



wwPDB NMR Structure Validation Summary Report ⓘ

Sep 9, 2026 – 02:28 am BST

PDB ID : 34AG / pdb_000034ag
BMRB ID : 35087
Title : Cu(II) - alpha-synuclein monomer complex - local structure of binding site
His50 with Gly47 as ligand
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Deposited on : 2026-09-03

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

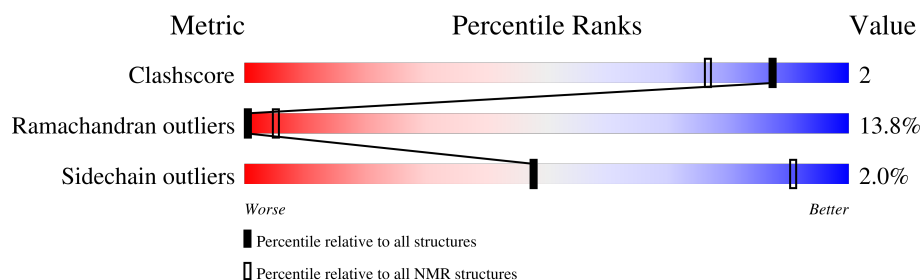
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 41%.

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	140	

2 Ensemble composition and analysis

This entry contains 5 models. Model 2 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:47-A:60 (14)	3.29	2

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

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

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

Cluster number	Models
1	1, 2, 5
Single-model clusters	3; 4

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 308 atoms, of which 159 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Alpha-synuclein.

Mol	Chain	Residues	Atoms					Trace
1	A	21	Total	C	H	N	O	0
			307	92	159	27	29	

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	
2	A	1	Total	Cu
			1	1

5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 5 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
Amber	refinement	20
CYANA	structure calculation	3.98.15

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	679
Number of shifts mapped to atoms	105
Number of unparsed shifts	0
Number of shifts with mapping errors	574
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	41%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU

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	0.91±0.01	0±0/97 (0.0± 0.0%)	1.76±0.12	1±1/130 (1.1± 1.0%)
All	All	0.91	0/485 (0.0%)	1.77	7/650 (1.1%)

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	48	VAL	CA-C-N	7.82	131.44	122.36	2	2
1	A	48	VAL	C-N-CA	7.82	131.44	122.36	2	2
1	A	48	VAL	N-CA-C	7.47	114.21	106.21	1	1
1	A	47	GLY	O-C-N	5.57	129.94	122.70	4	1
1	A	50	HIS	N-CA-C	5.05	117.44	111.33	2	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	97	103	103	0±0
All	All	490	515	515	2

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.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:THR:HG22	1:A:55:VAL:H	0.58	1.59	1	1
1:A:47:GLY:O	1:A:50:HIS:CE1	0.41	2.74	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	13/140 (9%)	7±1 (57±8%)	4±2 (29±12%)	2±1 (14±9%)	0	5
All	All	65/700 (9%)	37 (57%)	19 (29%)	9 (14%)	0	5

5 of 6 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	49	VAL	3
1	A	55	VAL	2
1	A	52	VAL	1
1	A	48	VAL	1
1	A	59	THR	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	10/103 (10%)	10±0 (98±4%)	0±0 (2±4%)	48	91
All	All	50/515 (10%)	49 (98%)	1 (2%)	48	91

All 1 unique residues with a non-rotameric sidechain are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	55	VAL	1

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 41% for the well-defined parts and 41% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	679
Number of shifts mapped to atoms	105
Number of unparsed shifts	0
Number of shifts with mapping errors	574
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 574) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	HA	3.955	0.00	1
1	A	1	MET	CA	55.259	0.00	1
1	A	2	ASP	HA	4.681	0.00	1
1	A	2	ASP	C	176.038	0.00	1
1	A	2	ASP	CA	54.198	0.00	1
1	A	3	VAL	H	8.287	0.00	1
1	A	3	VAL	HA	4.014	0.00	1
1	A	3	VAL	C	176.022	0.00	1
1	A	3	VAL	CA	62.643	0.00	1
1	A	3	VAL	N	120.598	0.00	1
1	A	4	PHE	H	8.375	0.00	1
1	A	4	PHE	HA	4.596	0.00	1
1	A	4	PHE	C	175.913	0.00	1
1	A	4	PHE	CA	57.988	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	PHE	N	123.761	0.00	1
1	A	5	MET	H	8.255	0.00	1
1	A	5	MET	HA	4.386	0.00	1
1	A	5	MET	C	176.013	0.00	1
1	A	5	MET	CA	55.312	0.00	1
1	A	5	MET	N	122.381	0.00	1
1	A	6	LYS	H	8.335	0.00	1
1	A	6	LYS	HA	4.2	0.00	1
1	A	6	LYS	C	177.216	0.00	1
1	A	6	LYS	CA	56.865	0.00	1
1	A	6	LYS	N	122.726	0.00	1
1	A	7	GLY	H	8.484	0.00	1
1	A	7	GLY	HA2	3.939	0.00	1
1	A	7	GLY	HA3	3.939	0.00	1
1	A	7	GLY	C	174.23	0.00	1
1	A	7	GLY	CA	45.274	0.00	1
1	A	7	GLY	N	110.251	0.00	1
1	A	8	LEU	H	8.106	0.00	1
1	A	8	LEU	HA	4.38	0.00	1
1	A	8	LEU	C	177.731	0.00	1
1	A	8	LEU	CA	55.114	0.00	1
1	A	8	LEU	N	121.582	0.00	1
1	A	9	SER	H	8.376	0.00	1
1	A	9	SER	HA	4.412	0.00	1
1	A	9	SER	C	174.62	0.00	1
1	A	9	SER	CA	58.371	0.00	1
1	A	9	SER	N	116.849	0.00	1
1	A	10	LYS	H	8.453	0.00	1
1	A	10	LYS	HA	4.364	0.00	1
1	A	10	LYS	C	176.752	0.00	1
1	A	10	LYS	CA	56.405	0.00	1
1	A	10	LYS	N	123.884	0.00	1
1	A	11	ALA	H	8.359	0.00	1
1	A	11	ALA	HA	4.247	0.00	1
1	A	11	ALA	C	177.986	0.00	1
1	A	11	ALA	CA	52.725	0.00	1
1	A	11	ALA	N	125.502	0.00	1
1	A	12	LYS	H	8.402	0.00	1
1	A	12	LYS	HA	4.266	0.00	1
1	A	12	LYS	C	176.776	0.00	1
1	A	12	LYS	CA	56.436	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	LYS	N	121.057	0.00	1
1	A	13	GLU	H	8.488	0.00	1
1	A	13	GLU	C	177.096	0.00	1
1	A	13	GLU	CA	56.768	0.00	1
1	A	13	GLU	N	122.411	0.00	1
1	A	14	GLY	H	8.545	0.00	1
1	A	14	GLY	C	174.08	0.00	1
1	A	14	GLY	CA	45.308	0.00	1
1	A	14	GLY	N	110.23	0.00	1
1	A	15	VAL	H	8.027	0.00	1
1	A	15	VAL	HA	4.084	0.00	1
1	A	15	VAL	C	176.561	0.00	1
1	A	15	VAL	CA	62.643	0.00	1
1	A	15	VAL	N	120.329	0.00	1
1	A	16	VAL	H	8.38	0.00	1
1	A	16	VAL	C	176.084	0.00	1
1	A	16	VAL	CA	62.55	0.00	1
1	A	16	VAL	N	125.527	0.00	1
1	A	17	ALA	H	8.506	0.00	1
1	A	17	ALA	HA	4.26	0.00	1
1	A	17	ALA	C	177.755	0.00	1
1	A	17	ALA	CA	52.629	0.00	1
1	A	17	ALA	N	128.59	0.00	1
1	A	18	ALA	H	8.375	0.00	1
1	A	18	ALA	HA	4.228	0.00	1
1	A	18	ALA	C	177.991	0.00	1
1	A	18	ALA	CA	52.77	0.00	1
1	A	18	ALA	N	123.761	0.00	1
1	A	19	ALA	H	8.374	0.00	1
1	A	19	ALA	HA	4.264	0.00	1
1	A	19	ALA	C	178.285	0.00	1
1	A	19	ALA	CA	52.847	0.00	1
1	A	19	ALA	N	123.35	0.00	1
1	A	20	GLU	H	8.378	0.00	1
1	A	20	GLU	C	177.01	0.00	1
1	A	20	GLU	CA	56.796	0.00	1
1	A	20	GLU	N	120.277	0.00	1
1	A	21	LYS	H	8.391	0.00	1
1	A	21	LYS	HA	4.323	0.00	1
1	A	21	LYS	C	177.245	0.00	1
1	A	21	LYS	CA	56.778	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	21	LYS	N	122.465	0.00	1
1	A	22	THR	H	8.193	0.00	1
1	A	22	THR	HA	4.269	0.00	1
1	A	22	THR	C	174.76	0.00	1
1	A	22	THR	CA	62.358	0.00	1
1	A	22	THR	N	115.676	0.00	1
1	A	23	LYS	H	8.405	0.00	1
1	A	23	LYS	HA	4.277	0.00	1
1	A	23	LYS	C	176.779	0.00	1
1	A	23	LYS	CA	56.806	0.00	1
1	A	23	LYS	N	123.923	0.00	1
1	A	24	GLN	H	8.488	0.00	1
1	A	24	GLN	HA	4.29	0.00	1
1	A	24	GLN	C	176.684	0.00	1
1	A	24	GLN	CA	56.308	0.00	1
1	A	24	GLN	N	122.411	0.00	1
1	A	25	GLY	H	8.538	0.00	1
1	A	25	GLY	HA2	3.978	0.00	1
1	A	25	GLY	HA3	3.978	0.00	1
1	A	25	GLY	C	174.332	0.00	1
1	A	25	GLY	CA	45.361	0.00	1
1	A	25	GLY	N	110.431	0.00	1
1	A	26	VAL	H	8.069	0.00	1
1	A	26	VAL	HA	4.065	0.00	1
1	A	26	VAL	C	176.487	0.00	1
1	A	26	VAL	CA	62.681	0.00	1
1	A	26	VAL	N	119.989	0.00	1
1	A	27	ALA	H	8.476	0.00	1
1	A	27	ALA	HA	4.283	0.00	1
1	A	27	ALA	C	178.243	0.00	1
1	A	27	ALA	CA	52.861	0.00	1
1	A	27	ALA	N	127.428	0.00	1
1	A	28	GLU	H	8.458	0.00	1
1	A	28	GLU	HA	4.194	0.00	1
1	A	28	GLU	C	176.754	0.00	1
1	A	28	GLU	CA	56.878	0.00	1
1	A	28	GLU	N	120.631	0.00	1
1	A	29	ALA	H	8.346	0.00	1
1	A	29	ALA	HA	4.262	0.00	1
1	A	29	ALA	C	177.838	0.00	1
1	A	29	ALA	CA	52.731	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	29	ALA	N	124.989	0.00	1
1	A	30	ALA	H	8.28	0.00	1
1	A	30	ALA	HA	4.287	0.00	1
1	A	30	ALA	C	178.552	0.00	1
1	A	30	ALA	CA	52.821	0.00	1
1	A	30	ALA	N	123.043	0.00	1
1	A	31	GLY	H	8.357	0.00	1
1	A	31	GLY	HA2	3.925	0.00	1
1	A	31	GLY	HA3	3.925	0.00	1
1	A	31	GLY	C	174.244	0.00	1
1	A	31	GLY	CA	45.328	0.00	1
1	A	31	GLY	N	107.844	0.00	1
1	A	32	LYS	H	8.151	0.00	1
1	A	32	LYS	HA	4.421	0.00	1
1	A	32	LYS	C	177.082	0.00	1
1	A	32	LYS	CA	56.242	0.00	1
1	A	32	LYS	N	120.772	0.00	1
1	A	33	THR	H	8.288	0.00	1
1	A	33	THR	HA	4.336	0.00	1
1	A	33	THR	C	174.721	0.00	1
1	A	33	THR	CA	61.99	0.00	1
1	A	33	THR	N	115.827	0.00	1
1	A	34	LYS	H	8.539	0.00	1
1	A	34	LYS	C	176.598	0.00	1
1	A	34	LYS	CA	56.565	0.00	1
1	A	34	LYS	N	124.012	0.00	1
1	A	35	GLU	H	8.536	0.00	1
1	A	35	GLU	HA	4.256	0.00	1
1	A	35	GLU	C	177.005	0.00	1
1	A	35	GLU	CA	56.521	0.00	1
1	A	35	GLU	N	122.23	0.00	1
1	A	36	GLY	H	8.484	0.00	1
1	A	36	GLY	HA2	3.951	0.00	1
1	A	36	GLY	HA3	3.951	0.00	1
1	A	36	GLY	C	174.067	0.00	1
1	A	36	GLY	CA	45.259	0.00	1
1	A	36	GLY	N	110.251	0.00	1
1	A	37	VAL	H	7.958	0.00	1
1	A	37	VAL	HA	4.058	0.00	1
1	A	37	VAL	C	176.025	0.00	1
1	A	37	VAL	CA	62.379	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	37	VAL	N	119.734	0.00	1
1	A	38	LEU	H	8.343	0.00	1
1	A	38	LEU	HA	4.345	0.00	1
1	A	38	LEU	C	176.716	0.00	1
1	A	38	LEU	CA	54.948	0.00	1
1	A	38	LEU	N	126.047	0.00	1
1	A	39	TYR	H	8.335	0.00	1
1	A	39	TYR	HA	4.582	0.00	1
1	A	39	TYR	C	175.623	0.00	1
1	A	39	TYR	CA	57.925	0.00	1
1	A	39	TYR	N	122.726	0.00	1
1	A	49	VAL	H	8.359	0.00	1
1	A	50	HIS	H	8.556	0.00	1
1	A	61	GLU	H	8.488	0.00	1
1	A	61	GLU	C	176.591	0.00	1
1	A	61	GLU	CA	56.602	0.00	1
1	A	61	GLU	N	122.411	0.00	1
1	A	62	GLN	H	8.488	0.00	1
1	A	62	GLN	HA	4.334	0.00	1
1	A	62	GLN	C	176.025	0.00	1
1	A	62	GLN	CA	55.816	0.00	1
1	A	62	GLN	N	122.411	0.00	1
1	A	63	VAL	H	8.34	0.00	1
1	A	63	VAL	HA	4.185	0.00	1
1	A	63	VAL	C	176.416	0.00	1
1	A	63	VAL	CA	62.353	0.00	1
1	A	63	VAL	N	122.234	0.00	1
1	A	64	THR	H	8.363	0.00	1
1	A	64	THR	HA	4.361	0.00	1
1	A	64	THR	C	174.082	0.00	1
1	A	64	THR	CA	61.861	0.00	1
1	A	64	THR	N	118.415	0.00	1
1	A	65	ASN	H	8.575	0.00	1
1	A	65	ASN	HA	4.775	0.00	1
1	A	65	ASN	C	175.304	0.00	1
1	A	65	ASN	CA	53.111	0.00	1
1	A	65	ASN	N	121.787	0.00	1
1	A	66	VAL	H	8.304	0.00	1
1	A	66	VAL	HA	4.115	0.00	1
1	A	66	VAL	C	176.94	0.00	1
1	A	66	VAL	CA	62.674	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	66	VAL	N	120.955	0.00	1
1	A	67	GLY	H	8.614	0.00	1
1	A	67	GLY	HA2	3.968	0.00	1
1	A	67	GLY	HA3	3.968	0.00	1
1	A	67	GLY	C	174.713	0.00	1
1	A	67	GLY	CA	45.369	0.00	1
1	A	67	GLY	N	112.79	0.00	1
1	A	68	GLY	H	8.277	0.00	1
1	A	68	GLY	HA2	3.942	0.00	1
1	A	68	GLY	HA3	3.942	0.00	1
1	A	68	GLY	C	173.772	0.00	1
1	A	68	GLY	CA	45.015	0.00	1
1	A	68	GLY	N	108.871	0.00	1
1	A	69	ALA	H	8.211	0.00	1
1	A	69	ALA	HA	4.345	0.00	1
1	A	69	ALA	C	177.725	0.00	1
1	A	69	ALA	CA	52.317	0.00	1
1	A	69	ALA	N	123.816	0.00	1
1	A	70	VAL	H	8.262	0.00	1
1	A	70	VAL	HA	4.085	0.00	1
1	A	70	VAL	C	176.405	0.00	1
1	A	70	VAL	CA	62.435	0.00	1
1	A	70	VAL	N	120.846	0.00	1
1	A	71	VAL	H	8.464	0.00	1
1	A	71	VAL	HA	4.213	0.00	1
1	A	71	VAL	C	176.352	0.00	1
1	A	71	VAL	CA	62.123	0.00	1
1	A	71	VAL	N	125.795	0.00	1
1	A	72	THR	H	8.375	0.00	1
1	A	72	THR	HA	4.358	0.00	1
1	A	72	THR	C	174.947	0.00	1
1	A	72	THR	CA	61.87	0.00	1
1	A	72	THR	N	118.98	0.00	1
1	A	73	GLY	H	8.493	0.00	1
1	A	73	GLY	HA2	3.986	0.00	1
1	A	73	GLY	HA3	3.986	0.00	1
1	A	73	GLY	C	174.042	0.00	1
1	A	73	GLY	CA	45.211	0.00	1
1	A	73	GLY	N	111.476	0.00	1
1	A	74	VAL	H	8.139	0.00	1
1	A	74	VAL	HA	4.185	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	74	VAL	C	176.628	0.00	1
1	A	74	VAL	CA	62.334	0.00	1
1	A	74	VAL	N	119.687	0.00	1
1	A	75	THR	H	8.366	0.00	1
1	A	75	THR	HA	4.306	0.00	1
1	A	75	THR	C	174.11	0.00	1
1	A	75	THR	CA	61.983	0.00	1
1	A	75	THR	N	119.349	0.00	1
1	A	76	ALA	H	8.438	0.00	1
1	A	76	ALA	HA	4.34	0.00	1
1	A	76	ALA	C	177.627	0.00	1
1	A	76	ALA	CA	52.439	0.00	1
1	A	76	ALA	N	127.655	0.00	1
1	A	77	VAL	H	8.218	0.00	1
1	A	77	VAL	HA	4.053	0.00	1
1	A	77	VAL	C	176.075	0.00	1
1	A	77	VAL	CA	62.261	0.00	1
1	A	77	VAL	N	120.403	0.00	1
1	A	78	ALA	H	8.48	0.00	1
1	A	78	ALA	HA	4.284	0.00	1
1	A	78	ALA	C	177.7	0.00	1
1	A	78	ALA	CA	52.49	0.00	1
1	A	78	ALA	N	128.4	0.00	1
1	A	79	GLN	H	8.458	0.00	1
1	A	79	GLN	HA	4.285	0.00	1
1	A	79	GLN	C	176.013	0.00	1
1	A	79	GLN	CA	55.675	0.00	1
1	A	79	GLN	N	120.631	0.00	1
1	A	80	LYS	H	8.501	0.00	1
1	A	80	LYS	HA	4.364	0.00	1
1	A	80	LYS	C	176.751	0.00	1
1	A	80	LYS	CA	56.341	0.00	1
1	A	80	LYS	N	123.541	0.00	1
1	A	81	THR	H	8.358	0.00	1
1	A	81	THR	HA	4.338	0.00	1
1	A	81	THR	C	174.481	0.00	1
1	A	81	THR	CA	61.987	0.00	1
1	A	81	THR	N	117.256	0.00	1
1	A	82	VAL	H	8.311	0.00	1
1	A	82	VAL	HA	4.113	0.00	1
1	A	82	VAL	C	176.215	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	82	VAL	CA	62.32	0.00	1
1	A	82	VAL	N	123.424	0.00	1
1	A	83	GLU	H	8.632	0.00	1
1	A	83	GLU	HA	4.256	0.00	1
1	A	83	GLU	C	177.094	0.00	1
1	A	83	GLU	CA	56.831	0.00	1
1	A	83	GLU	N	125.568	0.00	1
1	A	84	GLY	H	8.58	0.00	1
1	A	84	GLY	HA2	3.951	0.00	1
1	A	84	GLY	HA3	3.951	0.00	1
1	A	84	GLY	C	174.196	0.00	1
1	A	84	GLY	CA	45.258	0.00	1
1	A	84	GLY	N	110.857	0.00	1
1	A	85	ALA	H	8.31	0.00	1
1	A	85	ALA	HA	4.301	0.00	1
1	A	85	ALA	C	178.577	0.00	1
1	A	85	ALA	CA	52.917	0.00	1
1	A	85	ALA	N	123.987	0.00	1
1	A	86	GLY	H	8.55	0.00	1
1	A	86	GLY	HA2	3.964	0.00	1
1	A	86	GLY	HA3	3.964	0.00	1
1	A	86	GLY	C	174.337	0.00	1
1	A	86	GLY	CA	45.28	0.00	1
1	A	86	GLY	N	108.288	0.00	1
1	A	87	SER	H	8.193	0.00	1
1	A	87	SER	HA	4.459	0.00	1
1	A	87	SER	C	174.757	0.00	1
1	A	87	SER	CA	58.358	0.00	1
1	A	87	SER	N	115.676	0.00	1
1	A	88	ILE	H	8.252	0.00	1
1	A	88	ILE	HA	4.165	0.00	1
1	A	88	ILE	C	176.339	0.00	1
1	A	88	ILE	CA	61.278	0.00	1
1	A	88	ILE	N	123.013	0.00	1
1	A	89	ALA	H	8.409	0.00	1
1	A	89	ALA	HA	4.246	0.00	1
1	A	89	ALA	C	177.627	0.00	1
1	A	89	ALA	CA	52.614	0.00	1
1	A	89	ALA	N	128.312	0.00	1
1	A	90	ALA	H	8.277	0.00	1
1	A	90	ALA	HA	4.25	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	90	ALA	C	177.789	0.00	1
1	A	90	ALA	CA	52.442	0.00	1
1	A	90	ALA	N	123.5	0.00	1
1	A	91	ALA	H	8.353	0.00	1
1	A	91	ALA	HA	4.353	0.00	1
1	A	91	ALA	C	178.206	0.00	1
1	A	91	ALA	CA	52.614	0.00	1
1	A	91	ALA	N	123.608	0.00	1
1	A	92	THR	H	8.16	0.00	1
1	A	92	THR	HA	4.297	0.00	1
1	A	92	THR	C	175.213	0.00	1
1	A	92	THR	CA	62.043	0.00	1
1	A	92	THR	N	112.88	0.00	1
1	A	93	GLY	H	8.358	0.00	1
1	A	93	GLY	HA2	3.908	0.00	1
1	A	93	GLY	HA3	3.908	0.00	1
1	A	93	GLY	C	173.645	0.00	1
1	A	93	GLY	CA	45.143	0.00	1
1	A	93	GLY	N	110.801	0.00	1
1	A	94	PHE	H	8.133	0.00	1
1	A	94	PHE	HA	4.6	0.00	1
1	A	94	PHE	C	175.534	0.00	1
1	A	94	PHE	CA	57.894	0.00	1
1	A	94	PHE	N	120.451	0.00	1
1	A	95	VAL	H	8.109	0.00	1
1	A	95	VAL	HA	3.999	0.00	1
1	A	95	VAL	C	175.432	0.00	1
1	A	95	VAL	CA	62.015	0.00	1
1	A	95	VAL	N	124.148	0.00	1
1	A	96	LYS	H	8.455	0.00	1
1	A	96	LYS	HA	4.211	0.00	1
1	A	96	LYS	C	176.517	0.00	1
1	A	96	LYS	CA	56.46	0.00	1
1	A	96	LYS	N	126.683	0.00	1
1	A	97	LYS	H	8.539	0.00	1
1	A	97	LYS	HA	4.288	0.00	1
1	A	97	LYS	C	176.414	0.00	1
1	A	97	LYS	CA	56.49	0.00	1
1	A	97	LYS	N	124.012	0.00	1
1	A	98	ASP	H	8.457	0.00	1
1	A	98	ASP	HA	4.562	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	98	ASP	C	176.257	0.00	1
1	A	98	ASP	CA	54.416	0.00	1
1	A	98	ASP	N	121.421	0.00	1
1	A	99	GLN	H	8.403	0.00	1
1	A	99	GLN	HA	4.313	0.00	1
1	A	99	GLN	C	176.067	0.00	1
1	A	99	GLN	CA	55.854	0.00	1
1	A	99	GLN	N	120.344	0.00	1
1	A	100	LEU	H	8.361	0.00	1
1	A	100	LEU	HA	4.332	0.00	1
1	A	100	LEU	C	178.06	0.00	1
1	A	100	LEU	CA	55.351	0.00	1
1	A	100	LEU	N	122.983	0.00	1
1	A	101	GLY	H	8.529	0.00	1
1	A	101	GLY	HA2	3.939	0.00	1
1	A	101	GLY	HA3	3.939	0.00	1
1	A	101	GLY	C	174.125	0.00	1
1	A	101	GLY	CA	45.279	0.00	1
1	A	101	GLY	N	109.909	0.00	1
1	A	102	LYS	H	8.284	0.00	1
1	A	102	LYS	HA	4.306	0.00	1
1	A	102	LYS	C	176.525	0.00	1
1	A	102	LYS	CA	56.213	0.00	1
1	A	102	LYS	N	120.751	0.00	1
1	A	103	ASN	H	8.678	0.00	1
1	A	103	ASN	HA	4.692	0.00	1
1	A	103	ASN	C	175.364	0.00	1
1	A	103	ASN	CA	53.296	0.00	1
1	A	103	ASN	N	120.107	0.00	1
1	A	104	GLU	H	8.53	0.00	1
1	A	104	GLU	HA	4.295	0.00	1
1	A	104	GLU	C	176.605	0.00	1
1	A	104	GLU	CA	56.489	0.00	1
1	A	104	GLU	N	121.464	0.00	1
1	A	105	GLU	H	8.516	0.00	1
1	A	105	GLU	C	177.097	0.00	1
1	A	105	GLU	CA	56.52	0.00	1
1	A	105	GLU	N	121.926	0.00	1
1	A	106	GLY	H	8.484	0.00	1
1	A	106	GLY	HA2	3.926	0.00	1
1	A	106	GLY	HA3	3.926	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	106	GLY	C	173.476	0.00	1
1	A	106	GLY	CA	45.001	0.00	1
1	A	106	GLY	N	110.251	0.00	1
1	A	107	ALA	H	8.158	0.00	1
1	A	107	ALA	N	125.002	0.00	1
1	A	108	PRO	HA	4.43	0.00	1
1	A	108	PRO	C	177.087	0.00	1
1	A	108	PRO	CA	63.011	0.00	1
1	A	109	GLN	H	8.647	0.00	1
1	A	109	GLN	HA	4.298	0.00	1
1	A	109	GLN	C	176.037	0.00	1
1	A	109	GLN	CA	55.676	0.00	1
1	A	109	GLN	N	121.393	0.00	1
1	A	110	GLU	H	8.588	0.00	1
1	A	110	GLU	HA	4.287	0.00	1
1	A	110	GLU	C	176.797	0.00	1
1	A	110	GLU	CA	56.5	0.00	1
1	A	110	GLU	N	122.793	0.00	1
1	A	111	GLY	H	8.538	0.00	1
1	A	111	GLY	HA2	3.944	0.00	1
1	A	111	GLY	HA3	3.944	0.00	1
1	A	111	GLY	C	173.791	0.00	1
1	A	111	GLY	CA	45.242	0.00	1
1	A	111	GLY	N	110.431	0.00	1
1	A	112	ILE	H	8.06	0.00	1
1	A	112	ILE	HA	4.169	0.00	1
1	A	112	ILE	C	176.337	0.00	1
1	A	112	ILE	CA	60.876	0.00	1
1	A	112	ILE	N	120.352	0.00	1
1	A	113	LEU	H	8.476	0.00	1
1	A	113	LEU	HA	4.389	0.00	1
1	A	113	LEU	C	177.206	0.00	1
1	A	113	LEU	CA	54.983	0.00	1
1	A	113	LEU	N	127.428	0.00	1
1	A	114	GLU	H	8.488	0.00	1
1	A	114	GLU	HA	4.25	0.00	1
1	A	114	GLU	C	175.931	0.00	1
1	A	114	GLU	CA	56.43	0.00	1
1	A	114	GLU	N	122.411	0.00	1
1	A	115	ASP	H	8.419	0.00	1
1	A	115	ASP	HA	4.562	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	115	ASP	C	175.847	0.00	1
1	A	115	ASP	CA	54.279	0.00	1
1	A	115	ASP	N	121.766	0.00	1
1	A	116	MET	H	8.34	0.00	1
1	A	116	MET	N	122.234	0.00	1
1	A	117	PRO	HA	4.453	0.00	1
1	A	117	PRO	C	176.757	0.00	1
1	A	117	PRO	CA	62.88	0.00	1
1	A	118	VAL	H	8.374	0.00	1
1	A	118	VAL	HA	4.062	0.00	1
1	A	118	VAL	C	175.843	0.00	1
1	A	118	VAL	CA	61.945	0.00	1
1	A	118	VAL	N	121.114	0.00	1
1	A	119	ASP	H	8.6	0.00	1
1	A	119	ASP	N	126.371	0.00	1
1	A	120	PRO	HA	4.333	0.00	1
1	A	120	PRO	C	176.931	0.00	1
1	A	120	PRO	CA	63.43	0.00	1
1	A	121	ASP	H	8.431	0.00	1
1	A	121	ASP	HA	4.598	0.00	1
1	A	121	ASP	C	176.215	0.00	1
1	A	121	ASP	CA	54.506	0.00	1
1	A	121	ASP	N	119.567	0.00	1
1	A	122	ASN	H	8.177	0.00	1
1	A	122	ASN	HA	4.676	0.00	1
1	A	122	ASN	C	175.438	0.00	1
1	A	122	ASN	CA	53.395	0.00	1
1	A	122	ASN	N	119.3	0.00	1
1	A	123	GLU	H	8.419	0.00	1
1	A	123	GLU	HA	4.203	0.00	1
1	A	123	GLU	C	176.119	0.00	1
1	A	123	GLU	CA	56.248	0.00	1
1	A	123	GLU	N	121.766	0.00	1
1	A	124	ALA	H	8.281	0.00	1
1	A	124	ALA	HA	4.283	0.00	1
1	A	124	ALA	C	177.248	0.00	1
1	A	124	ALA	CA	52.317	0.00	1
1	A	124	ALA	N	124.753	0.00	1
1	A	125	TYR	H	8.103	0.00	1
1	A	125	TYR	HA	4.514	0.00	1
1	A	125	TYR	C	175.363	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	125	TYR	CA	57.754	0.00	1
1	A	125	TYR	N	120.676	0.00	1
1	A	126	GLU	H	8.194	0.00	1
1	A	126	GLU	HA	4.241	0.00	1
1	A	126	GLU	C	175.427	0.00	1
1	A	126	GLU	CA	55.544	0.00	1
1	A	126	GLU	N	124.201	0.00	1
1	A	127	MET	H	8.495	0.00	1
1	A	127	MET	N	124.223	0.00	1
1	A	128	PRO	HA	4.434	0.00	1
1	A	128	PRO	C	176.916	0.00	1
1	A	128	PRO	CA	62.978	0.00	1
1	A	129	SER	H	8.563	0.00	1
1	A	129	SER	HA	4.413	0.00	1
1	A	129	SER	C	174.845	0.00	1
1	A	129	SER	CA	58.242	0.00	1
1	A	129	SER	N	117.034	0.00	1
1	A	130	GLU	H	8.644	0.00	1
1	A	130	GLU	HA	4.32	0.00	1
1	A	130	GLU	C	176.507	0.00	1
1	A	130	GLU	CA	56.392	0.00	1
1	A	130	GLU	N	123.434	0.00	1
1	A	131	GLU	H	8.532	0.00	1
1	A	131	GLU	HA	4.244	0.00	1
1	A	131	GLU	C	177.022	0.00	1
1	A	131	GLU	CA	56.794	0.00	1
1	A	131	GLU	N	122.323	0.00	1
1	A	132	GLY	H	8.484	0.00	1
1	A	132	GLY	HA2	3.895	0.00	1
1	A	132	GLY	HA3	3.895	0.00	1
1	A	132	GLY	C	173.867	0.00	1
1	A	132	GLY	CA	45.122	0.00	1
1	A	132	GLY	N	110.251	0.00	1
1	A	133	TYR	H	8.108	0.00	1
1	A	133	TYR	HA	4.499	0.00	1
1	A	133	TYR	C	175.787	0.00	1
1	A	133	TYR	CA	58.124	0.00	1
1	A	133	TYR	N	120.386	0.00	1
1	A	134	GLN	H	8.252	0.00	1
1	A	134	GLN	HA	4.247	0.00	1
1	A	134	GLN	C	174.862	0.00	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	134	GLN	CA	55.346	0.00	1
1	A	134	GLN	N	123.013	0.00	1
1	A	135	ASP	H	8.286	0.00	1
1	A	135	ASP	HA	4.524	0.00	1
1	A	135	ASP	C	175.57	0.00	1
1	A	135	ASP	CA	54.204	0.00	1
1	A	135	ASP	N	121.945	0.00	1
1	A	136	TYR	H	8.103	0.00	1
1	A	136	TYR	HA	4.553	0.00	1
1	A	136	TYR	C	175.137	0.00	1
1	A	136	TYR	CA	57.552	0.00	1
1	A	136	TYR	N	120.676	0.00	1
1	A	137	GLU	H	8.325	0.00	1
1	A	137	GLU	N	125.613	0.00	1
1	A	138	PRO	HA	4.343	0.00	1
1	A	138	PRO	C	176.913	0.00	1
1	A	138	PRO	CA	62.861	0.00	1
1	A	139	GLU	H	8.575	0.00	1
1	A	139	GLU	HA	4.206	0.00	1
1	A	139	GLU	C	175.471	0.00	1
1	A	139	GLU	CA	56.592	0.00	1
1	A	139	GLU	N	121.787	0.00	1
1	A	140	ALA	H	8.07	0.00	1
1	A	140	ALA	HA	4.098	0.00	1
1	A	140	ALA	C	182.65	0.00	1
1	A	140	ALA	CA	53.795	0.00	1
1	A	140	ALA	N	131.128	0.00	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	135	-0.41 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	134	-0.46 ± 0.17	None needed (< 0.5 ppm)
^{15}N	133	-1.35 ± 0.44	Should be applied

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 41%, i.e. 71 atoms were assigned a chemical shift out of a possible 175. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	71/72 (99%)	29/30 (97%)	28/28 (100%)	14/14 (100%)
Sidechain	0/96 (0%)	0/64 (0%)	0/30 (0%)	0/2 (0%)
Aromatic	0/7 (0%)	0/4 (0%)	0/2 (0%)	0/1 (0%)
Overall	71/175 (41%)	29/98 (30%)	28/60 (47%)	14/17 (82%)

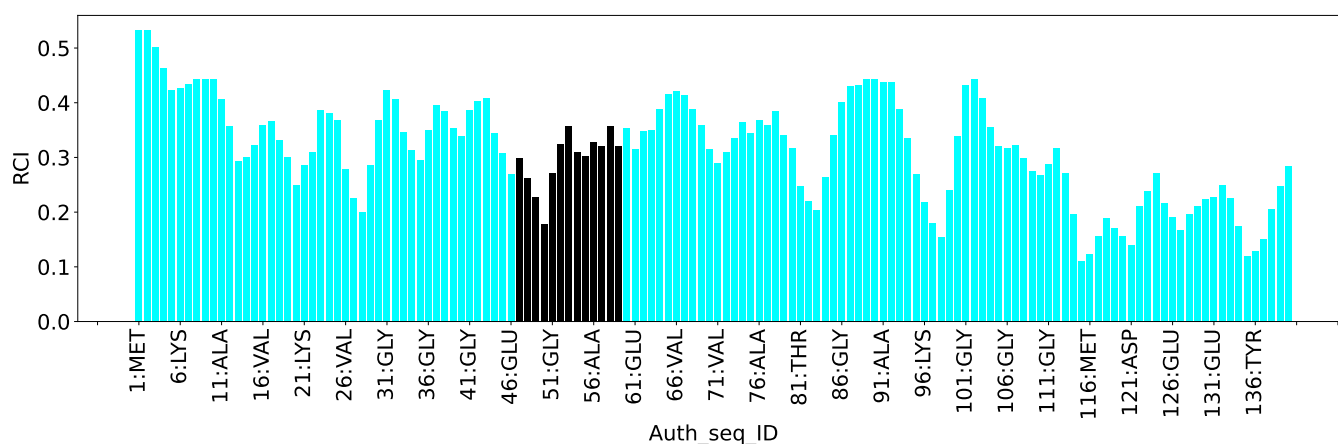
7.1.4 Statistically unusual chemical shifts [i](#)

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 [i](#)

8.1 Conformationally restricting restraints [i](#)

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	18
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	2
Long range ($ i-j \geq 5$)	16
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	18
Number of restraints per residue	0.1
Number of long range restraints per residue ¹	0.1

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 [i](#)

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 [i](#)

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 [i](#)

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

9 Distance violation analysis [i](#)

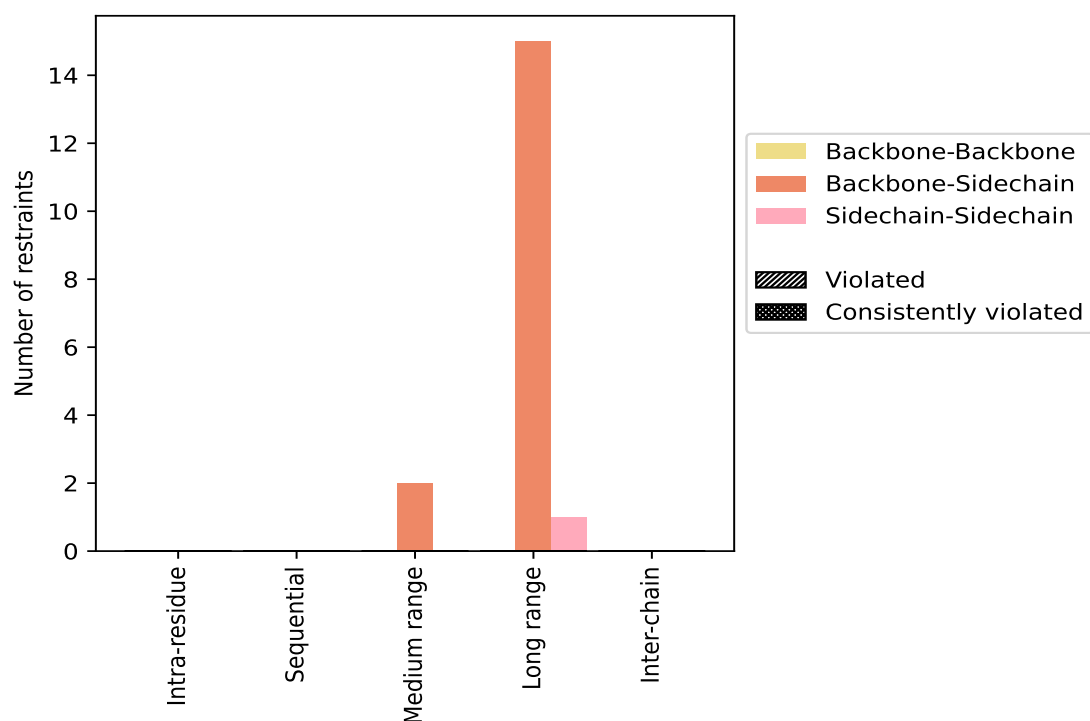
9.1 Summary of distance violations [i](#)

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.

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)	2	11.1	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	2	11.1	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)	16	88.9	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	15	83.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	1	5.6	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	18	100.0	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	17	94.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	1	5.6	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 [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

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

No violations found

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

No violations found

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

No violations found

9.5 All violated distance restraints [i](#)

No violations found

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found