



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:13 AM UTC

PDB ID : 1UUC / pdb_00001uuc
BMRB ID : 6110
Title : solution structure of a chimeric LEKTI-domain
Authors : Tidow, H.; Lauber, T.; Roesch, P.; Marx, U.C.
Deposited on : 2003-12-18

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

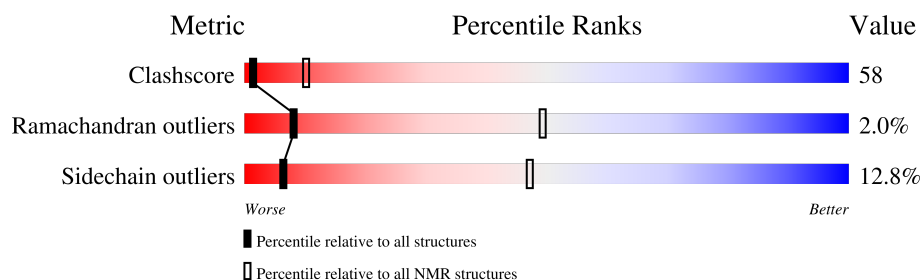
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 46%.

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	55	40% 47% 7% 5%

2 Ensemble composition and analysis

This entry contains 30 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:2-A:53 (52)	1.17	2

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 4 single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 5, 7, 8, 10, 12, 13, 14, 15, 16, 17, 18, 21, 22, 23, 24, 25, 26, 28
2	3, 6, 9, 19, 20
Single-model clusters	11; 27; 29; 30

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 442 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SERINE PROTEASE INHIBITOR KAZAL-TYPE 5.

Mol	Chain	Residues	Atoms					Trace
1	A	55	Total	C	N	O	S	0
			442	277	74	83	8	

There are 6 discrepancies between the modelled and reference sequences:

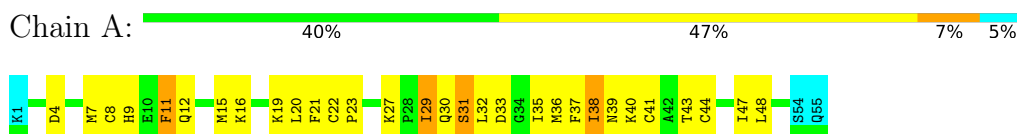
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASN	ASP	conflict	UNP Q9NQ38
A	3	GLU	SER	conflict	UNP Q9NQ38
A	4	ASP	LEU	conflict	UNP Q9NQ38
A	5	GLN	SER	conflict	UNP Q9NQ38
A	28	PRO	PHE	engineered mutation	UNP Q9NQ38
A	29	ILE	PHE	engineered mutation	UNP Q9NQ38

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.

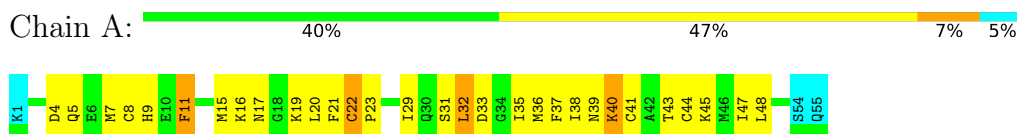
- Molecule 1: SERINE PROTEASE INHIBITOR KAZAL-TYPE 5



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

The representative model is number 2. Colouring as in section 4.1 above.

- Molecule 1: SERINE PROTEASE INHIBITOR KAZAL-TYPE 5



5 Refinement protocol and experimental data overview

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

Of the 160 calculated structures, 30 were deposited, based on the following criterion: *LOWEST ENERGY; LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
X-PLOR	refinement	3.8.5.1
NDEE; NMRVIEW	structure solution	5.1.4

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	346
Number of shifts mapped to atoms	56
Number of unparsed shifts	0
Number of shifts with mapping errors	290
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	46%

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	1.37±0.01	0±0/424 (0.0± 0.0%)	1.31±0.02	0±0/563 (0.0± 0.1%)
All	All	1.37	0/12720 (0.0%)	1.31	3/16890 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	34	GLY	N-CA-C	-5.12	108.56	115.21	21	2
1	A	11	PHE	CA-CB-CG	-5.09	108.71	113.80	29	1

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	417	0	415	48±8
All	All	12510	0	12450	1451

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 58.

5 of 456 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:ILE:HD13	1:A:30:GLN:N	1.01	1.71	18	5
1:A:7:MET:HE2	1:A:29:ILE:HD12	0.99	1.31	24	1
1:A:15:MET:SD	1:A:48:LEU:HD13	0.91	2.05	8	4
1:A:4:ASP:OD2	1:A:32:LEU:HD11	0.91	1.66	2	2
1:A:15:MET:HG3	1:A:48:LEU:HD13	0.86	1.45	18	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	52/55 (95%)	48±1 (92±2%)	3±1 (6±2%)	1±1 (2±2%)	8	49
All	All	1560/1650 (95%)	1437 (92%)	92 (6%)	31 (2%)	8	49

5 of 7 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	38	ILE	16
1	A	37	PHE	7
1	A	23	PRO	4
1	A	39	ASN	1
1	A	33	ASP	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	47/50 (94%)	41±1 (87±3%)	6±1 (13±3%)	6	47
All	All	1410/1500 (94%)	1230 (87%)	180 (13%)	6	47

5 of 19 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	29	ILE	29
1	A	11	PHE	26
1	A	27	LYS	17
1	A	31	SER	15
1	A	32	LEU	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 46% for the well-defined parts and 46% 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	346
Number of shifts mapped to atoms	56
Number of unparsed shifts	0
Number of shifts with mapping errors	290
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 290) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	LYS	HA	4.043	0.02	1
1	A	1	LYS	HB2	1.898	0.02	1
1	A	1	LYS	HD2	1.687	0.02	1
1	A	1	LYS	HE2	2.984	0.02	1
1	A	1	LYS	HG2	1.418	0.02	1
1	A	2	ASN	HA	4.658	0.02	1
1	A	2	ASN	HB2	2.887	0.02	2
1	A	2	ASN	HB3	2.792	0.02	2
1	A	2	ASN	HD21	7.676	0.02	2
1	A	2	ASN	HD22	6.965	0.02	2
1	A	3	GLU	H	8.928	0.02	1
1	A	3	GLU	HA	4.19	0.02	1
1	A	3	GLU	HB2	1.941	0.02	1
1	A	3	GLU	HG2	2.294	0.02	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	ASP	H	8.341	0.02	1
1	A	4	ASP	HA	4.45	0.02	1
1	A	4	ASP	HB2	2.654	0.02	1
1	A	5	GLN	H	8.159	0.02	1
1	A	5	GLN	HA	4.063	0.02	1
1	A	5	GLN	HB2	2.011	0.02	1
1	A	5	GLN	HG2	2.322	0.02	1
1	A	6	GLU	H	8.257	0.02	1
1	A	6	GLU	HA	4.09	0.02	1
1	A	6	GLU	HB2	2.037	0.02	1
1	A	6	GLU	HG2	2.294	0.02	1
1	A	7	MET	H	8.341	0.02	1
1	A	7	MET	HA	4.212	0.02	1
1	A	7	MET	HB2	2.286	0.02	1
1	A	7	MET	HG2	2.654	0.02	1
1	A	8	CYS	H	8.08	0.02	1
1	A	8	CYS	HA	4.148	0.02	1
1	A	8	CYS	HB2	2.932	0.02	1
1	A	9	HIS	H	8.111	0.02	1
1	A	9	HIS	HA	4.56	0.02	1
1	A	9	HIS	HB2	3.144	0.02	2
1	A	9	HIS	HB3	3.026	0.02	2
1	A	9	HIS	HD2	7.222	0.02	1
1	A	9	HIS	HE1	8.505	0.02	1
1	A	10	GLU	H	8.24	0.02	1
1	A	10	GLU	HA	4.23	0.02	1
1	A	10	GLU	HB2	1.925	0.02	1
1	A	10	GLU	HG2	2.191	0.02	1
1	A	11	PHE	H	7.62	0.02	1
1	A	11	PHE	HA	4.7	0.02	1
1	A	11	PHE	HB2	3.589	0.02	2
1	A	11	PHE	HB3	2.738	0.02	2
1	A	11	PHE	HD2	6.976	0.02	1
1	A	11	PHE	HE2	7.209	0.02	1
1	A	12	GLN	H	7.572	0.02	1
1	A	12	GLN	HA	3.831	0.02	1
1	A	12	GLN	HB2	2.074	0.02	1
1	A	12	GLN	HE21	7.383	0.02	2
1	A	12	GLN	HE22	6.826	0.02	2
1	A	12	GLN	HG2	2.437	0.02	1
1	A	13	ALA	H	7.943	0.02	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	13	ALA	HA	4.068	0.02	1
1	A	13	ALA	HB1	1.004	0.02	1
1	A	13	ALA	HB2	1.004	0.02	1
1	A	13	ALA	HB3	1.004	0.02	1
1	A	14	PHE	H	7.654	0.02	1
1	A	14	PHE	HA	4.74	0.02	1
1	A	14	PHE	HB2	3.877	0.02	2
1	A	14	PHE	HB3	2.979	0.02	2
1	A	14	PHE	HD2	7.403	0.02	1
1	A	14	PHE	HE2	7.461	0.02	1
1	A	15	MET	H	7.407	0.02	1
1	A	15	MET	HA	5.033	0.02	1
1	A	15	MET	HB2	2.085	0.02	1
1	A	15	MET	HG2	2.661	0.02	2
1	A	15	MET	HG3	2.338	0.02	2
1	A	16	LYS	H	9.37	0.02	1
1	A	16	LYS	HA	4.547	0.02	1
1	A	16	LYS	HB2	1.805	0.02	1
1	A	16	LYS	HG2	1.382	0.02	1
1	A	17	ASN	H	9.528	0.02	1
1	A	17	ASN	HA	4.381	0.02	1
1	A	17	ASN	HB2	3.066	0.02	2
1	A	17	ASN	HB3	2.82	0.02	2
1	A	17	ASN	HD21	7.624	0.02	2
1	A	17	ASN	HD22	6.977	0.02	2
1	A	18	GLY	H	8.746	0.02	1
1	A	18	GLY	HA2	4.093	0.02	2
1	A	18	GLY	HA3	3.498	0.02	2
1	A	19	LYS	H	7.678	0.02	1
1	A	19	LYS	HA	4.659	0.02	1
1	A	19	LYS	HB2	1.726	0.02	2
1	A	19	LYS	HB3	1.361	0.02	2
1	A	19	LYS	HD2	1.596	0.02	1
1	A	19	LYS	HG2	1.164	0.02	1
1	A	20	LEU	H	9.512	0.02	1
1	A	20	LEU	HA	4.53	0.02	1
1	A	20	LEU	HB2	1.707	0.02	2
1	A	20	LEU	HB3	1.278	0.02	2
1	A	20	LEU	HD11	0.672	0.02	1
1	A	20	LEU	HD12	0.672	0.02	1
1	A	20	LEU	HD13	0.672	0.02	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	20	LEU	HD21	0.672	0.02	1
1	A	20	LEU	HD22	0.672	0.02	1
1	A	20	LEU	HD23	0.672	0.02	1
1	A	20	LEU	HG	1.344	0.02	1
1	A	21	PHE	H	8.213	0.02	1
1	A	21	PHE	HA	4.637	0.02	1
1	A	21	PHE	HB2	3.036	0.02	1
1	A	21	PHE	HD2	7.131	0.02	1
1	A	21	PHE	HE2	7.314	0.02	1
1	A	22	CYS	H	8.307	0.02	1
1	A	22	CYS	HA	4.49	0.02	1
1	A	22	CYS	HB2	2.924	0.02	2
1	A	22	CYS	HB3	2.583	0.02	2
1	A	23	PRO	HA	4.369	0.02	1
1	A	23	PRO	HB2	1.889	0.02	1
1	A	23	PRO	HD2	3.435	0.02	2
1	A	23	PRO	HD3	3.231	0.02	2
1	A	23	PRO	HG2	1.73	0.02	1
1	A	24	GLN	H	8.329	0.02	1
1	A	24	GLN	HA	4.45	0.02	1
1	A	24	GLN	HB2	1.901	0.02	1
1	A	24	GLN	HG2	2.189	0.02	2
1	A	24	GLN	HG3	2.07	0.02	2
1	A	25	ASP	H	8.45	0.02	1
1	A	25	ASP	HA	4.96	0.02	1
1	A	25	ASP	HB2	2.582	0.02	1
1	A	26	LYS	H	8.305	0.02	1
1	A	26	LYS	HA	4.255	0.02	1
1	A	26	LYS	HB2	1.856	0.02	1
1	A	26	LYS	HD2	1.695	0.02	1
1	A	26	LYS	HG2	1.385	0.02	1
1	A	27	LYS	H	8.117	0.02	1
1	A	27	LYS	HA	4.511	0.02	1
1	A	27	LYS	HB2	1.768	0.02	2
1	A	27	LYS	HB3	1.705	0.02	2
1	A	27	LYS	HG2	1.409	0.02	1
1	A	28	PRO	HA	4.391	0.02	1
1	A	28	PRO	HB2	2.24	0.02	1
1	A	28	PRO	HD2	3.732	0.02	2
1	A	28	PRO	HD3	3.587	0.02	2
1	A	28	PRO	HG2	1.975	0.02	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	29	ILE	H	8.036	0.02	1
1	A	29	ILE	HA	4.14	0.02	1
1	A	29	ILE	HB	1.833	0.02	1
1	A	29	ILE	HD11	0.886	0.02	1
1	A	29	ILE	HD12	0.886	0.02	1
1	A	29	ILE	HD13	0.886	0.02	1
1	A	29	ILE	HG12	1.461	0.02	1
1	A	29	ILE	HG21	1.169	0.02	1
1	A	29	ILE	HG22	1.169	0.02	1
1	A	29	ILE	HG23	1.169	0.02	1
1	A	30	GLN	H	8.431	0.02	1
1	A	30	GLN	HA	4.397	0.02	1
1	A	30	GLN	HB2	2.091	0.02	2
1	A	30	GLN	HB3	1.954	0.02	2
1	A	30	GLN	HE21	7.532	0.02	2
1	A	30	GLN	HE22	6.828	0.02	2
1	A	30	GLN	HG2	2.321	0.02	1
1	A	31	SER	H	8.232	0.02	1
1	A	31	SER	HA	4.515	0.02	1
1	A	31	SER	HB2	4.008	0.02	2
1	A	31	SER	HB3	3.85	0.02	2
1	A	32	LEU	H	8.57	0.02	1
1	A	32	LEU	HA	4.252	0.02	1
1	A	32	LEU	HB2	1.9	0.02	1
1	A	32	LEU	HD11	0.937	0.02	2
1	A	32	LEU	HD12	0.937	0.02	2
1	A	32	LEU	HD13	0.937	0.02	2
1	A	32	LEU	HD21	0.881	0.02	2
1	A	32	LEU	HD22	0.881	0.02	2
1	A	32	LEU	HD23	0.881	0.02	2
1	A	32	LEU	HG	1.661	0.02	1
1	A	33	ASP	H	8.319	0.02	1
1	A	33	ASP	HA	4.49	0.02	1
1	A	33	ASP	HB2	2.638	0.02	1
1	A	34	GLY	H	8.15	0.02	1
1	A	34	GLY	HA2	3.987	0.02	2
1	A	34	GLY	HA3	3.856	0.02	2
1	A	35	ILE	H	7.972	0.02	1
1	A	35	ILE	HA	3.987	0.02	1
1	A	35	ILE	HB	1.9	0.02	1
1	A	35	ILE	HD11	0.842	0.02	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	35	ILE	HD12	0.842	0.02	1
1	A	35	ILE	HD13	0.842	0.02	1
1	A	35	ILE	HG12	1.502	0.02	2
1	A	35	ILE	HG13	1.15	0.02	2
1	A	36	MET	H	8.332	0.02	1
1	A	36	MET	HA	4.54	0.02	1
1	A	36	MET	HB2	2.08	0.02	1
1	A	36	MET	HG2	2.864	0.02	2
1	A	36	MET	HG3	2.604	0.02	2
1	A	37	PHE	H	8.214	0.02	1
1	A	37	PHE	HA	4.496	0.02	1
1	A	37	PHE	HB2	3.162	0.02	1
1	A	37	PHE	HD2	6.978	0.02	1
1	A	37	PHE	HE2	7.208	0.02	1
1	A	37	PHE	HZ	7.244	0.02	1
1	A	38	ILE	H	8.08	0.02	1
1	A	38	ILE	HA	3.824	0.02	1
1	A	38	ILE	HB	1.897	0.02	1
1	A	38	ILE	HG12	1.583	0.02	2
1	A	38	ILE	HG13	1.267	0.02	2
1	A	38	ILE	HG21	0.878	0.02	1
1	A	38	ILE	HG22	0.878	0.02	1
1	A	38	ILE	HG23	0.878	0.02	1
1	A	39	ASN	H	8.332	0.02	1
1	A	39	ASN	HA	4.54	0.02	1
1	A	39	ASN	HB2	2.856	0.02	1
1	A	39	ASN	HD21	7.616	0.02	2
1	A	39	ASN	HD22	6.928	0.02	2
1	A	40	LYS	H	8.434	0.02	1
1	A	40	LYS	HA	3.951	0.02	1
1	A	40	LYS	HB2	1.778	0.02	1
1	A	40	LYS	HD2	1.635	0.02	1
1	A	40	LYS	HE2	2.981	0.02	1
1	A	40	LYS	HG2	1.42	0.02	1
1	A	41	CYS	H	8.201	0.02	1
1	A	41	CYS	HA	4.523	0.02	1
1	A	41	CYS	HB2	2.894	0.02	2
1	A	41	CYS	HB3	2.47	0.02	2
1	A	42	ALA	H	7.787	0.02	1
1	A	42	ALA	HA	3.826	0.02	1
1	A	42	ALA	HB1	1.409	0.02	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	42	ALA	HB2	1.409	0.02	1
1	A	42	ALA	HB3	1.409	0.02	1
1	A	43	THR	H	7.796	0.02	1
1	A	43	THR	HA	3.946	0.02	1
1	A	43	THR	HB	4.205	0.02	1
1	A	43	THR	HG21	1.183	0.02	1
1	A	43	THR	HG22	1.183	0.02	1
1	A	43	THR	HG23	1.183	0.02	1
1	A	44	CYS	H	8.114	0.02	1
1	A	44	CYS	HA	4.497	0.02	1
1	A	44	CYS	HB2	2.683	0.02	1
1	A	45	LYS	H	8.371	0.02	1
1	A	45	LYS	HA	3.743	0.02	1
1	A	45	LYS	HB2	1.903	0.02	1
1	A	45	LYS	HD2	1.715	0.02	1
1	A	45	LYS	HG2	1.388	0.02	1
1	A	46	MET	H	7.4	0.02	1
1	A	46	MET	HA	4.189	0.02	1
1	A	46	MET	HB2	2.173	0.02	1
1	A	46	MET	HG2	2.677	0.02	1
1	A	47	ILE	H	7.408	0.02	1
1	A	47	ILE	HA	3.746	0.02	1
1	A	47	ILE	HB	1.935	0.02	1
1	A	47	ILE	HG12	1.68	0.02	2
1	A	47	ILE	HG13	1.179	0.02	2
1	A	47	ILE	HG21	0.846	0.02	1
1	A	47	ILE	HG22	0.846	0.02	1
1	A	47	ILE	HG23	0.846	0.02	1
1	A	48	LEU	H	8.658	0.02	1
1	A	48	LEU	HA	4.124	0.02	1
1	A	48	LEU	HB2	1.79	0.02	1
1	A	48	LEU	HD11	0.862	0.02	1
1	A	48	LEU	HD12	0.862	0.02	1
1	A	48	LEU	HD13	0.862	0.02	1
1	A	48	LEU	HD21	0.862	0.02	1
1	A	48	LEU	HD22	0.862	0.02	1
1	A	48	LEU	HD23	0.862	0.02	1
1	A	48	LEU	HG	1.637	0.02	1
1	A	49	GLU	H	8.063	0.02	1
1	A	49	GLU	HA	4.072	0.02	1
1	A	49	GLU	HB2	2.087	0.02	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	49	GLU	HG2	2.655	0.02	2
1	A	49	GLU	HG3	2.471	0.02	2
1	A	50	LYS	H	7.539	0.02	1
1	A	50	LYS	HA	4.181	0.02	1
1	A	50	LYS	HB2	1.924	0.02	1
1	A	50	LYS	HD2	1.684	0.02	1
1	A	50	LYS	HG2	1.479	0.02	1
1	A	51	GLU	H	7.962	0.02	1
1	A	51	GLU	HA	4.18	0.02	1
1	A	51	GLU	HB2	2.093	0.02	2
1	A	51	GLU	HB3	1.999	0.02	2
1	A	51	GLU	HG2	2.405	0.02	1
1	A	52	ALA	H	7.899	0.02	1
1	A	52	ALA	HA	4.271	0.02	1
1	A	52	ALA	HB1	1.424	0.02	1
1	A	52	ALA	HB2	1.424	0.02	1
1	A	52	ALA	HB3	1.424	0.02	1
1	A	53	LYS	H	7.94	0.02	1
1	A	53	LYS	HA	4.35	0.02	1
1	A	53	LYS	HB2	1.826	0.02	1
1	A	53	LYS	HD2	1.694	0.02	1
1	A	53	LYS	HG2	1.438	0.02	1
1	A	54	SER	H	8.207	0.02	1
1	A	54	SER	HA	4.76	0.02	1
1	A	54	SER	HB2	3.885	0.02	1
1	A	55	GLN	H	7.938	0.02	1
1	A	55	GLN	HA	4.154	0.02	1
1	A	55	GLN	HB2	2.11	0.02	2
1	A	55	GLN	HB3	1.916	0.02	2
1	A	55	GLN	HG2	2.293	0.02	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	51	-0.50 ± 0.29	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 46%, i.e. 331 atoms were assigned a chemical shift out of a possible 713. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	152/258 (59%)	103/104 (99%)	0/104 (0%)	49/50 (98%)
Sidechain	168/409 (41%)	163/262 (62%)	0/132 (0%)	5/15 (33%)
Aromatic	11/46 (24%)	11/24 (46%)	0/22 (0%)	0/0 (—%)
Overall	331/713 (46%)	277/390 (71%)	0/258 (0%)	54/65 (83%)

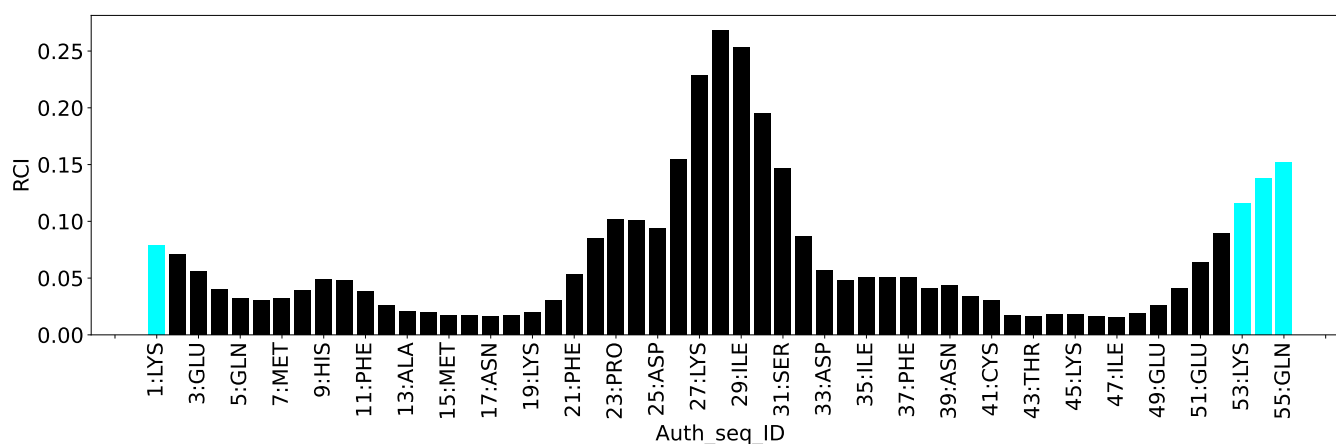
7.1.4 Statistically unusual chemical shifts [i](#)

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	518
Intra-residue ($ i-j =0$)	152
Sequential ($ i-j =1$)	167
Medium range ($ i-j >1$ and $ i-j <5$)	99
Long range ($ i-j \geq 5$)	100
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	9.4
Number of long range restraints per residue ¹	1.8

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)	16.6	0.2
0.2-0.5 (Medium)	31.8	0.5
>0.5 (Large)	43.4	3.04

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

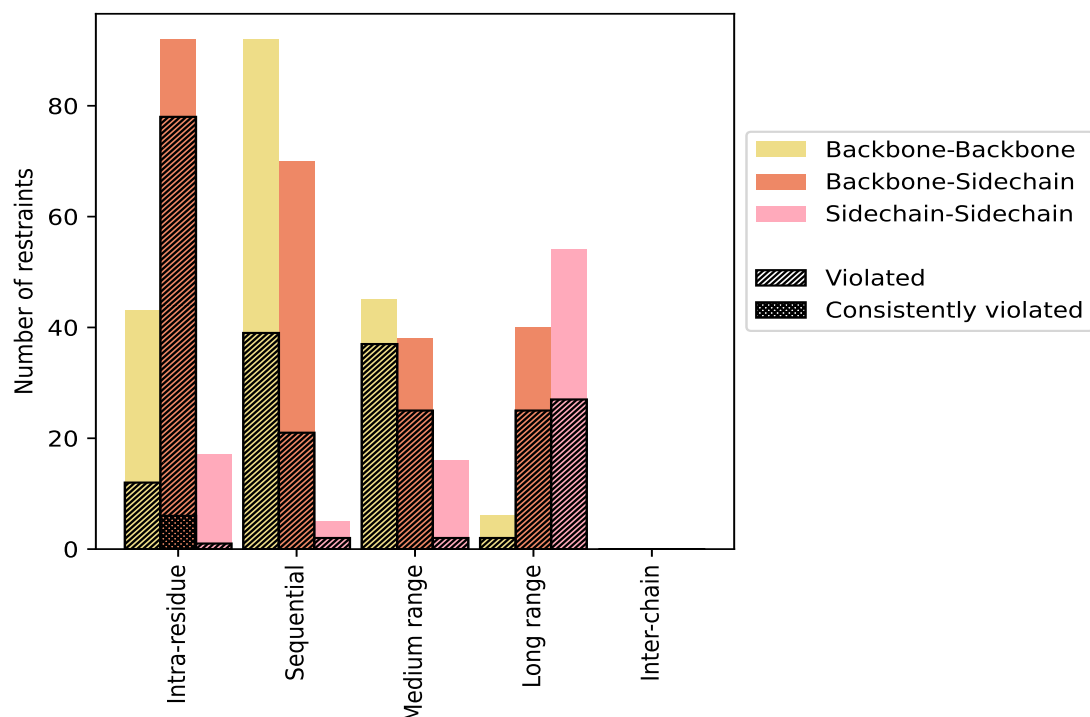
9.1 Summary of distance violations ⓘ

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)	152	29.3	91	59.9	17.6	6	3.9	1.2
Backbone-Backbone	43	8.3	12	27.9	2.3	0	0.0	0.0
Backbone-Sidechain	92	17.8	78	84.8	15.1	6	6.5	1.2
Sidechain-Sidechain	17	3.3	1	5.9	0.2	0	0.0	0.0
Sequential (i-j =1)	167	32.2	62	37.1	12.0	0	0.0	0.0
Backbone-Backbone	92	17.8	39	42.4	7.5	0	0.0	0.0
Backbone-Sidechain	70	13.5	21	30.0	4.1	0	0.0	0.0
Sidechain-Sidechain	5	1.0	2	40.0	0.4	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	99	19.1	64	64.6	12.4	0	0.0	0.0
Backbone-Backbone	45	8.7	37	82.2	7.1	0	0.0	0.0
Backbone-Sidechain	38	7.3	25	65.8	4.8	0	0.0	0.0
Sidechain-Sidechain	16	3.1	2	12.5	0.4	0	0.0	0.0
Long range (i-j ≥5)	100	19.3	54	54.0	10.4	0	0.0	0.0
Backbone-Backbone	6	1.2	2	33.3	0.4	0	0.0	0.0
Backbone-Sidechain	40	7.7	25	62.5	4.8	0	0.0	0.0
Sidechain-Sidechain	54	10.4	27	50.0	5.2	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	518	100.0	271	52.3	52.3	6	1.2	1.2
Backbone-Backbone	186	35.9	90	48.4	17.4	0	0.0	0.0
Backbone-Sidechain	240	46.3	149	62.1	28.8	6	2.5	1.2
Sidechain-Sidechain	92	17.8	32	34.8	6.2	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	42	13	26	20	0	101	0.61	2.31	0.49	0.44
2	42	7	19	16	0	84	0.64	2.59	0.5	0.44
3	44	7	20	18	0	89	0.65	2.6	0.54	0.51
4	47	9	22	14	0	92	0.61	2.5	0.5	0.42
5	44	12	31	14	0	101	0.62	2.66	0.51	0.44
6	44	4	18	11	0	77	0.58	2.54	0.48	0.42
7	48	8	19	13	0	88	0.65	2.37	0.55	0.46
8	43	10	22	8	0	83	0.63	2.74	0.55	0.46
9	52	15	22	17	0	106	0.68	2.95	0.57	0.51
10	49	11	22	16	0	98	0.59	2.6	0.46	0.44

Continued on next page...

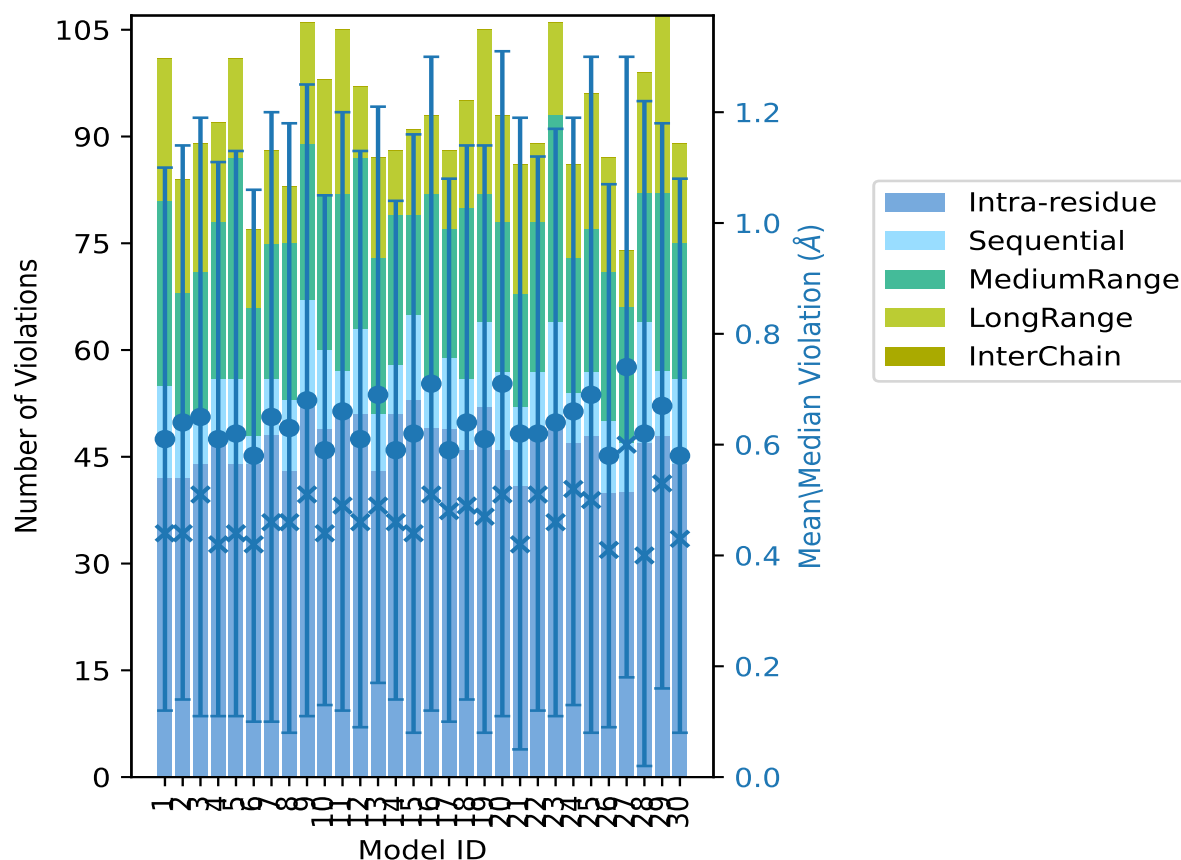
Continued from previous page...

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				
11	51	6	25	23	0	105	0.66	2.48	0.54	0.49
12	51	12	24	10	0	97	0.61	2.65	0.52	0.46
13	43	8	22	14	0	87	0.69	2.57	0.52	0.49
14	51	7	21	9	0	88	0.59	2.33	0.45	0.46
15	53	12	14	12	0	91	0.62	2.46	0.54	0.44
16	49	7	26	11	0	93	0.71	2.7	0.59	0.51
17	49	10	18	11	0	88	0.59	2.6	0.49	0.48
18	46	10	24	15	0	95	0.64	2.29	0.5	0.49
19	52	12	18	23	0	105	0.61	3.03	0.53	0.47
20	46	11	21	15	0	93	0.71	3.0	0.6	0.51
21	41	11	16	18	0	86	0.62	2.95	0.57	0.42
22	49	8	21	11	0	89	0.62	2.93	0.5	0.51
23	50	14	29	13	0	106	0.64	2.82	0.53	0.46
24	47	7	19	13	0	86	0.66	2.86	0.53	0.52
25	48	9	20	19	0	96	0.69	2.95	0.61	0.5
26	40	10	21	16	0	87	0.58	2.29	0.49	0.41
27	40	7	19	8	0	74	0.74	2.66	0.56	0.6
28	47	17	18	17	0	99	0.62	3.04	0.6	0.4
29	48	9	25	25	0	107	0.67	2.49	0.51	0.53
30	44	12	19	14	0	89	0.58	2.6	0.5	0.43

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 247(IR:61, SQ:105, MR:35, LR:46, 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	%
2	14	3	9	0	28	1	3.3
2	11	5	5	0	23	2	6.7
4	5	4	2	0	15	3	10.0
2	8	5	7	0	22	4	13.3
2	4	4	2	0	12	5	16.7
2	2	3	3	0	10	6	20.0

Continued on next page...

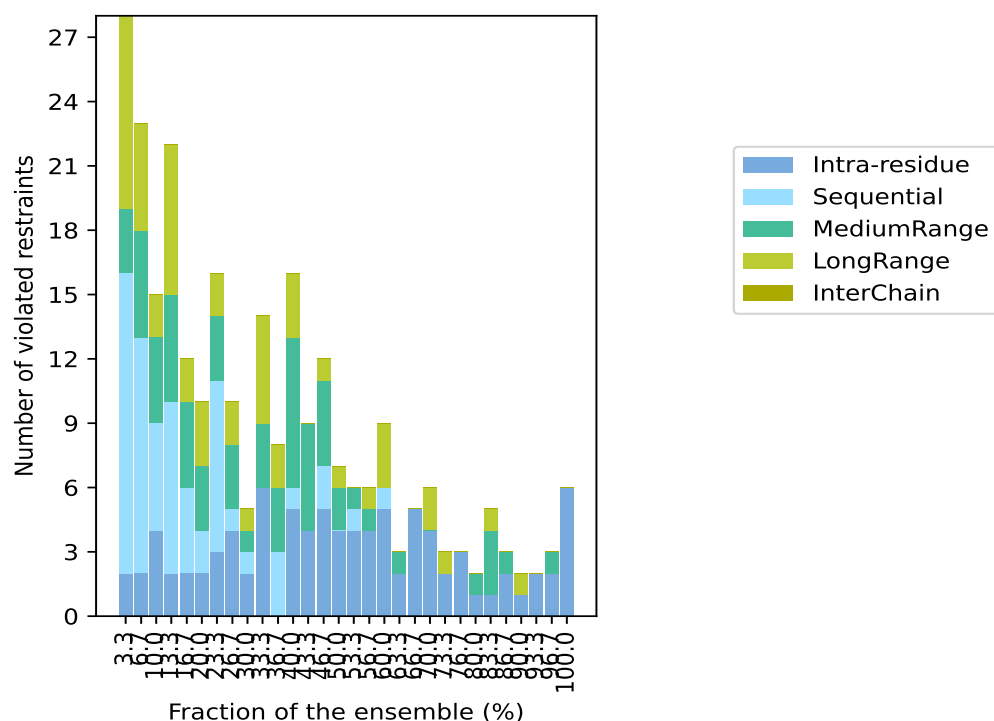
Continued from previous page...

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
3	8	3	2	0	16	7	23.3
4	1	3	2	0	10	8	26.7
2	1	1	1	0	5	9	30.0
6	0	3	5	0	14	10	33.3
0	3	3	2	0	8	11	36.7
5	1	7	3	0	16	12	40.0
4	0	5	0	0	9	13	43.3
5	2	4	1	0	12	14	46.7
4	0	2	1	0	7	15	50.0
4	1	1	0	0	6	16	53.3
4	0	1	1	0	6	17	56.7
5	1	0	3	0	9	18	60.0
2	0	1	0	0	3	19	63.3
5	0	0	0	0	5	20	66.7
4	0	0	2	0	6	21	70.0
2	0	0	1	0	3	22	73.3
3	0	0	0	0	3	23	76.7
1	0	1	0	0	2	24	80.0
1	0	3	1	0	5	25	83.3
2	0	1	0	0	3	26	86.7
1	0	0	1	0	2	27	90.0
2	0	0	0	0	2	28	93.3
2	0	1	0	0	3	29	96.7
6	0	0	0	0	6	30	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](#)

No violations found

9.5 All violated distance restraints [i](#)

No violations found

10 Dihedral-angle violation analysis

No dihedral-angle restraints found