wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2ROP
BMRB ID	:	11041
Title	:	Solution structure of domains 3 and 4 of human ATP7B
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Deposited on	:	2008-04-04

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

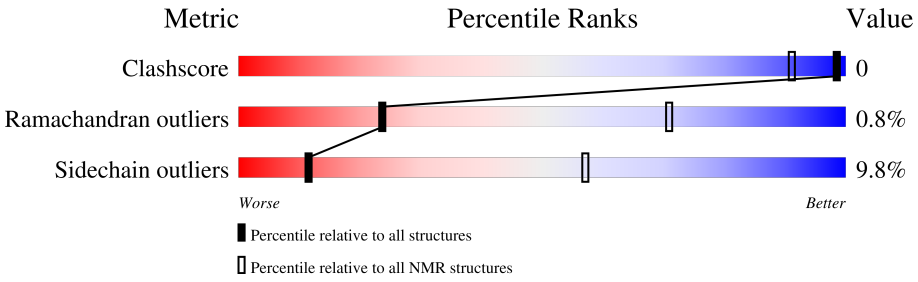
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 90%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	202	66% · 30%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:20-A:90, A:120-A:190 (142)	0.63	4

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2109 atoms, of which 1066 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Copper-transporting ATPase 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	142	2109	651	1066	173	209	10	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	ALA	SER	SEE REMARK 999	UNP P35670

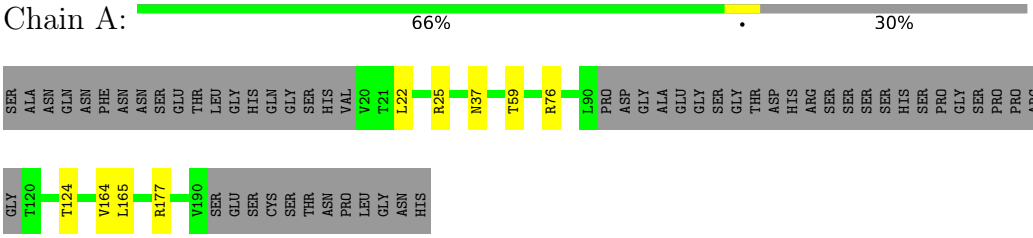
4 Residue-property plots (i)

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: Copper-transporting ATPase 2

Chain A:

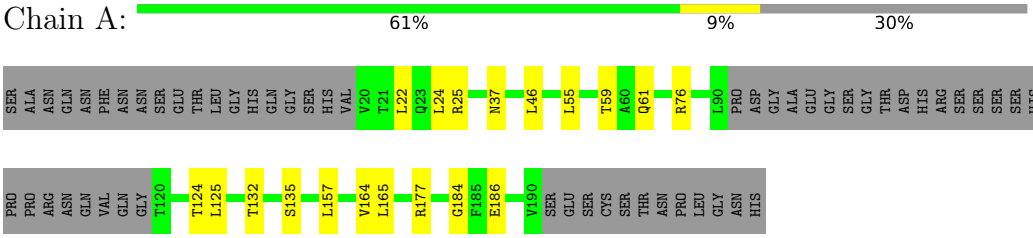


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 4. Colouring as in section 4.1 above.

• Molecule 1: Copper-transporting ATPase 2

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	refinement	2.1

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	2032
Number of shifts mapped to atoms	1650
Number of unparsed shifts	0
Number of shifts with mapping errors	382
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

6 Model quality

6.1 Standard geometry

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	0.58±0.01	0±0/1053 (0.0± 0.0%)	1.03±0.02	2±1/1430 (0.2± 0.1%)
All	All	0.58	0/21060 (0.0%)	1.03	47/28600 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.2
All	All	0	1

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	76	ARG	NE-CZ-NH1	9.59	125.09	120.30	18	16
1	A	25	ARG	NE-CZ-NH1	9.54	125.07	120.30	4	14
1	A	177	ARG	NE-CZ-NH1	7.62	124.11	120.30	14	14
1	A	177	ARG	NE-CZ-NH2	-5.77	117.41	120.30	9	2
1	A	22	LEU	CB-CG-CD2	5.13	119.72	111.00	13	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	177	ARG	Sidechain	1

6.2 Too-close contacts

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	1043	1066	1064	0±1
All	All	20860	21320	21280	6

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:LEU:HD12	1:A:23:GLN:H	0.55	1.60	5	1
1:A:42:ILE:CD1	1:A:78:ILE:HG22	0.45	2.41	15	2
1:A:42:ILE:HD12	1:A:78:ILE:HG22	0.44	1.89	2	1
1:A:131:MET:SD	1:A:157:LEU:HD22	0.40	2.55	7	1
1:A:23:GLN:NE2	1:A:61:GLN:HE22	0.40	2.15	10	1

6.3 Torsion angles

6.3.1 Protein backbone

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	138/202 (68%)	126±2 (92±2%)	11±2 (8±2%)	1±1 (1±1%)	24	71
All	All	2760/4040 (68%)	2527 (92%)	211 (8%)	22 (1%)	24	71

5 of 9 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	46	LEU	4
1	A	121	CYS	4
1	A	132	THR	4

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Mol	Chain	Res	Type	Models (Total)
1	A	184	GLY	3
1	A	130	GLY	2

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	120/170 (71%)	108±3 (90±2%)	12±3 (10±2%)	11	57
All	All	2400/3400 (71%)	2164 (90%)	236 (10%)	11	57

5 of 50 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	124	THR	20
1	A	164	VAL	20
1	A	165	LEU	18
1	A	22	LEU	11
1	A	37	ASN	11

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 90% 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	2032
Number of shifts mapped to atoms	1650
Number of unparsed shifts	0
Number of shifts with mapping errors	382
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 382) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	10	GLU	CA	56.835	0.3	1
1	A	10	GLU	CB	29.924	0.3	1
1	A	10	GLU	CG	31.664	0.3	1
1	A	10	GLU	H	8.463	0.020	1
1	A	10	GLU	HA	4.338	0.020	1
1	A	10	GLU	HB2	2.287	0.020	2
1	A	10	GLU	HB3	2.002	0.020	2
1	A	10	GLU	HG2	2.082	0.020	1
1	A	10	GLU	HG3	2.082	0.020	1
1	A	10	GLU	N	122.42	0.3	1
1	A	11	THR	C	174.641	0.3	1
1	A	11	THR	CA	61.855	0.3	1
1	A	11	THR	CB	69.374	0.3	1
1	A	11	THR	CG2	21.376	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	THR	H	8.119	0.020	1
1	A	11	THR	HA	4.305	0.020	1
1	A	11	THR	HB	4.4	0.020	1
1	A	11	THR	N	114.426	0.3	1
1	A	11	THR	HG21	1.175	0.020	1
1	A	11	THR	HG22	1.175	0.020	1
1	A	11	THR	HG23	1.175	0.020	1
1	A	12	LEU	C	177.752	0.3	1
1	A	12	LEU	CA	55.281	0.3	1
1	A	12	LEU	CB	41.949	0.3	1
1	A	12	LEU	CG	26.85	0.3	1
1	A	12	LEU	CD1	24.608	0.3	1
1	A	12	LEU	CD2	23.244	0.3	1
1	A	12	LEU	H	8.178	0.020	1
1	A	12	LEU	HA	4.305	0.020	1
1	A	12	LEU	HB2	1.649	0.020	1
1	A	12	LEU	HB3	1.649	0.020	1
1	A	12	LEU	HG	1.618	0.020	1
1	A	12	LEU	N	124.126	0.3	1
1	A	12	LEU	HD11	0.937	0.020	2
1	A	12	LEU	HD12	0.937	0.020	2
1	A	12	LEU	HD13	0.937	0.020	2
1	A	12	LEU	HD21	0.839	0.020	2
1	A	12	LEU	HD22	0.839	0.020	2
1	A	12	LEU	HD23	0.839	0.020	2
1	A	13	GLY	C	173.958	0.3	1
1	A	13	GLY	CA	45.083	0.3	1
1	A	13	GLY	H	8.343	0.020	1
1	A	13	GLY	HA2	3.958	0.020	2
1	A	13	GLY	HA3	3.891	0.020	2
1	A	13	GLY	N	109.016	0.3	1
1	A	16	GLY	CA	45.176	0.3	1
1	A	16	GLY	H	8.505	0.020	1
1	A	16	GLY	N	110.208	0.3	1
1	A	18	HIS	CA	55.22	0.3	1
1	A	18	HIS	CB	29.373	0.3	1
1	A	18	HIS	HA	4.089	0.020	1
1	A	18	HIS	HB2	4.09	0.020	1
1	A	18	HIS	HB3	4.09	0.020	1
1	A	19	VAL	C	175.056	0.3	1
1	A	19	VAL	CA	61.2	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	19	VAL	CB	33.7	0.3	1
1	A	19	VAL	CG1	21.1	0.3	1
1	A	19	VAL	CG2	20.4	0.3	1
1	A	19	VAL	H	7.743	0.020	1
1	A	19	VAL	HA	4.296	0.020	1
1	A	19	VAL	HB	1.748	0.020	1
1	A	19	VAL	N	117.676	0.3	1
1	A	19	VAL	HG11	0.656	0.020	2
1	A	19	VAL	HG12	0.656	0.020	2
1	A	19	VAL	HG13	0.656	0.020	2
1	A	19	VAL	HG21	0.72	0.020	2
1	A	19	VAL	HG22	0.72	0.020	2
1	A	19	VAL	HG23	0.72	0.020	2
1	A	91	PRO	CA	63.033	0.3	1
1	A	91	PRO	CB	32.0	0.3	1
1	A	91	PRO	CG	27.23	0.3	1
1	A	91	PRO	CD	50.3	0.3	1
1	A	91	PRO	HA	4.491	0.020	1
1	A	91	PRO	HB2	2.359	0.020	1
1	A	91	PRO	HB3	2.359	0.020	1
1	A	91	PRO	HG2	2.03	0.020	1
1	A	91	PRO	HG3	2.03	0.020	1
1	A	91	PRO	HD2	3.78	0.020	2
1	A	91	PRO	HD3	3.653	0.020	2
1	A	92	ASP	C	176.966	0.3	1
1	A	92	ASP	CA	54.515	0.3	1
1	A	92	ASP	CB	40.7	0.3	1
1	A	92	ASP	H	8.531	0.020	1
1	A	92	ASP	HA	4.538	0.020	1
1	A	92	ASP	HB2	2.688	0.020	1
1	A	92	ASP	HB3	2.688	0.020	1
1	A	92	ASP	N	120.3	0.3	1
1	A	93	GLY	C	174.137	0.3	1
1	A	93	GLY	CA	44.9	0.3	1
1	A	93	GLY	H	8.49	0.020	1
1	A	93	GLY	HA2	3.97	0.020	1
1	A	93	GLY	HA3	3.97	0.020	1
1	A	93	GLY	N	109.8	0.3	1
1	A	94	ALA	C	177.896	0.3	1
1	A	94	ALA	CA	52.5	0.3	1
1	A	94	ALA	CB	19.0	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	94	ALA	H	8.142	0.020	1
1	A	94	ALA	HA	4.334	0.020	1
1	A	94	ALA	N	123.396	0.3	1
1	A	94	ALA	HB1	1.404	0.020	1
1	A	94	ALA	HB2	1.404	0.020	1
1	A	94	ALA	HB3	1.404	0.020	1
1	A	95	GLU	C	177.005	0.3	1
1	A	95	GLU	CA	56.8	0.3	1
1	A	95	GLU	CB	29.685	0.3	1
1	A	95	GLU	CG	35.9	0.3	1
1	A	95	GLU	H	8.639	0.020	1
1	A	95	GLU	HA	4.265	0.020	1
1	A	95	GLU	HB2	2.083	0.020	1
1	A	95	GLU	HB3	2.083	0.020	1
1	A	95	GLU	HG2	2.292	0.020	1
1	A	95	GLU	HG3	2.292	0.020	1
1	A	95	GLU	N	119.963	0.3	1
1	A	96	GLY	C	174.259	0.3	1
1	A	96	GLY	CA	45.2	0.3	1
1	A	96	GLY	H	8.42	0.020	1
1	A	96	GLY	HA2	4.042	0.020	1
1	A	96	GLY	HA3	4.042	0.020	1
1	A	96	GLY	N	109.943	0.3	1
1	A	97	SER	C	175.037	0.3	1
1	A	97	SER	CA	58.524	0.3	1
1	A	97	SER	CB	63.9	0.3	1
1	A	97	SER	H	8.304	0.020	1
1	A	97	SER	HA	4.489	0.020	1
1	A	97	SER	HB2	3.902	0.020	1
1	A	97	SER	HB3	3.902	0.020	1
1	A	97	SER	N	115.677	0.3	1
1	A	98	GLY	C	174.4	0.3	1
1	A	98	GLY	CA	45.38	0.3	1
1	A	98	GLY	H	8.585	0.020	1
1	A	98	GLY	HA2	4.049	0.020	1
1	A	98	GLY	HA3	4.049	0.020	1
1	A	98	GLY	N	110.918	0.3	1
1	A	99	THR	C	174.182	0.3	1
1	A	99	THR	CA	61.5	0.3	1
1	A	99	THR	CB	69.489	0.3	1
1	A	99	THR	CG2	21.2	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	99	THR	H	8.083	0.020	1
1	A	99	THR	HA	4.3	0.020	1
1	A	99	THR	HB	4.214	0.020	1
1	A	99	THR	N	112.963	0.3	1
1	A	99	THR	HG21	1.133	0.020	1
1	A	99	THR	HG22	1.133	0.020	1
1	A	99	THR	HG23	1.133	0.020	1
1	A	100	ASP	C	175.619	0.3	1
1	A	100	ASP	CA	53.874	0.3	1
1	A	100	ASP	CB	40.9	0.3	1
1	A	100	ASP	H	8.373	0.020	1
1	A	100	ASP	HA	4.571	0.020	1
1	A	100	ASP	HB2	2.644	0.020	1
1	A	100	ASP	HB3	2.644	0.020	1
1	A	100	ASP	N	122.26	0.3	1
1	A	101	HIS	C	174.86	0.3	1
1	A	101	HIS	CA	55.9	0.3	1
1	A	101	HIS	CB	29.5	0.3	1
1	A	101	HIS	H	8.267	0.020	1
1	A	101	HIS	HA	4.667	0.020	1
1	A	101	HIS	HB2	3.12	0.020	2
1	A	101	HIS	HB3	3.24	0.020	2
1	A	101	HIS	HD2	7.188	0.020	1
1	A	101	HIS	N	118.773	0.3	1
1	A	102	ARG	C	176.484	0.3	1
1	A	102	ARG	CA	56.024	0.3	1
1	A	102	ARG	CB	30.577	0.3	1
1	A	102	ARG	CG	26.7	0.3	1
1	A	102	ARG	CD	43.3	0.3	1
1	A	102	ARG	H	8.332	0.020	1
1	A	102	ARG	HA	4.314	0.020	1
1	A	102	ARG	HB2	1.815	0.020	1
1	A	102	ARG	HB3	1.815	0.020	1
1	A	102	ARG	HG2	1.595	0.020	1
1	A	102	ARG	HG3	1.595	0.020	1
1	A	102	ARG	HD2	3.194	0.020	1
1	A	102	ARG	HD3	3.194	0.020	1
1	A	102	ARG	N	121.841	0.3	1
1	A	103	SER	C	174.675	0.3	1
1	A	103	SER	CA	58.172	0.3	1
1	A	103	SER	CB	63.8	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	103	SER	H	8.428	0.020	1
1	A	103	SER	HA	4.506	0.020	1
1	A	103	SER	HB2	3.891	0.020	1
1	A	103	SER	HB3	3.891	0.020	1
1	A	103	SER	N	116.734	0.3	1
1	A	104	SER	C	174.884	0.3	1
1	A	104	SER	CA	58.198	0.3	1
1	A	104	SER	CB	63.677	0.3	1
1	A	104	SER	H	8.423	0.020	1
1	A	104	SER	HA	4.48	0.020	1
1	A	104	SER	HB2	3.897	0.020	1
1	A	104	SER	HB3	3.897	0.020	1
1	A	104	SER	N	117.8	0.3	1
1	A	105	SER	CA	58.294	0.3	1
1	A	105	SER	CB	63.793	0.3	1
1	A	105	SER	H	8.277	0.020	1
1	A	105	SER	HA	4.428	0.020	1
1	A	105	SER	HB2	3.86	0.020	1
1	A	105	SER	HB3	3.86	0.020	1
1	A	105	SER	N	117.394	0.3	1
1	A	109	PRO	CA	63.53	0.3	1
1	A	109	PRO	CB	31.747	0.3	1
1	A	109	PRO	CG	29.137	0.3	1
1	A	109	PRO	CD	50.288	0.3	1
1	A	109	PRO	HA	4.7	0.020	1
1	A	109	PRO	HB2	2.006	0.020	1
1	A	109	PRO	HB3	2.006	0.020	1
1	A	109	PRO	HG2	2.031	0.020	1
1	A	109	PRO	HG3	2.031	0.020	1
1	A	109	PRO	HD2	3.617	0.020	1
1	A	109	PRO	HD3	3.617	0.020	1
1	A	110	GLY	C	173.79	0.3	1
1	A	110	GLY	CA	45.0	0.3	1
1	A	110	GLY	H	8.494	0.020	1
1	A	110	GLY	HA2	3.951	0.020	1
1	A	110	GLY	HA3	3.951	0.020	1
1	A	110	GLY	N	109.378	0.3	1
1	A	111	SER	C	171.809	0.3	1
1	A	111	SER	CA	56.435	0.3	1
1	A	111	SER	CB	63.271	0.3	1
1	A	111	SER	H	8.114	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	111	SER	HA	4.768	0.020	1
1	A	111	SER	HB2	3.851	0.020	2
1	A	111	SER	HB3	3.785	0.020	2
1	A	111	SER	N	116.919	0.3	1
1	A	116	GLN	CA	55.4	0.3	1
1	A	116	GLN	CB	29.6	0.3	1
1	A	116	GLN	CG	33.6	0.3	1
1	A	116	GLN	HA	4.339	0.020	1
1	A	116	GLN	HB2	2.342	0.020	1
1	A	116	GLN	HB3	2.342	0.020	1
1	A	116	GLN	HG2	2.33	0.020	1
1	A	116	GLN	HG3	2.33	0.020	1
1	A	116	GLN	NE2	117.0	0.3	1
1	A	117	VAL	C	175.948	0.3	1
1	A	117	VAL	CA	62.1	0.3	1
1	A	117	VAL	CB	32.1	0.3	1
1	A	117	VAL	CG1	20.7	0.3	1
1	A	117	VAL	H	8.196	0.020	1
1	A	117	VAL	HA	4.077	0.020	1
1	A	117	VAL	HB	2.03	0.020	1
1	A	117	VAL	N	121.631	0.3	1
1	A	117	VAL	HG11	0.911	0.020	1
1	A	117	VAL	HG12	0.911	0.020	1
1	A	117	VAL	HG13	0.911	0.020	1
1	A	117	VAL	HG21	0.911	0.020	1
1	A	117	VAL	HG22	0.911	0.020	1
1	A	117	VAL	HG23	0.911	0.020	1
1	A	118	GLN	C	176.107	0.3	1
1	A	118	GLN	CA	55.769	0.3	1
1	A	118	GLN	CB	29.5	0.3	1
1	A	118	GLN	CG	33.7	0.3	1
1	A	118	GLN	H	8.523	0.020	1
1	A	118	GLN	HA	4.363	0.020	1
1	A	118	GLN	HB2	2.05	0.020	2
1	A	118	GLN	HB3	2.05	0.020	2
1	A	118	GLN	HG2	2.364	0.020	1
1	A	118	GLN	HG3	2.364	0.020	1
1	A	118	GLN	HE21	7.513	0.020	1
1	A	118	GLN	HE22	6.864	0.020	1
1	A	118	GLN	N	124.625	0.3	1
1	A	118	GLN	NE2	112.427	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	119	GLY	C	173.824	0.3	1
1	A	119	GLY	CA	44.9	0.3	1
1	A	119	GLY	H	8.426	0.020	1
1	A	119	GLY	HA2	4.022	0.020	1
1	A	119	GLY	HA3	4.022	0.020	1
1	A	119	GLY	N	110.442	0.3	1
1	A	191	SER	C	173.902	0.3	1
1	A	191	SER	CA	57.801	0.3	1
1	A	191	SER	CB	64.057	0.3	1
1	A	191	SER	H	8.14	0.020	1
1	A	191	SER	HA	4.632	0.020	1
1	A	191	SER	HB2	3.915	0.020	2
1	A	191	SER	HB3	3.841	0.020	2
1	A	191	SER	N	116.583	0.3	1
1	A	192	GLU	C	175.729	0.3	1
1	A	192	GLU	CA	57.101	0.3	1
1	A	192	GLU	CB	30.706	0.3	1
1	A	192	GLU	CG	35.905	0.3	1
1	A	192	GLU	H	8.728	0.020	1
1	A	192	GLU	HA	4.596	0.020	1
1	A	192	GLU	HB2	2.138	0.020	2
1	A	192	GLU	HB3	2.046	0.020	2
1	A	192	GLU	HG2	2.285	0.020	1
1	A	192	GLU	HG3	2.285	0.020	1
1	A	192	GLU	N	123.773	0.3	1
1	A	193	SER	C	174.088	0.3	1
1	A	193	SER	CA	57.709	0.3	1
1	A	193	SER	CB	64.009	0.3	1
1	A	193	SER	H	8.584	0.020	1
1	A	193	SER	HA	4.644	0.020	1
1	A	193	SER	HB2	3.886	0.020	1
1	A	193	SER	HB3	3.886	0.020	1
1	A	193	SER	N	116.41	0.3	1
1	A	194	CYS	C	174.603	0.3	1
1	A	194	CYS	CA	58.201	0.3	1
1	A	194	CYS	CB	28.086	0.3	1
1	A	194	CYS	H	8.541	0.020	1
1	A	194	CYS	HA	4.738	0.020	1
1	A	194	CYS	HB2	2.981	0.020	1
1	A	194	CYS	HB3	2.981	0.020	1
1	A	194	CYS	N	121.323	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	195	SER	C	174.563	0.3	1
1	A	195	SER	CA	58.262	0.3	1
1	A	195	SER	CB	63.758	0.3	1
1	A	195	SER	H	8.525	0.020	1
1	A	195	SER	HA	4.543	0.020	1
1	A	195	SER	HB2	3.88	0.020	1
1	A	195	SER	HB3	3.88	0.020	1
1	A	195	SER	N	119.503	0.3	1
1	A	196	THR	C	173.915	0.3	1
1	A	196	THR	CA	61.504	0.3	1
1	A	196	THR	CB	69.502	0.3	1
1	A	196	THR	CG2	21.507	0.3	1
1	A	196	THR	H	8.175	0.020	1
1	A	196	THR	HA	4.348	0.020	1
1	A	196	THR	HB	4.21	0.020	1
1	A	196	THR	N	115.176	0.3	1
1	A	196	THR	HG21	1.176	0.020	1
1	A	196	THR	HG22	1.176	0.020	1
1	A	196	THR	HG23	1.176	0.020	1
1	A	197	ASN	C	173.467	0.3	1
1	A	197	ASN	CA	51.128	0.3	1
1	A	197	ASN	CB	38.504	0.3	1
1	A	197	ASN	H	8.392	0.020	1
1	A	197	ASN	HA	4.979	0.020	1
1	A	197	ASN	HB2	2.85	0.020	2
1	A	197	ASN	HB3	2.693	0.020	2
1	A	197	ASN	N	121.668	0.3	1
1	A	197	ASN	ND2	112.192	0.3	1
1	A	198	PRO	C	177.07	0.3	1
1	A	198	PRO	CA	63.3	0.3	1
1	A	198	PRO	CB	31.8	0.3	1
1	A	198	PRO	CG	26.929	0.3	1
1	A	198	PRO	CD	50.487	0.3	1
1	A	198	PRO	HA	4.418	0.020	1
1	A	198	PRO	HB2	2.294	0.020	2
1	A	198	PRO	HB3	1.95	0.020	2
1	A	198	PRO	HG2	2.009	0.020	1
1	A	198	PRO	HG3	2.009	0.020	1
1	A	198	PRO	HD2	3.756	0.020	2
1	A	198	PRO	HD3	3.817	0.020	2
1	A	199	LEU	C	177.83	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	199	LEU	CA	55.031	0.3	1
1	A	199	LEU	CB	41.606	0.3	1
1	A	199	LEU	CD1	23.001	0.3	1
1	A	199	LEU	CD2	24.687	0.3	1
1	A	199	LEU	H	8.248	0.020	1
1	A	199	LEU	HA	4.33	0.020	1
1	A	199	LEU	HB2	1.633	0.020	1
1	A	199	LEU	HB3	1.633	0.020	1
1	A	199	LEU	N	120.361	0.3	1
1	A	199	LEU	HD11	0.848	0.020	2
1	A	199	LEU	HD12	0.848	0.020	2
1	A	199	LEU	HD13	0.848	0.020	2
1	A	199	LEU	HD21	0.91	0.020	2
1	A	199	LEU	HD22	0.91	0.020	2
1	A	199	LEU	HD23	0.91	0.020	2
1	A	200	GLY	C	173.533	0.3	1
1	A	200	GLY	CA	45.043	0.3	1
1	A	200	GLY	H	8.113	0.020	1
1	A	200	GLY	HA2	3.921	0.020	1
1	A	200	GLY	HA3	3.921	0.020	1
1	A	200	GLY	N	108.366	0.3	1
1	A	201	ASN	C	174.212	0.3	1
1	A	201	ASN	CA	53.11	0.3	1
1	A	201	ASN	CB	38.789	0.3	1
1	A	201	ASN	H	8.261	0.020	1
1	A	201	ASN	HA	4.771	0.020	1
1	A	201	ASN	HB2	2.707	0.020	2
1	A	201	ASN	HB3	2.802	0.020	2
1	A	201	ASN	HD21	7.598	0.020	1
1	A	201	ASN	HD22	6.912	0.020	1
1	A	201	ASN	N	118.586	0.3	1
1	A	201	ASN	ND2	112.8	0.3	1
1	A	202	HIS	C	178.707	0.3	1
1	A	202	HIS	CA	57.194	0.3	1
1	A	202	HIS	CB	29.6	0.3	1
1	A	202	HIS	H	8.039	0.020	1
1	A	202	HIS	HA	4.464	0.020	1
1	A	202	HIS	HB2	3.245	0.020	2
1	A	202	HIS	HB3	3.094	0.020	2
1	A	202	HIS	N	123.752	0.3	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	180	-0.12 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	163	0.32 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	156	-0.09 ± 0.13	None needed (< 0.5 ppm)
^{15}N	168	0.42 ± 0.46	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 90%, i.e. 1650 atoms were assigned a chemical shift out of a possible 1835. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	674/707 (95%)	281/287 (98%)	261/284 (92%)	132/136 (97%)
Sidechain	960/1076 (89%)	665/712 (93%)	283/337 (84%)	12/27 (44%)
Aromatic	16/52 (31%)	11/26 (42%)	5/24 (21%)	0/2 (0%)
Overall	1650/1835 (90%)	957/1025 (93%)	549/645 (85%)	144/165 (87%)

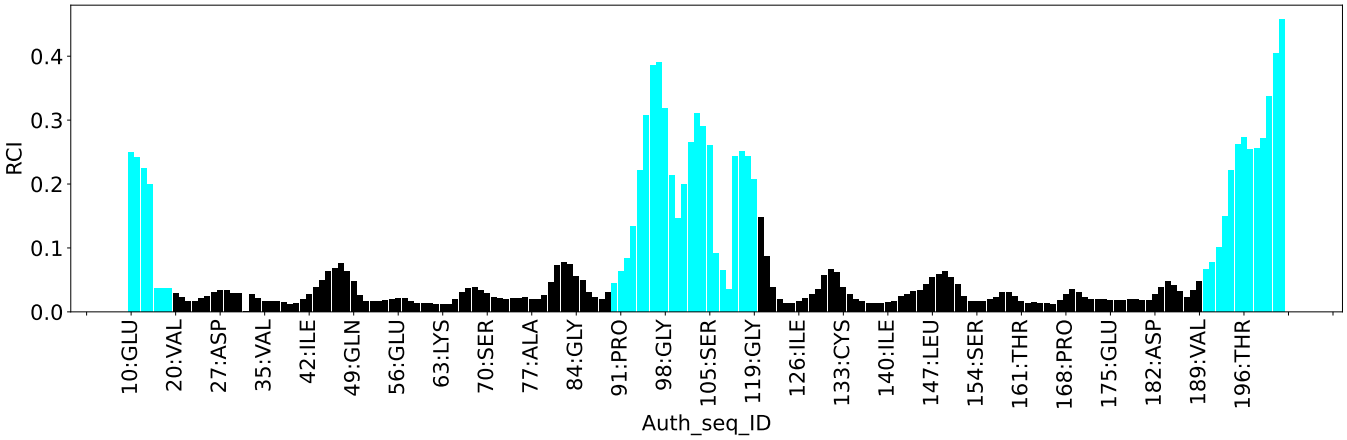
7.1.4 Statistically unusual chemical shifts (i)

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:


RCI
0.0
0.1
0.2
0.3
0.4
10:GLU
20:VAL
27:ASP
35:VAL
42:ILE
49:GLN
56:GLU
63:LYS
70:SER
77:ALA
84:GLY
91:PRO
98:GLY
105:SER
119:GLY
126:ILE
133:CYS
140:ILE
147:LEU
154:SER
161:THR
168:PRO
175:GLU
182:ASP
189:VAL
196:THR
Auth_seq_ID

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	2205
Intra-residue (|i-j|=0)	429
Sequential (|i-j|=1)	743
Medium range (|i-j|>1 and |i-j|<5)	393
Long range (|i-j|≥5)	640
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	276
Number of restraints per residue	10.9
Number of long range restraints per residue[1]	3.2

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

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)	6.8	0.2
0.2-0.5 (Medium)	1.8	0.5
>0.5 (Large)	3.5	1.78

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

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

9 Distance violation analysis (i)

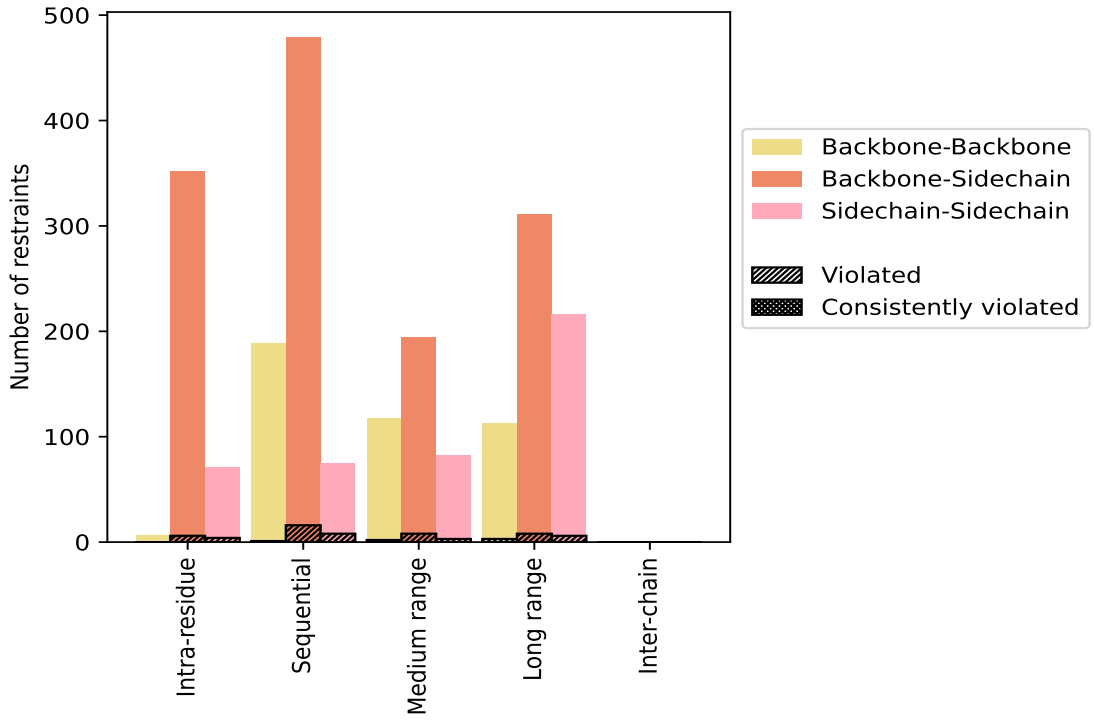
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	429	19.5	10	2.3	0.5	0	0.0	0.0
Backbone-Backbone	6	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	352	16.0	6	1.7	0.3	0	0.0	0.0
Sidechain-Sidechain	71	3.2	4	5.6	0.2	0	0.0	0.0
Sequential (|i-j|=1)	743	33.7	25	3.4	1.1	0	0.0	0.0
Backbone-Backbone	189	8.6	1	0.5	0.0	0	0.0	0.0
Backbone-Sidechain	479	21.7	16	3.3	0.7	0	0.0	0.0
Sidechain-Sidechain	75	3.4	8	10.7	0.4	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	393	17.8	13	3.3	0.6	0	0.0	0.0
Backbone-Backbone	117	5.3	2	1.7	0.1	0	0.0	0.0
Backbone-Sidechain	194	8.8	8	4.1	0.4	0	0.0	0.0
Sidechain-Sidechain	82	3.7	3	3.7	0.1	0	0.0	0.0
Long range (|i-j|≥5)	640	29.0	17	2.7	0.8	0	0.0	0.0
Backbone-Backbone	113	5.1	3	2.7	0.1	0	0.0	0.0
Backbone-Sidechain	311	14.1	8	2.6	0.4	0	0.0	0.0
Sidechain-Sidechain	216	9.8	6	2.8	0.3	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	2205	100.0	65	2.9	2.9	0	0.0	0.0
Backbone-Backbone	425	19.3	6	1.4	0.3	0	0.0	0.0
Backbone-Sidechain	1336	60.6	38	2.8	1.7	0	0.0	0.0
Sidechain-Sidechain	444	20.1	21	4.7	1.0	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

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	3	6	1	1	0	11	0.33	1.62	0.42	0.18
2	3	7	0	2	0	12	0.4	1.37	0.39	0.17
3	3	3	2	3	0	11	0.4	1.06	0.37	0.16
4	2	5	1	3	0	11	0.41	1.52	0.49	0.15
5	2	5	0	1	0	8	0.44	1.58	0.51	0.16
6	2	7	3	3	0	15	0.45	1.34	0.44	0.2
7	0	10	3	3	0	16	0.59	1.71	0.56	0.29
8	1	4	0	2	0	7	0.32	1.01	0.32	0.14
9	2	4	0	4	0	10	0.43	1.54	0.45	0.14
10	2	7	1	1	0	11	0.56	1.78	0.6	0.21
11	3	4	0	3	0	10	0.56	1.67	0.58	0.16

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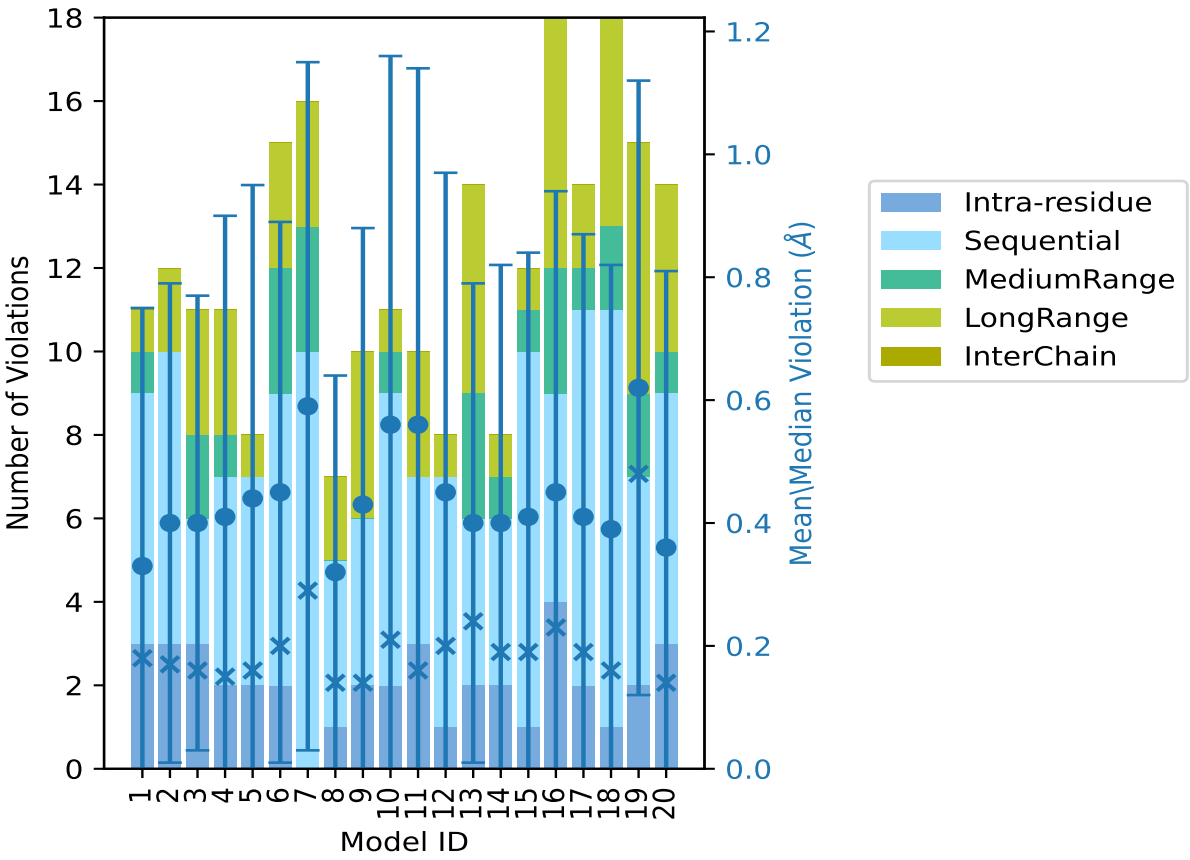
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	1	6	0	1	0	8	0.45	1.65	0.52	0.2
13	2	4	3	5	0	14	0.4	1.4	0.39	0.24
14	2	4	1	1	0	8	0.4	1.28	0.42	0.19
15	1	9	1	1	0	12	0.41	1.64	0.43	0.19
16	4	5	3	6	0	18	0.45	1.64	0.49	0.23
17	2	9	1	2	0	14	0.41	1.49	0.46	0.19
18	1	10	2	5	0	18	0.39	1.7	0.43	0.16
19	2	5	2	6	0	15	0.62	1.69	0.5	0.48
20	3	6	1	4	0	14	0.36	1.68	0.45	0.14

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

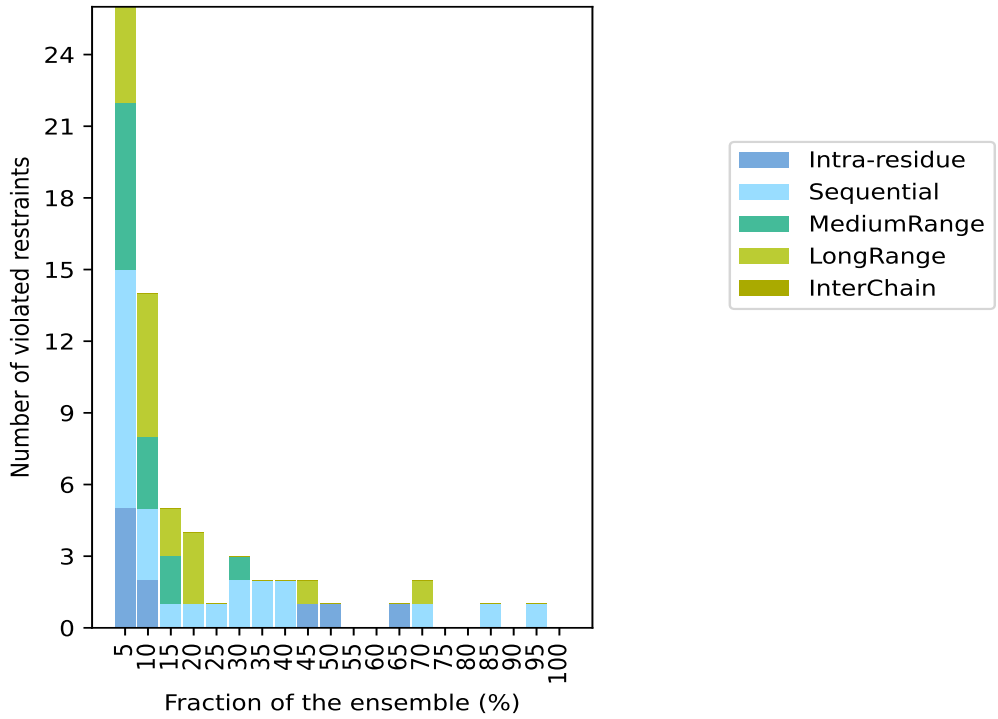
9.3 Distance violation statistics for the ensemble (i)

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, 2140(IR:419, SQ:718, MR:380, LR:623, 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]	%
5	10	7	4	0	26	1	5.0
2	3	3	6	0	14	2	10.0
0	1	2	2	0	5	3	15.0
0	1	0	3	0	4	4	20.0
0	1	0	0	0	1	5	25.0
0	2	1	0	0	3	6	30.0
0	2	0	0	0	2	7	35.0
0	2	0	0	0	2	8	40.0
1	0	0	1	0	2	9	45.0
1	0	0	0	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
1	0	0	0	0	1	13	65.0
0	1	0	1	0	2	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	1	0	0	0	1	17	85.0
0	0	0	0	0	0	18	90.0
0	1	0	0	0	1	19	95.0
0	0	0	0	0	0	20	100.0

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

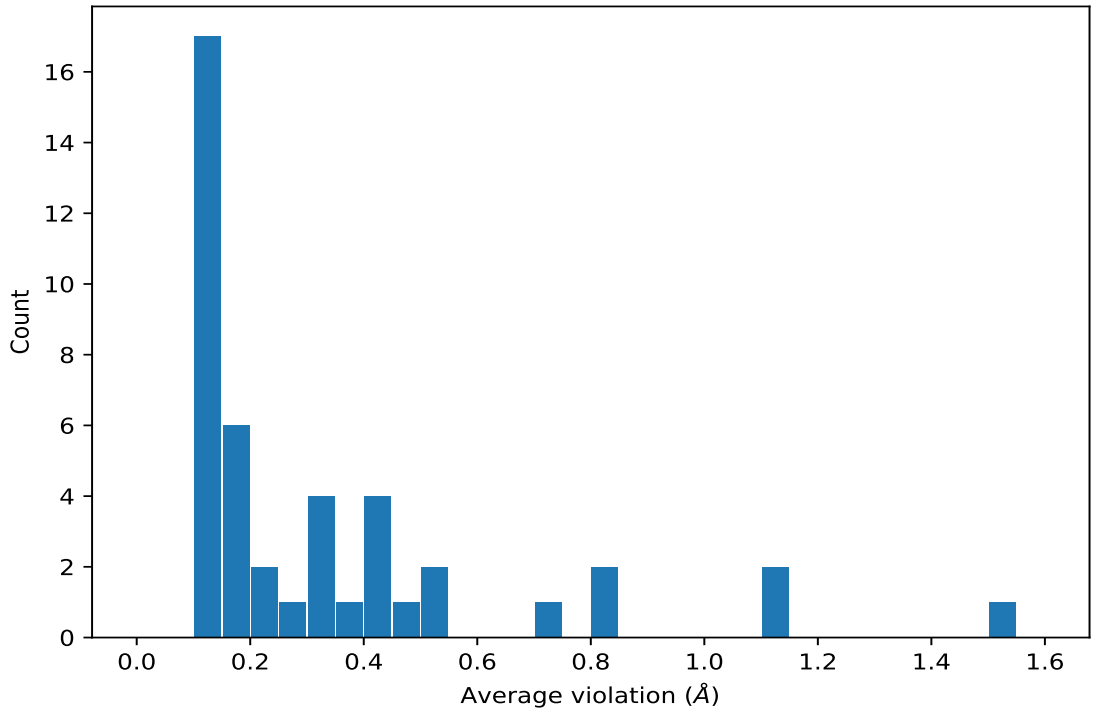
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance 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



9.4.2 Table: Most violated distance restraints (i)

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

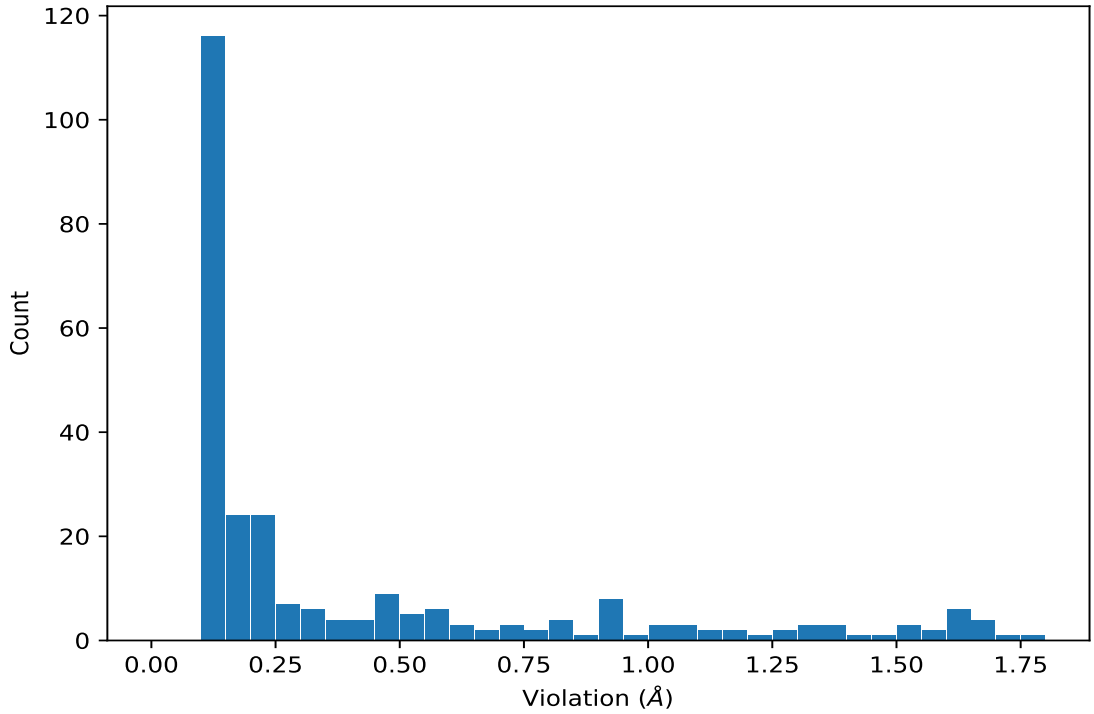
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1565)	1:A:145:SER:HB3	1:A:146:GLN:HE22	19	1.1	0.44	1.01
(1,1657)	1:A:151:GLN:HE22	1:A:152:GLN:HA	17	1.53	0.12	1.54
(1,430)	1:A:40:GLU:HG2	1:A:41:ASN:HD22	14	0.82	0.23	0.87
(1,144)	1:A:23:GLN:HE21	1:A:61:GLN:HA	14	0.74	0.28	0.66
(1,1680)	1:A:152:GLN:HB3	1:A:152:GLN:HG3	13	0.13	0.01	0.13
(1,1579)	1:A:146:GLN:HB3	1:A:146:GLN:HE22	10	0.2	0.03	0.2
(1,1744)	1:A:155:VAL:HB	1:A:163:THR:H	9	0.14	0.02	0.15
(1,369)	1:A:37:ASN:HB3	1:A:37:ASN:HD22	9	0.13	0.01	0.13
(1,1656)	1:A:151:GLN:HE22	1:A:152:GLN:H	8	0.2	0.07	0.19
(1,1896)	1:A:167:ASN:HD21	1:A:168:PRO:HD3	8	0.15	0.02	0.16

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1565)	1:A:145:SER:HB3	1:A:146:GLN:HE22	10	1.78
(1,1658)	1:A:151:GLN:HE22	1:A:152:GLN:HB2	7	1.71
(1,1657)	1:A:151:GLN:HE22	1:A:152:GLN:HA	18	1.7
(1,1565)	1:A:145:SER:HB3	1:A:146:GLN:HE22	19	1.69
(1,1657)	1:A:151:GLN:HE22	1:A:152:GLN:HA	20	1.68
(1,1565)	1:A:145:SER:HB3	1:A:146:GLN:HE22	11	1.67
(1,1657)	1:A:151:GLN:HE22	1:A:152:GLN:HA	10	1.65
(1,1657)	1:A:151:GLN:HE22	1:A:152:GLN:HA	12	1.65
(1,1657)	1:A:151:GLN:HE22	1:A:152:GLN:HA	15	1.64
(1,1565)	1:A:145:SER:HB3	1:A:146:GLN:HE22	16	1.64

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value