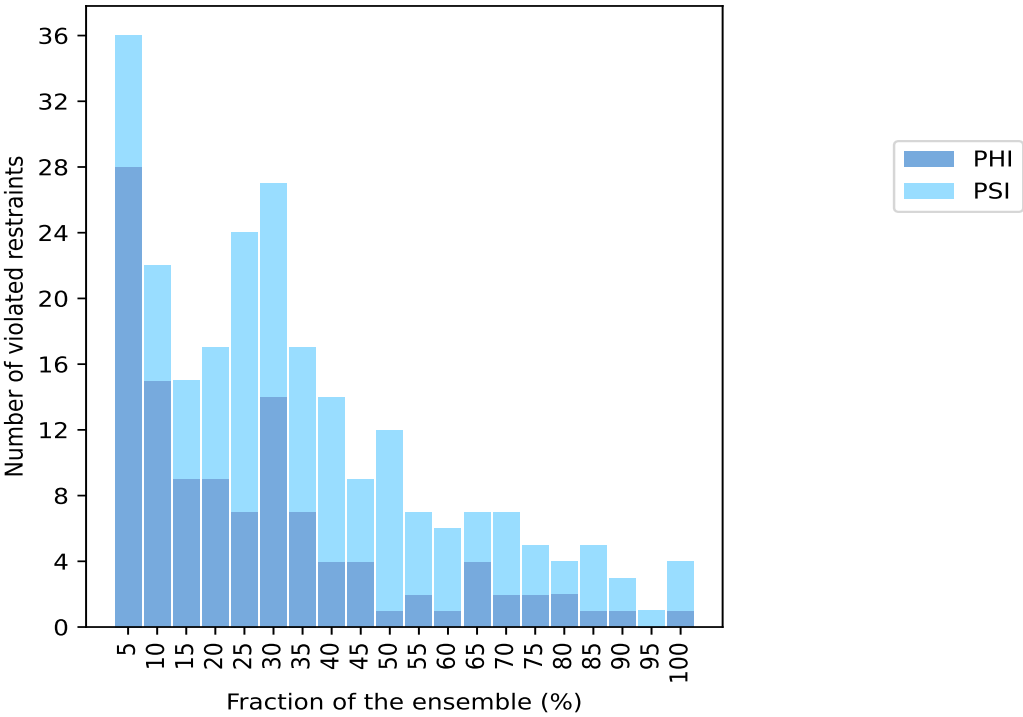
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
1	5	6	12	60.0
4	3	7	13	65.0
2	5	7	14	70.0
2	3	5	15	75.0
2	2	4	16	80.0
1	4	5	17	85.0
1	2	3	18	90.0
0	1	1	19	95.0
1	3	4	20	100.0

¹ Number of models with violations

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

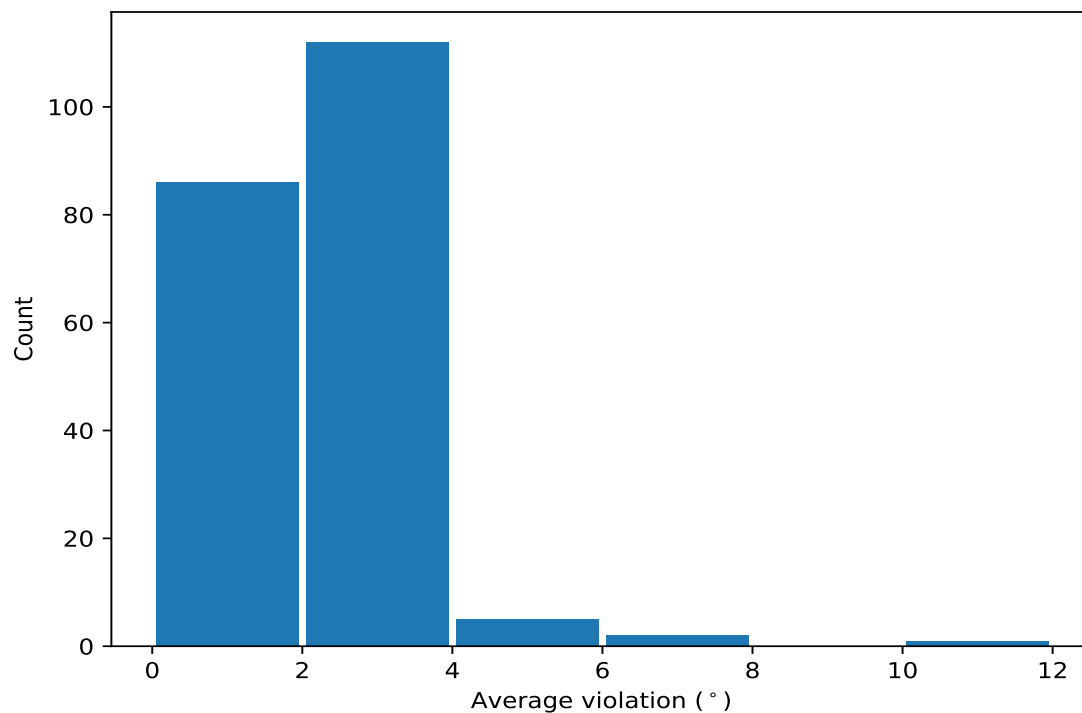


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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.

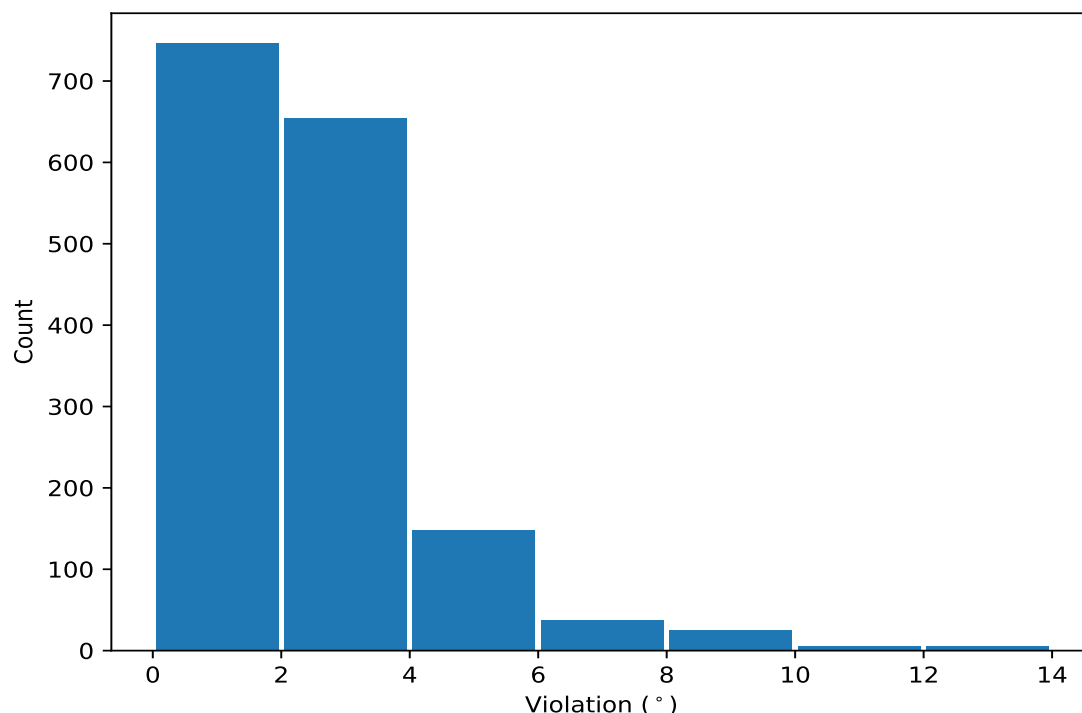
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,118)	1:67:A:THR:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	20	10.1	2.01	9.96
(1,117)	1:67:A:THR:N	1:67:A:THR:CA	1:67:A:THR:C	1:68:A:GLY:N	20	6.81	2.11	7.58
(1,119)	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	1:69:A:VAL:N	20	3.88	1.85	3.85
(1,74)	1:45:A:VAL:N	1:45:A:VAL:CA	1:45:A:VAL:C	1:46:A:LYS:N	20	3.21	1.28	2.99
(1,141)	1:79:A:GLU:N	1:79:A:GLU:CA	1:79:A:GLU:C	1:80:A:LEU:N	19	3.76	1.37	3.71
(1,32)	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	1:18:A:LEU:N	18	4.0	1.52	3.78
(1,252)	1:142:A:VAL:N	1:142:A:VAL:CA	1:142:A:VAL:C	1:143:A:LYS:N	18	3.46	0.99	3.3
(1,195)	1:106:A:LYS:C	1:107:A:ALA:N	1:107:A:ALA:CA	1:107:A:ALA:C	18	3.46	1.53	3.19
(1,66)	1:38:A:GLU:N	1:38:A:GLU:CA	1:38:A:GLU:C	1:39:A:GLU:N	17	4.51	2.27	4.48
(1,167)	1:92:A:ILE:N	1:92:A:ILE:CA	1:92:A:ILE:C	1:93:A:GLU:N	17	4.32	1.36	4.12

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 (°)
(1,118)	1:67:A:THR:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	11	13.97
(1,118)	1:67:A:THR:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	2	12.91
(1,118)	1:67:A:THR:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	16	12.74
(1,118)	1:67:A:THR:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	12	12.35
(1,118)	1:67:A:THR:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	3	12.19
(1,118)	1:67:A:THR:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	1	11.46
(1,118)	1:67:A:THR:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	4	10.95
(1,118)	1:67:A:THR:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	20	10.85
(1,118)	1:67:A:THR:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	18	10.57
(1,118)	1:67:A:THR:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	10	10.06