



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 5IXF / pdb_00005ixf
BMRB ID : 30041
Title : Solution structure of the STAM2 SH3 with AMSH derived peptide complex
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Deposited on : 2016-03-23

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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
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

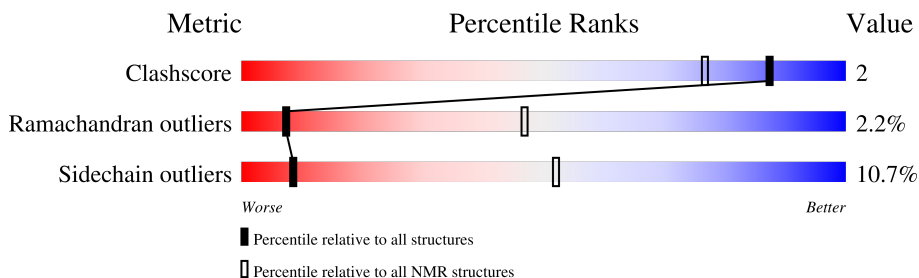
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 50%.

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	109	60% (green), 38% (grey), 2% (yellow)
2	B	14	71% (green), 14% (yellow), 7% (orange), 7% (cyan)

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 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:203-A:270, B:1-B:13 (81)	1.15	3

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, 3, 4
2	6, 10
Single-model clusters	5; 7; 8; 9

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1305 atoms, of which 648 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Signal transducing adapter molecule 2.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	68	1091	353	535	95	108	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	expression tag	UNP O75886
A	165	ALA	-	expression tag	UNP O75886
A	166	MET	-	expression tag	UNP O75886
A	167	GLY	-	expression tag	UNP O75886
A	168	MET	-	expression tag	UNP O75886
A	261	ASP	ASN	conflict	UNP O75886

- Molecule 2 is a protein called STAM-binding protein.

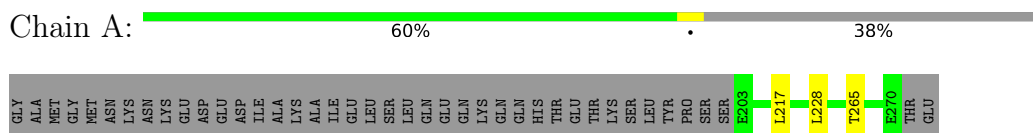
Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	14	214	64	113	19	18	0

4 Residue-property plots

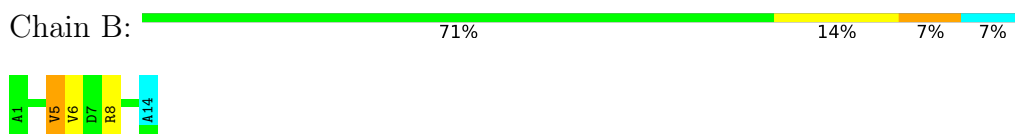
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Signal transducing adapter molecule 2



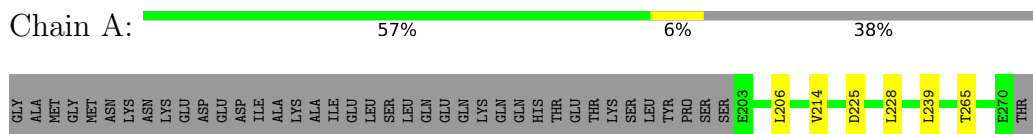
- Molecule 2: STAM-binding protein



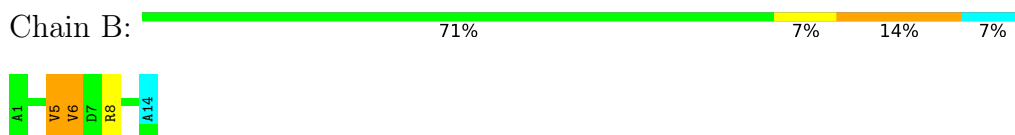
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 3. Colouring as in section 4.1 above.

- Molecule 1: Signal transducing adapter molecule 2



- Molecule 2: STAM-binding protein



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 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	structure calculation	
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	888
Number of shifts mapped to atoms	560
Number of unparsed shifts	0
Number of shifts with mapping errors	328
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	50%

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	556	535	532	2±2
2	B	95	108	108	2±1
All	All	6510	6430	6400	26

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 2.

5 of 22 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:245:ASN:O	1:A:259:PRO:HA	0.60	1.96	9	2
2:B:5:VAL:O	2:B:6:VAL:HB	0.59	1.96	2	3
1:A:261:ASP:HB3	2:B:5:VAL:HG23	0.56	1.76	5	1
2:B:4:PRO:O	2:B:5:VAL:HB	0.50	2.07	6	1
1:A:218:TYR:CD1	2:B:5:VAL:HB	0.49	2.42	1	2

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	66/109 (61%)	57±3 (87±4%)	8±3 (13±4%)	0±0 (0±1%)	26	74
2	B	12/14 (86%)	7±2 (55±13%)	4±1 (33±11%)	1±1 (12±9%)	1	7
All	All	780/1230 (63%)	638 (82%)	125 (16%)	17 (2%)	7	47

5 of 8 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	5	VAL	7
2	B	6	VAL	3
2	B	3	PRO	2
2	B	7	ASP	1
1	A	222	ALA	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	60/96 (62%)	54±2 (89±3%)	6±2 (11±3%)	8	52
2	B	11/11 (100%)	10±1 (89±5%)	1±1 (11±5%)	8	52
All	All	710/1070 (66%)	634 (89%)	76 (11%)	8	52

5 of 29 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	217	LEU	8
1	A	265	THR	8
1	A	228	LEU	7
2	B	8	ARG	6
1	A	247	TRP	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 i

The completeness of assignment taking into account all chemical shift lists is 50% for the well-defined parts and 49% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *allshifts_nmrstar_resultat2.bmr*

7.1.1 Bookkeeping i

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

Total number of shifts	888
Number of shifts mapped to atoms	560
Number of unparsed shifts	0
Number of shifts with mapping errors	328
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 328) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	165	ALA	HA	4.241	0.00	1
1	A	165	ALA	HB1	1.277	0.00	1
1	A	165	ALA	HB2	1.277	0.00	1
1	A	165	ALA	HB3	1.277	0.00	1
1	A	165	ALA	C	178.019	.	1
1	A	165	ALA	CA	52.282	0.00	1
1	A	165	ALA	CB	19.327	0.00	1
1	A	166	MET	H	8.461	0.00	1
1	A	166	MET	HA	4.365	0.00	1
1	A	166	MET	HB2	1.989	0.00	1
1	A	166	MET	HB3	1.921	0.00	1
1	A	166	MET	C	176.956	.	1
1	A	166	MET	CA	55.334	0.00	1
1	A	166	MET	CB	31.901	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	166	MET	N	119.749	0.00	1
1	A	167	GLY	H	8.367	0.00	1
1	A	167	GLY	HA2	3.838	0.00	2
1	A	167	GLY	HA3	3.838	0.00	2
1	A	167	GLY	C	174.287	.	1
1	A	167	GLY	CA	45.306	0.00	1
1	A	167	GLY	N	110.154	0.00	1
1	A	168	MET	H	8.152	0.00	1
1	A	168	MET	HA	4.356	0.00	1
1	A	168	MET	HB2	1.962	0.00	1
1	A	168	MET	HB3	1.889	0.00	1
1	A	168	MET	C	176.455	.	1
1	A	168	MET	CA	55.195	0.00	1
1	A	168	MET	CB	31.786	0.00	1
1	A	168	MET	N	119.629	0.00	1
1	A	169	ASN	H	8.416	0.00	1
1	A	169	ASN	HB2	2.753	0.00	1
1	A	169	ASN	HB3	2.654	0.00	1
1	A	169	ASN	CA	53.191	0.00	1
1	A	169	ASN	CB	38.648	0.00	1
1	A	169	ASN	N	119.793	0.00	1
1	A	170	LYS	H	8.237	0.00	1
1	A	170	LYS	HA	4.179	0.00	1
1	A	170	LYS	HB2	1.721	0.00	1
1	A	170	LYS	HB3	1.629	0.00	1
1	A	170	LYS	C	176.455	.	1
1	A	170	LYS	CA	56.138	0.00	1
1	A	170	LYS	CB	32.891	0.00	1
1	A	170	LYS	N	121.91	0.01	1
1	A	171	ASN	H	8.435	0.00	1
1	A	171	ASN	HA	4.569	0.00	1
1	A	171	ASN	CA	53.191	0.00	1
1	A	171	ASN	CB	38.648	0.00	1
1	A	171	ASN	N	119.712	0.00	1
1	A	172	LYS	H	8.237	0.00	1
1	A	172	LYS	HA	4.094	0.00	1
1	A	172	LYS	HB2	1.723	0.00	1
1	A	172	LYS	HB3	1.692	0.00	1
1	A	172	LYS	HD2	1.568	0.00	2
1	A	172	LYS	HD3	1.568	0.00	2
1	A	172	LYS	HG2	1.322	0.00	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	172	LYS	HG3	1.322	0.00	2
1	A	172	LYS	C	177.148	.	1
1	A	172	LYS	CA	57.354	0.22	1
1	A	172	LYS	CB	32.559	0.00	1
1	A	172	LYS	CD	28.777	0.00	1
1	A	172	LYS	CG	24.367	0.00	1
1	A	172	LYS	N	121.91	0.01	1
1	A	173	GLU	H	8.329	0.14	1
1	A	173	GLU	HB2	1.94	0.00	1
1	A	173	GLU	HB3	1.87	0.00	1
1	A	173	GLU	C	177.615	.	1
1	A	173	GLU	CB	29.615	0.00	1
1	A	173	GLU	N	120.433	0.39	1
1	A	174	ASP	H	8.136	0.00	1
1	A	174	ASP	HA	4.407	0.00	1
1	A	174	ASP	HB2	2.584	0.00	2
1	A	174	ASP	HB3	2.584	0.00	2
1	A	174	ASP	C	177.555	.	1
1	A	174	ASP	CA	55.074	0.00	1
1	A	174	ASP	CB	40.566	0.00	1
1	A	174	ASP	N	119.881	0.00	1
1	A	175	GLU	H	8.099	0.00	1
1	A	175	GLU	HA	4.061	0.00	1
1	A	175	GLU	HB2	1.92	0.00	2
1	A	175	GLU	HB3	1.92	0.00	2
1	A	175	GLU	C	177.338	.	1
1	A	175	GLU	CA	57.505	0.00	1
1	A	175	GLU	CB	30.088	0.00	1
1	A	175	GLU	N	121.414	0.00	1
1	A	176	ASP	H	8.28	0.00	1
1	A	176	ASP	HA	4.43	0.00	1
1	A	176	ASP	HB2	2.588	0.00	2
1	A	176	ASP	HB3	2.588	0.00	2
1	A	176	ASP	C	178.014	.	1
1	A	176	ASP	CA	55.23	0.00	1
1	A	176	ASP	CB	40.517	0.00	1
1	A	176	ASP	N	121.171	0.00	1
1	A	177	ILE	H	7.902	0.00	1
1	A	177	ILE	HA	3.867	0.00	1
1	A	177	ILE	HB	1.811	0.00	1
1	A	177	ILE	HG12	1.28	0.18	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	177	ILE	HG13	1.28	0.18	2
1	A	177	ILE	HG21	0.83	0.00	1
1	A	177	ILE	HG22	0.83	0.00	1
1	A	177	ILE	HG23	0.83	0.00	1
1	A	177	ILE	C	177.201	.	1
1	A	177	ILE	CA	62.855	0.00	1
1	A	177	ILE	CB	38.26	0.00	1
1	A	177	ILE	CG1	28.11	0.00	1
1	A	177	ILE	CG2	17.189	0.00	1
1	A	177	ILE	N	122.202	0.00	1
1	A	178	ALA	H	7.98	0.00	1
1	A	178	ALA	HA	4.075	0.00	1
1	A	178	ALA	HB1	1.334	0.00	1
1	A	178	ALA	HB2	1.334	0.00	1
1	A	178	ALA	HB3	1.334	0.00	1
1	A	178	ALA	CA	53.824	0.00	1
1	A	178	ALA	CB	18.39	0.00	1
1	A	178	ALA	N	124.358	0.00	1
1	A	179	LYS	H	7.967	0.00	1
1	A	179	LYS	HA	4.063	0.00	1
1	A	179	LYS	HB2	1.747	0.00	2
1	A	179	LYS	HB3	1.747	0.00	2
1	A	179	LYS	HD2	1.585	0.00	2
1	A	179	LYS	HD3	1.585	0.00	2
1	A	179	LYS	C	177.531	.	1
1	A	179	LYS	CA	57.196	0.00	1
1	A	179	LYS	CB	32.385	0.00	1
1	A	179	LYS	CD	28.852	0.00	1
1	A	179	LYS	N	119.404	0.00	1
1	A	180	ALA	H	7.861	0.00	1
1	A	180	ALA	HA	4.111	0.00	1
1	A	180	ALA	HB1	1.353	0.00	1
1	A	180	ALA	HB2	1.353	0.00	1
1	A	180	ALA	HB3	1.353	0.00	1
1	A	180	ALA	C	171.664	.	1
1	A	180	ALA	CA	53.738	0.00	1
1	A	180	ALA	CB	18.499	0.00	1
1	A	180	ALA	N	123.501	0.00	1
1	A	181	ILE	H	7.978	0.00	1
1	A	181	ILE	HA	3.822	0.00	1
1	A	181	ILE	HB	1.788	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	181	ILE	HG12	1.291	0.23	2
1	A	181	ILE	HG13	1.291	0.23	2
1	A	181	ILE	HG21	0.793	0.00	1
1	A	181	ILE	HG22	0.793	0.00	1
1	A	181	ILE	HG23	0.793	0.00	1
1	A	181	ILE	C	177.67	.	1
1	A	181	ILE	CA	62.918	0.00	1
1	A	181	ILE	CB	38.317	0.00	1
1	A	181	ILE	CG1	28.123	0.00	1
1	A	181	ILE	CG2	17.036	0.00	1
1	A	181	ILE	N	120.246	0.00	1
1	A	182	GLU	H	8.065	0.00	1
1	A	182	GLU	HA	4.03	0.00	1
1	A	182	GLU	HB2	1.957	0.00	2
1	A	182	GLU	HB3	1.957	0.00	2
1	A	182	GLU	C	178.084	.	1
1	A	182	GLU	CA	57.962	0.00	1
1	A	182	GLU	CB	29.71	0.00	1
1	A	182	GLU	N	122.896	0.00	1
1	A	183	LEU	H	8.117	0.00	1
1	A	183	LEU	HA	4.126	0.00	1
1	A	183	LEU	HB2	1.611	0.00	1
1	A	183	LEU	HB3	1.502	0.00	1
1	A	183	LEU	HG	0.798	0.00	1
1	A	183	LEU	CA	56.294	0.00	1
1	A	183	LEU	CB	41.644	0.00	1
1	A	183	LEU	CG	26.768	0.00	1
1	A	183	LEU	N	121.496	0.00	1
1	A	184	SER	H	8.068	0.00	1
1	A	184	SER	HA	4.253	0.00	1
1	A	184	SER	HB2	3.868	0.00	2
1	A	184	SER	HB3	3.868	0.00	2
1	A	184	SER	C	175.875	.	1
1	A	184	SER	CA	59.566	0.00	1
1	A	184	SER	CB	63.066	0.00	1
1	A	184	SER	N	115.977	0.00	1
1	A	185	LEU	H	7.984	0.00	1
1	A	185	LEU	HA	4.128	0.00	1
1	A	185	LEU	HB2	1.668	0.00	1
1	A	185	LEU	HB3	1.474	0.00	1
1	A	185	LEU	HG	0.795	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	185	LEU	CA	56.17	0.00	1
1	A	185	LEU	CB	41.468	0.00	1
1	A	185	LEU	CG	26.713	0.00	1
1	A	185	LEU	N	122.708	0.00	1
1	A	186	GLN	H	7.954	0.00	1
1	A	186	GLN	HA	4.067	0.00	1
1	A	186	GLN	HB2	2.004	0.00	2
1	A	186	GLN	HB3	2.004	0.00	2
1	A	186	GLN	HG2	2.322	0.00	2
1	A	186	GLN	HG3	2.322	0.00	2
1	A	186	GLN	C	177.332	.	1
1	A	186	GLN	CA	57.042	0.00	1
1	A	186	GLN	CB	28.771	0.00	1
1	A	186	GLN	CG	33.574	0.00	1
1	A	186	GLN	N	119.135	0.00	1
1	A	187	GLU	H	8.082	0.00	1
1	A	187	GLU	HA	4.13	0.00	1
1	A	187	GLU	HB2	1.751	0.00	1
1	A	187	GLU	HB3	1.689	0.00	1
1	A	187	GLU	C	177.211	.	1
1	A	187	GLU	CA	57.245	0.00	1
1	A	187	GLU	CB	30.048	0.00	1
1	A	187	GLU	N	120.554	0.00	1
1	A	188	GLN	H	8.112	0.00	1
1	A	188	GLN	HA	4.111	0.00	1
1	A	188	GLN	HB2	2.032	0.00	1
1	A	188	GLN	HB3	1.937	0.00	1
1	A	188	GLN	C	176.888	.	1
1	A	188	GLN	CA	56.476	0.00	1
1	A	188	GLN	CB	28.973	0.00	1
1	A	188	GLN	N	120.128	0.00	1
1	A	189	LYS	H	8.026	0.00	1
1	A	189	LYS	HA	4.06	0.00	1
1	A	189	LYS	HB2	1.944	0.00	2
1	A	189	LYS	HB3	1.944	0.00	2
1	A	189	LYS	C	177.211	.	1
1	A	189	LYS	CA	56.743	0.00	1
1	A	189	LYS	CB	32.758	0.00	1
1	A	189	LYS	N	121.034	0.00	1
1	A	190	GLN	H	8.098	0.00	1
1	A	190	GLN	HA	3.857	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	190	GLN	HB2	1.923	0.00	1
1	A	190	GLN	HB3	1.832	0.00	1
1	A	190	GLN	CA	56.057	0.00	1
1	A	190	GLN	CB	29.379	0.00	1
1	A	190	GLN	N	120.12	0.01	1
1	A	191	GLN	H	8.302	0.00	1
1	A	191	GLN	HA	4.15	0.00	1
1	A	191	GLN	HB2	1.959	0.00	1
1	A	191	GLN	HB3	1.89	0.00	1
1	A	191	GLN	HG2	2.265	0.00	2
1	A	191	GLN	HG3	2.265	0.00	2
1	A	191	GLN	C	176.26	.	1
1	A	191	GLN	CA	55.899	0.00	1
1	A	191	GLN	CB	29.715	0.58	1
1	A	191	GLN	CG	33.631	0.00	1
1	A	191	GLN	N	120.312	0.01	1
1	A	192	HIS	H	8.177	0.00	1
1	A	192	HIS	HA	4.607	0.00	1
1	A	192	HIS	HB2	3.092	0.00	1
1	A	192	HIS	HB3	3.017	0.00	1
1	A	192	HIS	C	175.352	.	1
1	A	192	HIS	CA	55.798	0.00	1
1	A	192	HIS	CB	30.057	0.00	1
1	A	192	HIS	N	120.598	0.00	1
1	A	193	THR	H	8.03	0.00	1
1	A	193	THR	HA	4.182	0.00	1
1	A	193	THR	HB	4.055	0.00	1
1	A	193	THR	C	174.479	.	1
1	A	193	THR	CA	61.832	0.00	1
1	A	193	THR	CB	69.687	0.00	1
1	A	193	THR	N	116.042	0.00	1
1	A	194	GLU	H	8.48	0.00	1
1	A	194	GLU	HA	4.248	0.00	1
1	A	194	GLU	HB2	1.963	0.00	1
1	A	194	GLU	HB3	1.851	0.00	1
1	A	194	GLU	C	176.742	.	1
1	A	194	GLU	CA	56.249	0.00	1
1	A	194	GLU	CB	30.255	0.00	1
1	A	194	GLU	N	123.639	0.00	1
1	A	195	THR	H	8.19	0.00	1
1	A	195	THR	HA	4.17	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	195	THR	HB	4.068	0.00	1
1	A	195	THR	CA	62.189	0.00	1
1	A	195	THR	CB	69.476	0.00	1
1	A	195	THR	N	116.546	0.01	1
1	A	196	LYS	H	8.274	0.00	1
1	A	196	LYS	HA	4.219	0.00	1
1	A	196	LYS	HB2	1.705	0.00	1
1	A	196	LYS	HB3	1.634	0.00	1
1	A	196	LYS	HG2	1.301	0.00	2
1	A	196	LYS	HG3	1.301	0.00	2
1	A	196	LYS	C	176.605	.	1
1	A	196	LYS	CA	55.986	0.00	1
1	A	196	LYS	CB	32.875	0.00	1
1	A	196	LYS	CG	28.823	0.00	1
1	A	196	LYS	N	124.19	0.00	1
1	A	197	SER	H	8.212	0.00	1
1	A	197	SER	HB2	3.687	0.00	2
1	A	197	SER	HB3	3.687	0.00	2
1	A	197	SER	C	174.38	.	1
1	A	197	SER	CA	58.055	0.00	1
1	A	197	SER	CB	63.515	0.00	1
1	A	197	SER	N	116.982	0.00	1
1	A	198	LEU	H	8.107	0.00	1
1	A	198	LEU	HA	4.117	0.00	1
1	A	198	LEU	HB2	1.331	0.00	1
1	A	198	LEU	HB3	1.216	0.00	1
1	A	198	LEU	C	176.714	.	1
1	A	198	LEU	CA	54.929	0.00	1
1	A	198	LEU	CB	42.061	0.00	1
1	A	198	LEU	N	124.044	0.00	1
1	A	199	TYR	H	7.964	0.00	1
1	A	199	TYR	N	120.408	0.00	1
1	A	200	PRO	HA	4.342	0.00	1
1	A	200	PRO	HB2	2.169	0.00	2
1	A	200	PRO	HB3	2.169	0.00	2
1	A	200	PRO	HD2	3.609	0.00	1
1	A	200	PRO	HG2	1.852	0.00	2
1	A	200	PRO	HG3	1.852	0.00	2
1	A	200	PRO	C	177.178	.	1
1	A	200	PRO	CA	63.025	0.00	1
1	A	200	PRO	CB	31.871	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	200	PRO	CD	50.495	0.00	1
1	A	200	PRO	CG	27.115	0.00	1
1	A	201	SER	H	8.339	0.00	1
1	A	201	SER	HA	3.845	0.00	1
1	A	201	SER	HB2	3.765	0.00	2
1	A	201	SER	HB3	3.765	0.00	2
1	A	201	SER	C	174.992	.	1
1	A	201	SER	CA	58.599	0.00	1
1	A	201	SER	CB	63.473	0.00	1
1	A	201	SER	N	116.208	0.00	1
1	A	202	SER	H	8.289	0.00	1
1	A	202	SER	HA	4.334	0.00	1
1	A	202	SER	HB2	3.812	0.00	1
1	A	202	SER	HB3	3.743	0.00	1
1	A	202	SER	C	174.662	.	1
1	A	202	SER	CA	58.605	0.00	1
1	A	202	SER	CB	63.343	0.00	1
1	A	202	SER	N	117.585	0.01	1
1	A	271	THR	H	8.044	0.00	1
1	A	271	THR	HA	4.221	0.00	1
1	A	271	THR	HB	4.129	0.00	1
1	A	271	THR	C	173.782	.	1
1	A	271	THR	CA	61.496	0.00	1
1	A	271	THR	CB	69.674	0.00	1
1	A	271	THR	N	114.646	0.00	1
1	A	272	GLU	H	7.911	0.00	1
1	A	272	GLU	N	127.933	0.00	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	104	0.30 ± 0.33	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	99	-0.17 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	92	0.18 ± 0.34	None needed (< 0.5 ppm)
^{15}N	104	-0.11 ± 0.48	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 50%, i.e. 560 atoms were assigned a chemical shift out of a possible 1126. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	328/402 (82%)	134/163 (82%)	128/162 (79%)	66/77 (86%)
Sidechain	232/635 (37%)	150/409 (37%)	82/200 (41%)	0/26 (0%)
Aromatic	0/89 (0%)	0/44 (0%)	0/39 (0%)	0/6 (0%)
Overall	560/1126 (50%)	284/616 (46%)	210/401 (52%)	66/109 (61%)

7.1.4 Statistically unusual chemical shifts [i](#)

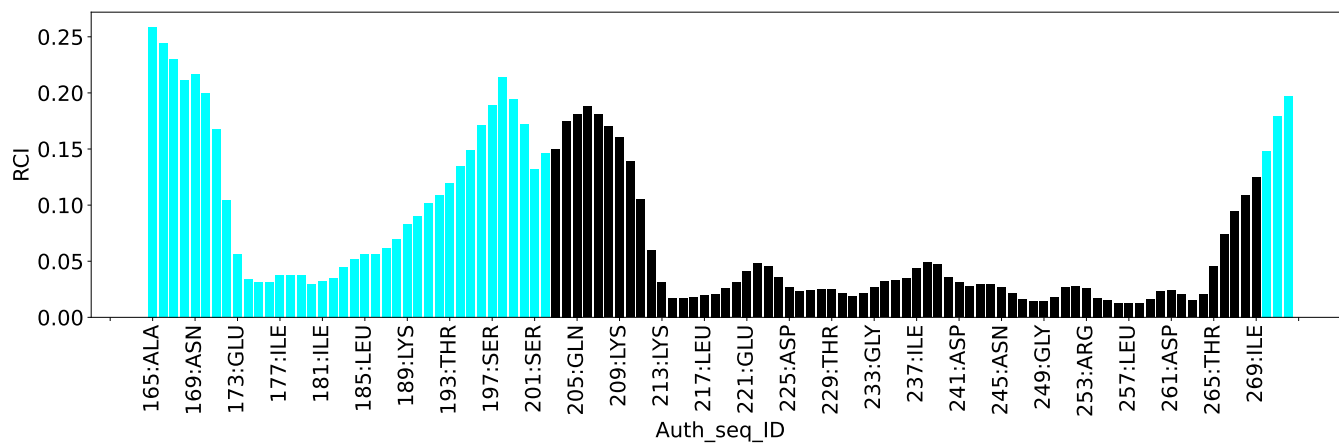
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	241	ASP	HB3	0.65	1.32 – 4.00	-7.5
1	A	254	GLY	N	128.09	91.59 – 127.52	5.2

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	14
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	14
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.1
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)	0.2	0.18
0.2-0.5 (Medium)	0.2	0.26
>0.5 (Large)	3.5	15.05

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis [i](#)

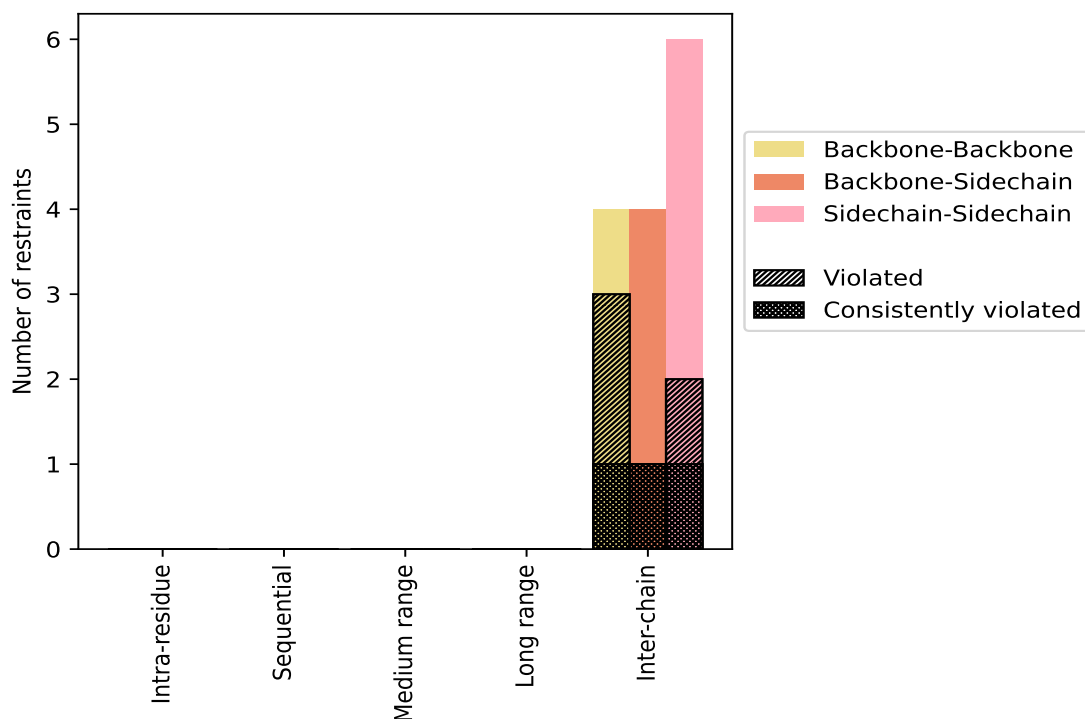
9.1 Summary of distance violations [i](#)

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)	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	14	100.0	6	42.9	42.9	3	21.4	21.4
Backbone-Backbone	4	28.6	3	75.0	21.4	1	25.0	7.1
Backbone-Sidechain	4	28.6	1	25.0	7.1	1	25.0	7.1
Sidechain-Sidechain	6	42.9	2	33.3	14.3	1	16.7	7.1
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	14	100.0	6	42.9	42.9	3	21.4	21.4
Backbone-Backbone	4	28.6	3	75.0	21.4	1	25.0	7.1
Backbone-Sidechain	4	28.6	1	25.0	7.1	1	25.0	7.1
Sidechain-Sidechain	6	42.9	2	33.3	14.3	1	16.7	7.1

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 disulfid bonds are counted in their appropriate category on the x-axis

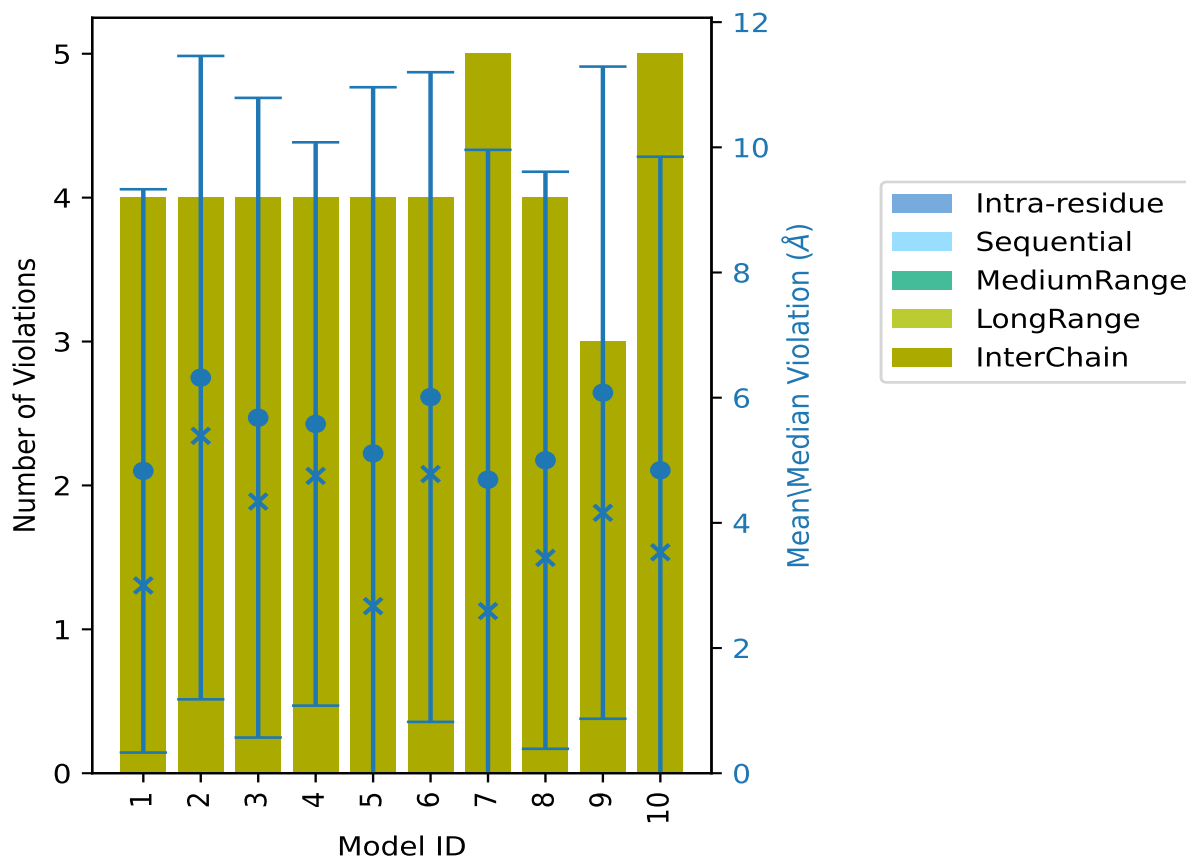
9.2 Distance violation statistics for each model [i](#)

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	4	4	4.83	12.43	4.5	3.0
2	0	0	0	0	4	4	6.32	14.4	5.14	5.39
3	0	0	0	0	4	4	5.68	13.93	5.11	4.34
4	0	0	0	0	4	4	5.58	12.66	4.5	4.75
5	0	0	0	0	4	4	5.11	14.88	5.85	2.67
6	0	0	0	0	4	4	6.01	14.36	5.19	4.78
7	0	0	0	0	5	5	4.69	15.05	5.27	2.59
8	0	0	0	0	4	4	5.0	12.47	4.61	3.44
9	0	0	0	0	3	3	6.08	13.19	5.21	4.16
10	0	0	0	0	5	5	4.84	14.31	5.01	3.53

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, 8(IR:0, SQ:0, MR:0, LR:0, IC:8) 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	1	1	1	10.0
0	0	0	0	1	1	2	20.0
0	0	0	0	0	0	3	30.0

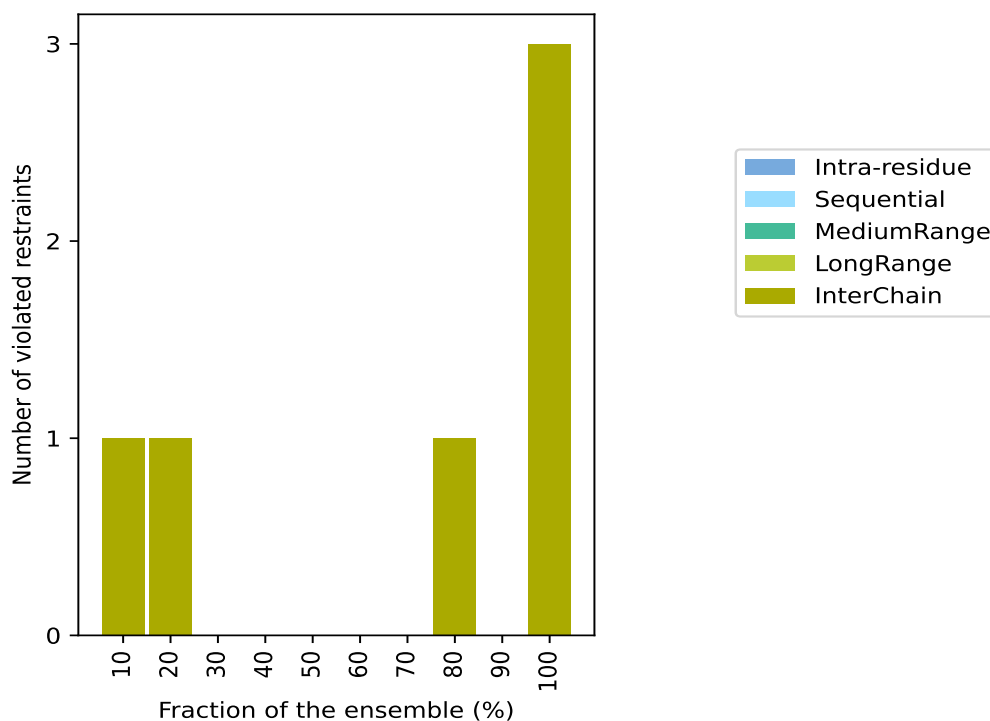
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	4	40.0
0	0	0	0	0	0	5	50.0
0	0	0	0	0	0	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	1	1	8	80.0
0	0	0	0	0	0	9	90.0
0	0	0	0	3	3	10	100.0

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

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

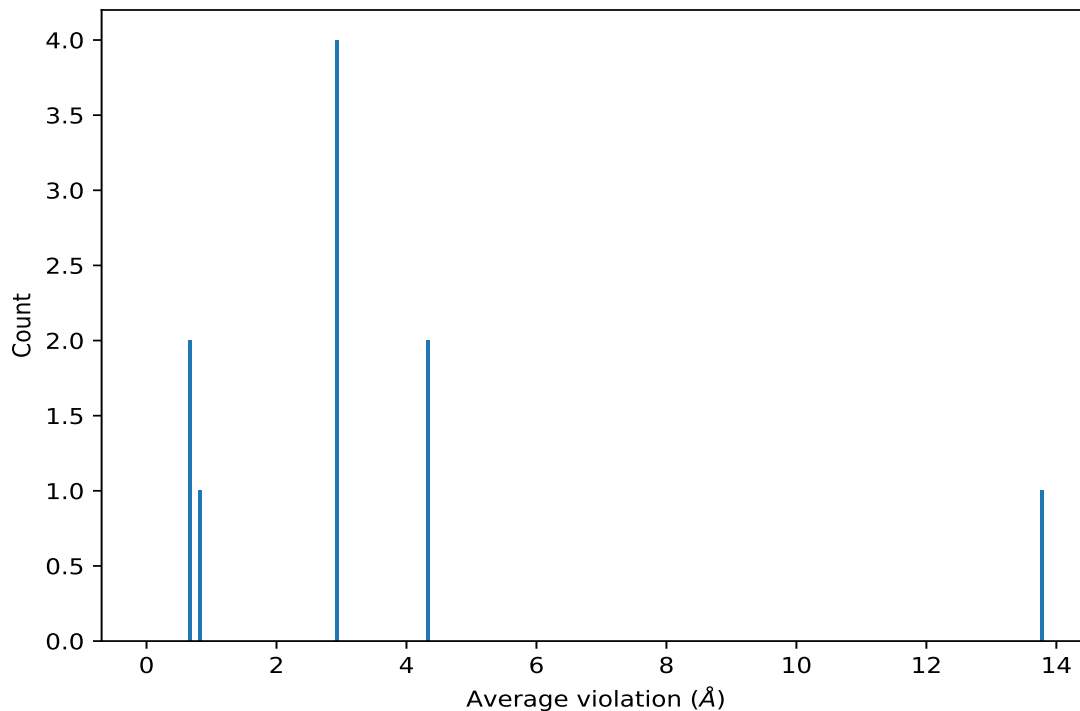


9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean 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.

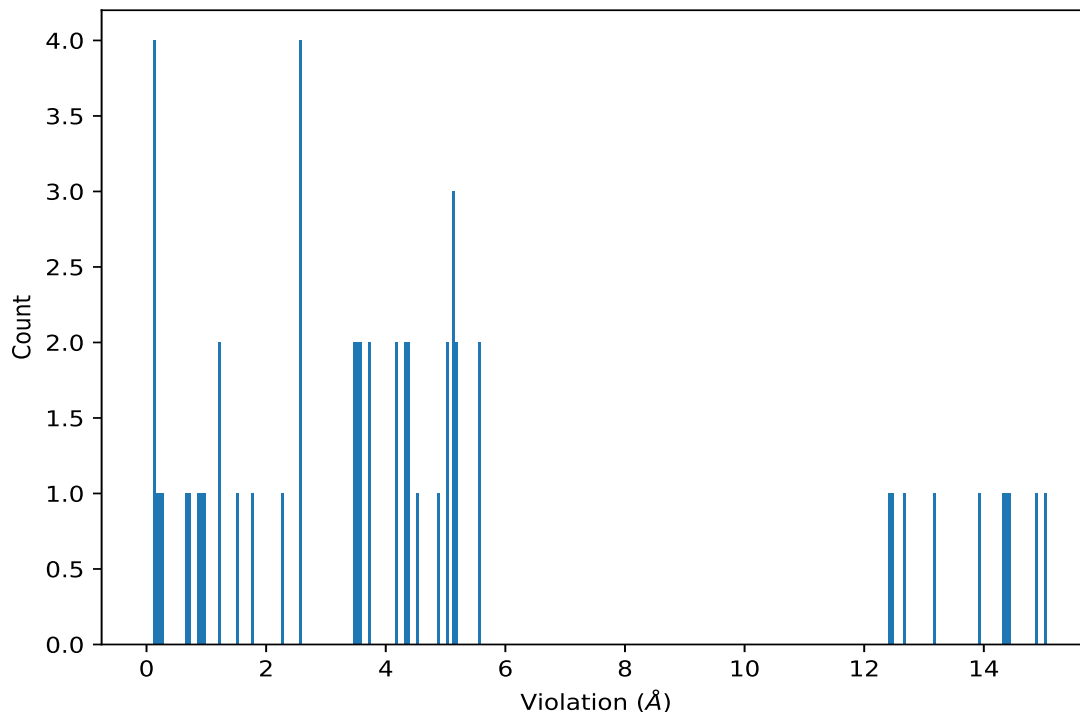
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4)	1:266:A:ASN:HA	2:2:B:LYS:HA	10	13.77	0.95	14.12
(1,2)	1:244:A:ALA:HA	2:11:B:LYS:HG2	10	4.3	0.71	4.26
(1,2)	1:244:A:ALA:HA	2:11:B:LYS:HG3	10	4.3	0.71	4.26
(1,6)	1:218:A:TYR:HD1	2:8:B:ARG:HH22	10	2.9	2.08	2.76
(1,6)	1:218:A:TYR:HD1	2:8:B:ARG:HH21	10	2.9	2.08	2.76
(1,6)	1:218:A:TYR:HD1	2:8:B:ARG:HH11	10	2.9	2.08	2.76
(1,6)	1:218:A:TYR:HD2	2:8:B:ARG:HH21	10	2.9	2.08	2.76
(1,13)	1:260:A:SER:H	2:6:B:VAL:HA	8	0.8	0.83	0.25
(1,9)	1:243:A:ASP:H	2:13:B:GLY:HA2	2	0.66	0.56	0.66
(1,9)	1:243:A:ASP:H	2:13:B:GLY:HA3	2	0.66	0.56	0.66

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)
(1,4)	1:266:A:ASN:HA	2:2:B:LYS:HA	7	15.05
(1,4)	1:266:A:ASN:HA	2:2:B:LYS:HA	5	14.88
(1,4)	1:266:A:ASN:HA	2:2:B:LYS:HA	2	14.4
(1,4)	1:266:A:ASN:HA	2:2:B:LYS:HA	6	14.36
(1,4)	1:266:A:ASN:HA	2:2:B:LYS:HA	10	14.31
(1,4)	1:266:A:ASN:HA	2:2:B:LYS:HA	3	13.93
(1,4)	1:266:A:ASN:HA	2:2:B:LYS:HA	9	13.19
(1,4)	1:266:A:ASN:HA	2:2:B:LYS:HA	4	12.66
(1,4)	1:266:A:ASN:HA	2:2:B:LYS:HA	8	12.47
(1,4)	1:266:A:ASN:HA	2:2:B:LYS:HA	1	12.43

10 Dihedral-angle violation analysis

No dihedral-angle restraints found