wwPDB NMR Structure Validation Summary Report

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PDB ID	:	9XH1 / pdb_00009xh1
BMRB ID	:	36807
Title	:	Cup s 7 NMR structure
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Deposited on	:	2025-10-31

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:

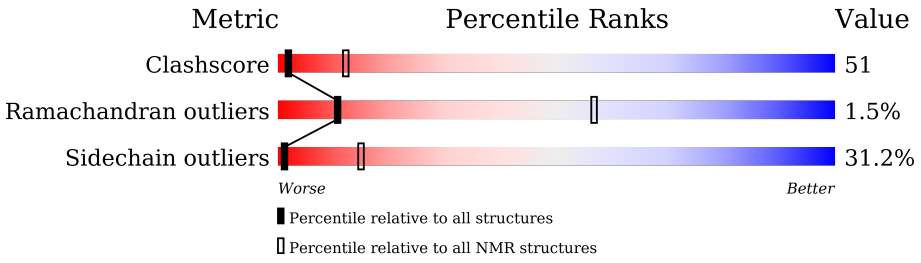
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.3.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 1%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	63	24% 59% 13% 5%

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:4-A:63 (60)	1.04	5

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, 6, 7, 10, 11, 12, 13, 14, 15, 16, 18, 19, 20
2	9, 17
Single-model clusters	8

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 898 atoms, of which 432 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cypmaclein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	63	898	276	432	90	88	12	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ILE	LEU	conflict	UNP C0HLQ2

4 Residue-property plots (i)

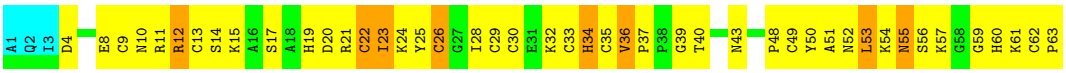
4.1 Average score per residue in the NMR ensemble

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: Cypmaclein

Chain A:





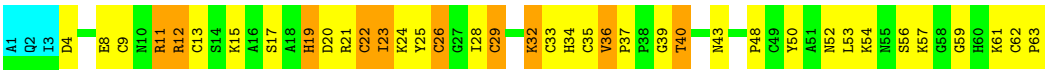
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 5. Colouring as in section 4.1 above.

- Molecule 1: Cypmaclein

Chain A:





5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 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	structure calculation	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	213
Number of shifts mapped to atoms	5
Number of unparsed shifts	0
Number of shifts with mapping errors	208
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

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	0.84±0.00	0±0/452 (0.0± 0.0%)	1.22±0.02	0±0/605 (0.0± 0.1%)
All	All	0.84	0/9040 (0.0%)	1.22	3/12100 (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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	37	PRO	O-C-N	7.11	124.49	121.15	20	2
1	A	55	ASN	CB-CA-C	-5.11	108.02	114.40	6	1

There are no chirality outliers.

There are no planarity outliers.

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	444	408	411	43±7
All	All	8880	8160	8224	869

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 51.

5 of 277 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:CYS:SG	1:A:62:CYS:SG	0.99	2.61	11	2
1:A:38:PRO:CG	1:A:46:VAL:HG21	0.81	2.06	13	3
1:A:35:CYS:O	1:A:36:VAL:HG13	0.80	1.76	2	17
1:A:12:ARG:HH11	1:A:21:ARG:CZ	0.80	1.90	6	3
1:A:53:LEU:HD11	1:A:61:LYS:HB3	0.79	1.54	2	1

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	59/63 (94%)	44±2 (75±4%)	14±2 (24±4%)	1±1 (2±2%)	11	57
All	All	1180/1260 (94%)	881 (75%)	281 (24%)	18 (2%)	11	57

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	10	ASN	5
1	A	43	ASN	3
1	A	14	SER	3
1	A	11	ARG	2
1	A	22	CYS	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	51/53 (96%)	35±3 (69±6%)	16±3 (31±6%)	1	15
All	All	1020/1060 (96%)	702 (69%)	318 (31%)	1	15

5 of 41 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	22	CYS	20
1	A	23	ILE	20
1	A	26	CYS	15
1	A	36	VAL	15
1	A	55	ASN	13

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 1% for the well-defined parts and 1% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_ output*

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	213
Number of shifts mapped to atoms	5
Number of unparsed shifts	0
Number of shifts with mapping errors	208
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 208) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	AIB	H1	8.154	0.000	.
1	A	1	AIB	HB11	1.319	0.000	.
1	A	1	AIB	HB12	1.319	0.000	.
1	A	1	AIB	HB13	1.319	0.000	.
1	A	1	AIB	HB21	1.262	0.002	.
1	A	1	AIB	HB22	1.262	0.002	.
1	A	1	AIB	HB23	1.262	0.002	.
1	A	2	ALA	H	8.152	0.002	1
1	A	2	ALA	HA	3.878	0.004	1
1	A	2	ALA	HB1	1.083	0.002	1
1	A	2	ALA	HB2	1.083	0.002	1
1	A	2	ALA	HB3	1.083	0.002	1
1	A	3	AIB	H	8.388	0.001	1
1	A	3	AIB	HB11	1.106	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	AIB	HB12	1.106	0.000	.
1	A	3	AIB	HB13	1.106	0.000	.
1	A	3	AIB	HB21	1.091	0.003	.
1	A	3	AIB	HB22	1.091	0.003	.
1	A	3	AIB	HB23	1.091	0.003	.
1	A	4	GLN	H	7.719	0.001	1
1	A	4	GLN	HA	3.743	0.003	1
1	A	4	GLN	HB2	1.77	0.002	.
1	A	4	GLN	HB3	1.728	0.003	.
1	A	4	GLN	HE21	7.356	0.001	.
1	A	4	GLN	HE22	6.759	0.000	.
1	A	4	GLN	HG2	2.113	0.003	.
1	A	4	GLN	HG3	2.028	0.001	.
1	A	5	ALA	H	7.871	0.003	1
1	A	5	ALA	HA	3.882	0.003	1
1	A	5	ALA	HB1	1.118	0.000	1
1	A	5	ALA	HB2	1.118	0.000	1
1	A	5	ALA	HB3	1.118	0.000	1
1	A	6	ARG	H	7.906	0.004	1
1	A	6	ARG	HA	3.891	0.007	1
1	A	6	ARG	HB2	1.57	0.000	.
1	A	6	ARG	HB3	1.525	0.000	.
1	A	6	ARG	HG2	1.399	0.000	.
1	A	6	ARG	HG3	1.321	0.000	.
1	A	7	ARG	H	7.914	0.007	1
1	A	7	ARG	HA	3.859	0.002	1
1	A	7	ARG	HB2	1.573	0.000	.
1	A	7	ARG	HB3	1.524	0.002	.
1	A	7	ARG	HD2	2.87	0.009	.
1	A	7	ARG	HE	6.977	0.001	1
1	A	7	ARG	HG2	1.4	0.000	.
1	A	7	ARG	HG3	1.276	0.003	.
1	A	8	ASN	H	8.266	0.001	1
1	A	8	ASN	HA	4.2	0.002	1
1	A	8	ASN	HB2	2.541	0.002	.
1	A	8	ASN	HB3	2.489	0.002	.
1	A	8	ASN	HD21	7.517	0.006	.
1	A	8	ASN	HD22	6.794	0.006	.
1	A	9	AIB	H	7.989	0.002	1
1	A	9	AIB	HB11	1.175	0.006	.
1	A	9	AIB	HB12	1.175	0.006	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	9	AIB	HB13	1.175	0.006	.
1	A	9	AIB	HB21	1.102	0.002	.
1	A	9	AIB	HB22	1.102	0.002	.
1	A	9	AIB	HB23	1.102	0.002	.
1	A	10	ALA	H	7.668	0.007	1
1	A	10	ALA	HA	3.779	0.003	1
1	A	10	ALA	HB1	1.109	0.004	1
1	A	10	ALA	HB2	1.109	0.004	1
1	A	10	ALA	HB3	1.109	0.004	1
1	A	11	AIB	H	7.766	0.003	1
1	A	11	AIB	HB11	1.233	0.003	.
1	A	11	AIB	HB12	1.233	0.003	.
1	A	11	AIB	HB13	1.233	0.003	.
1	A	11	AIB	HB21	1.164	0.001	.
1	A	11	AIB	HB22	1.164	0.001	.
1	A	11	AIB	HB23	1.164	0.001	.
1	A	12	GLN	H	7.633	0.003	1
1	A	12	GLN	HA	3.761	0.005	1
1	A	12	GLN	HB2	1.861	0.004	.
1	A	12	GLN	HB3	1.709	0.006	.
1	A	12	GLN	HE21	7.262	0.003	.
1	A	12	GLN	HE22	6.725	0.000	.
1	A	12	GLN	HG2	2.104	0.017	.
1	A	13	ALA	H	7.704	0.003	1
1	A	13	ALA	HA	3.903	0.004	1
1	A	13	ALA	HB1	1.205	0.001	1
1	A	13	ALA	HB2	1.205	0.001	1
1	A	13	ALA	HB3	1.205	0.001	1
1	A	14	ARG	H	7.664	0.004	1
1	A	14	ARG	HA	3.905	0.001	1
1	A	14	ARG	HB2	1.6	0.003	.
1	A	14	ARG	HB3	1.511	0.000	.
1	A	14	ARG	HD2	2.859	0.000	.
1	A	14	ARG	HG2	1.385	0.001	.
1	A	14	ARG	HG3	1.314	0.001	.
1	A	15	ARG	H	7.809	0.003	1
1	A	15	ARG	HA	3.86	0.004	1
1	A	15	ARG	HB3	1.518	0.004	.
1	A	15	ARG	HD2	2.859	0.003	.
1	A	15	ARG	HE	6.934	0.006	1
1	A	15	ARG	HG2	1.378	0.004	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	15	ARG	HG3	1.272	0.003	.
1	A	16	ASN	H	8.185	0.002	1
1	A	16	ASN	HA	4.201	0.003	1
1	A	16	ASN	HB2	2.52	0.004	.
1	A	16	ASN	HB3	2.442	0.001	.
1	A	16	ASN	HD21	7.428	0.001	.
1	A	16	ASN	HD22	6.751	0.001	.
1	A	17	AIB	H	7.894	0.003	1
1	A	17	AIB	HB11	1.183	0.001	.
1	A	17	AIB	HB12	1.183	0.001	.
1	A	17	AIB	HB13	1.183	0.001	.
1	A	17	AIB	HB21	1.114	0.001	.
1	A	17	AIB	HB22	1.114	0.001	.
1	A	17	AIB	HB23	1.114	0.001	.
1	A	19	AIB	H	7.623	0.002	1
1	A	19	AIB	HB11	1.125	0.000	.
1	A	19	AIB	HB12	1.125	0.000	.
1	A	19	AIB	HB13	1.125	0.000	.
1	A	19	AIB	HB21	1.12	0.000	.
1	A	19	AIB	HB22	1.12	0.000	.
1	A	19	AIB	HB23	1.12	0.000	.
1	A	20	GLN	H	7.68	0.004	1
1	A	20	GLN	HA	3.686	0.002	1
1	A	20	GLN	HB2	1.854	0.004	.
1	A	20	GLN	HB3	1.76	0.001	.
1	A	20	GLN	HG2	2.106	0.000	.
1	A	21	ALA	H	7.634	0.002	1
1	A	21	ALA	HA	3.9	0.004	1
1	A	21	ALA	HB1	1.16	0.003	1
1	A	21	ALA	HB2	1.16	0.003	1
1	A	21	ALA	HB3	1.16	0.003	1
1	A	22	ARG	H	7.631	0.003	1
1	A	22	ARG	HA	3.863	0.003	1
1	A	22	ARG	HB2	1.647	0.002	.
1	A	22	ARG	HB3	1.591	0.004	.
1	A	22	ARG	HD2	2.863	0.002	.
1	A	22	ARG	HE	6.948	0.002	1
1	A	22	ARG	HG2	1.439	0.000	.
1	A	22	ARG	HG3	1.321	0.004	.
1	A	23	ARG	H	7.758	0.004	1
1	A	23	ARG	HA	3.833	0.004	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	23	ARG	HB2	1.587	0.002	.
1	A	23	ARG	HB3	1.47	0.003	.
1	A	23	ARG	HD2	2.873	0.020	.
1	A	23	ARG	HE	6.979	0.003	1
1	A	23	ARG	HG2	1.278	0.003	.
1	A	24	ASN	H	8.262	0.002	1
1	A	24	ASN	HA	4.154	0.002	1
1	A	24	ASN	HB2	2.529	0.005	.
1	A	24	ASN	HD21	7.529	0.001	.
1	A	24	ASN	HD22	6.84	0.004	.
1	A	25	AIB	H	7.941	0.003	1
1	A	25	AIB	HB11	1.194	0.010	.
1	A	25	AIB	HB12	1.194	0.010	.
1	A	25	AIB	HB13	1.194	0.010	.
1	A	25	AIB	HB21	1.131	0.005	.
1	A	25	AIB	HB22	1.131	0.005	.
1	A	25	AIB	HB23	1.131	0.005	.
1	A	26	ALA	H	7.521	0.002	1
1	A	26	ALA	HA	3.776	0.008	1
1	A	26	ALA	HB1	1.126	0.005	1
1	A	26	ALA	HB2	1.126	0.005	1
1	A	26	ALA	HB3	1.126	0.005	1
1	A	27	AIB	H	7.825	0.001	1
1	A	27	AIB	HB11	1.258	0.003	.
1	A	27	AIB	HB12	1.258	0.003	.
1	A	27	AIB	HB13	1.258	0.003	.
1	A	27	AIB	HB21	8.115	.	.
1	A	27	AIB	HB22	8.115	.	.
1	A	27	AIB	HB23	8.115	.	.
1	A	28	GLN	H	7.683	0.003	1
1	A	28	GLN	HA	3.682	0.003	1
1	A	28	GLN	HB2	1.858	0.002	.
1	A	28	GLN	HB3	1.765	0.003	.
1	A	28	GLN	HE21	7.263	0.004	.
1	A	28	GLN	HE22	6.678	0.000	.
1	A	28	GLN	HG2	2.098	0.004	.
1	A	29	ALA	H	7.672	0.004	1
1	A	29	ALA	HA	3.87	0.013	1
1	A	29	ALA	HB1	1.208	0.003	1
1	A	29	ALA	HB2	1.208	0.003	1
1	A	29	ALA	HB3	1.208	0.003	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	ARG	H	7.685	0.006	1
1	A	30	ARG	HA	3.904	0.002	1
1	A	30	ARG	HB2	1.642	0.006	.
1	A	30	ARG	HB3	1.589	0.000	.
1	A	30	ARG	HG2	1.443	0.000	.
1	A	31	ARG	H	7.728	0.002	1
1	A	31	ARG	HA	3.832	0.003	1
1	A	31	ARG	HB2	1.585	0.003	.
1	A	31	ARG	HB3	1.469	0.001	.
1	A	31	ARG	HD2	2.89	0.000	.
1	A	31	ARG	HG2	1.287	0.000	.
1	A	32	ASN	H	8.234	0.002	1
1	A	32	ASN	HA	4.155	0.004	1
1	A	32	ASN	HB2	2.517	0.004	.
1	A	32	ASN	HD21	7.513	0.009	.
1	A	32	ASN	HD22	6.828	0.007	.
1	A	33	AIB	H	7.895	0.003	1
1	A	33	AIB	HB11	1.184	0.000	.
1	A	33	AIB	HB12	1.184	0.000	.
1	A	33	AIB	HB13	1.184	0.000	.
1	A	33	AIB	HB21	1.115	0.000	.
1	A	33	AIB	HB22	1.115	0.000	.
1	A	33	AIB	HB23	1.115	0.000	.
1	A	35	AIB	H	7.518	0.001	1
1	A	35	AIB	HB11	1.198	0.000	.
1	A	35	AIB	HB12	1.198	0.000	.
1	A	35	AIB	HB13	1.198	0.000	.
1	A	35	AIB	HB21	1.127	0.001	.
1	A	35	AIB	HB22	1.127	0.001	.
1	A	35	AIB	HB23	1.127	0.001	.

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 1%, i.e. 5 atoms were assigned a chemical shift out of a possible 723. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	2/297 (1%)	2/121 (2%)	0/120 (0%)	0/56 (0%)
Sidechain	3/387 (1%)	3/246 (1%)	0/121 (0%)	0/20 (0%)
Aromatic	0/39 (0%)	0/20 (0%)	0/16 (0%)	0/3 (0%)
Overall	5/723 (1%)	5/387 (1%)	0/257 (0%)	0/79 (0%)

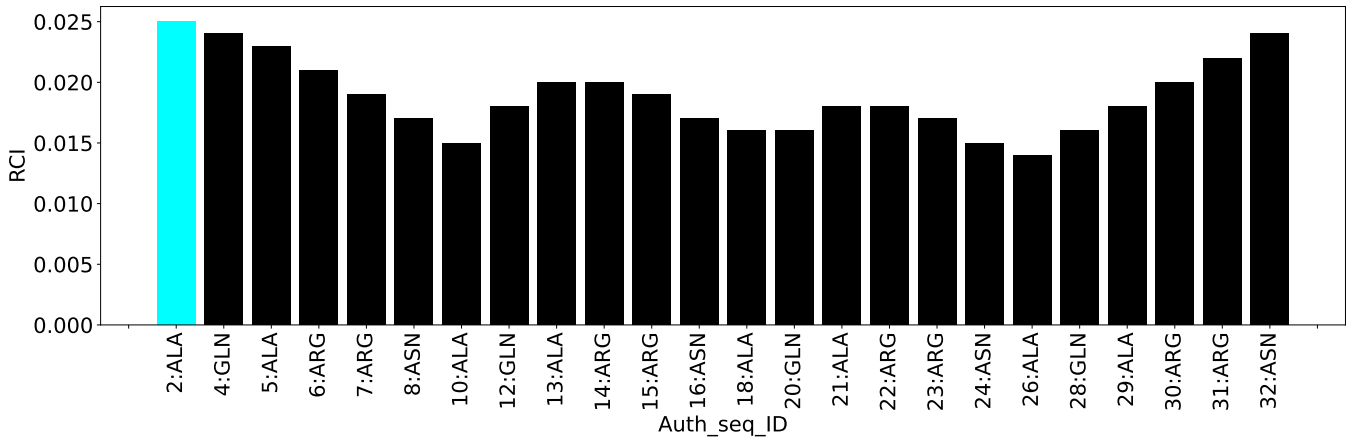
7.1.4 Statistically unusual chemical shifts (i)

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	609
Intra-residue (|i-j|=0)	189
Sequential (|i-j|=1)	189
Medium range (|i-j|>1 and |i-j|<5)	231
Long range (|i-j|≥5)	0
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	606
Number of restraints per residue	17.4
Number of long range restraints per residue[1]	0.0

[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.There are no distance violations

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)

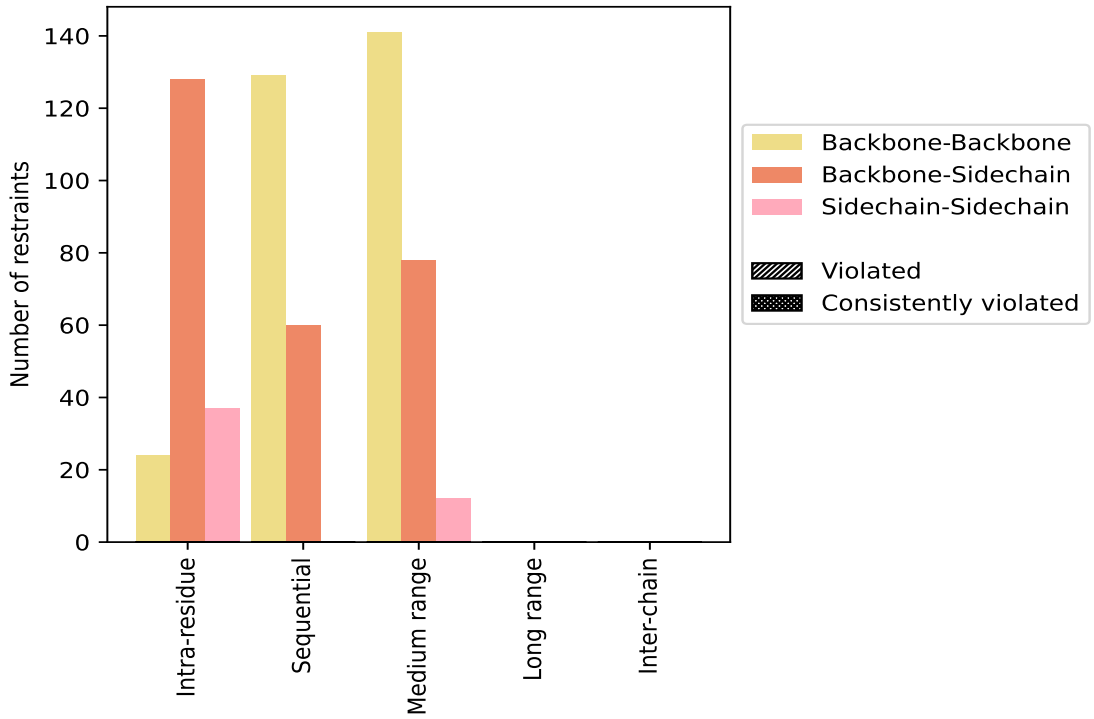
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	189	31.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	24	3.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	128	21.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	37	6.1	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	189	31.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	129	21.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	60	9.9	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)	231	37.9	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	141	23.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	78	12.8	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	12	2.0	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	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	609	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	294	48.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	266	43.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	49	8.0	0	0.0	0.0	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

No violations found

9.3 Distance violation statistics for the ensemble

No violations found

9.4 Most violated distance restraints in the ensemble

No violations found

9.5 All violated distance restraints

No violations found

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found