



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 07:24 AM UTC

PDB ID : 5UK6 / pdb_00005uk6
Title : Structure of Anabaena Sensory Rhodopsin Determined by Solid State NMR Spectroscopy and DEER
Authors : Milikisiyants, S.; Wang, S.; Munro, R.A.; Donohue, M.; Ward, M.E.; Brown, L.S.; Smirnova, T.I.; Ladizhansky, V.; Smirnov, A.I.
Deposited on : 2017-01-20

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

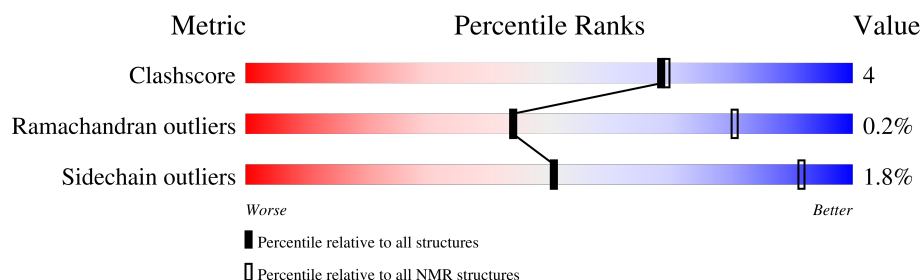
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 12%.

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	235	74% 6% 17% .
1	B	235	77% . 17% .
1	C	235	74% 6% 18% .

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models).

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:6-A:148, A:164-A:185, A:197-A:209, A:211-A:221, B:6-B:148, B:164-B:186, B:197-B:209, B:211-B:221, C:6-C:29, C:33-C:148, C:164-C:185, C:196-C:209, C:211-C:221 (566)	1.05	3

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

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

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

Cluster number	Models
1	1, 2, 3, 7, 8, 10
2	5, 6, 9
Single-model clusters	4

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11223 atoms, of which 5559 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Bacteriorhodopsin.

Mol	Chain	Residues	Atoms						Trace
1	A	229	Total	C	H	N	O	S	0
			3741	1268	1853	298	311	11	
1	B	229	Total	C	H	N	O	S	0
			3741	1268	1853	298	311	11	
1	C	229	Total	C	H	N	O	S	0
			3741	1268	1853	298	311	11	

There are 18 discrepancies between the modelled and reference sequences:

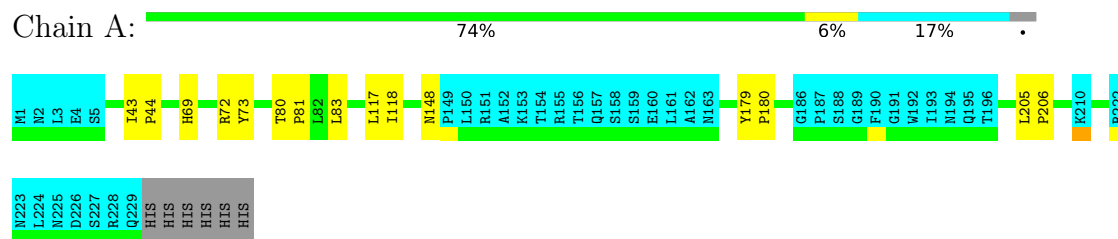
Chain	Residue	Modelled	Actual	Comment	Reference
A	230	HIS	-	expression tag	UNP Q8YSC4
A	231	HIS	-	expression tag	UNP Q8YSC4
A	232	HIS	-	expression tag	UNP Q8YSC4
A	233	HIS	-	expression tag	UNP Q8YSC4
A	234	HIS	-	expression tag	UNP Q8YSC4
A	235	HIS	-	expression tag	UNP Q8YSC4
B	230	HIS	-	expression tag	UNP Q8YSC4
B	231	HIS	-	expression tag	UNP Q8YSC4
B	232	HIS	-	expression tag	UNP Q8YSC4
B	233	HIS	-	expression tag	UNP Q8YSC4
B	234	HIS	-	expression tag	UNP Q8YSC4
B	235	HIS	-	expression tag	UNP Q8YSC4
C	230	HIS	-	expression tag	UNP Q8YSC4
C	231	HIS	-	expression tag	UNP Q8YSC4
C	232	HIS	-	expression tag	UNP Q8YSC4
C	233	HIS	-	expression tag	UNP Q8YSC4
C	234	HIS	-	expression tag	UNP Q8YSC4
C	235	HIS	-	expression tag	UNP Q8YSC4

4 Residue-property plots

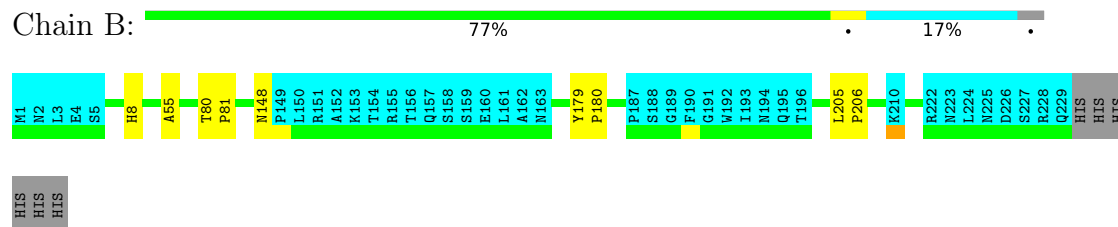
4.1 Average score per residue in the NMR ensemble

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

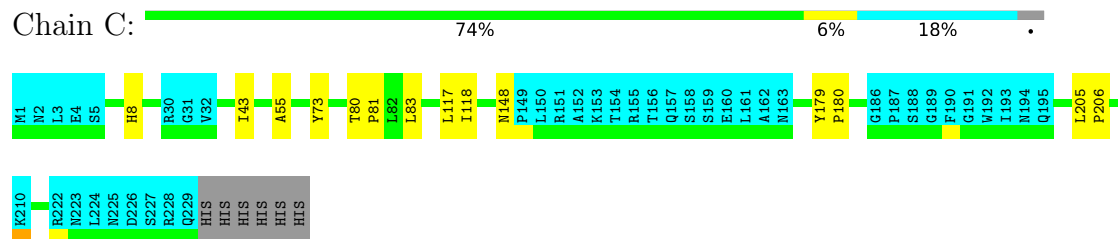
- Molecule 1: Bacteriorhodopsin



- Molecule 1: Bacteriorhodopsin

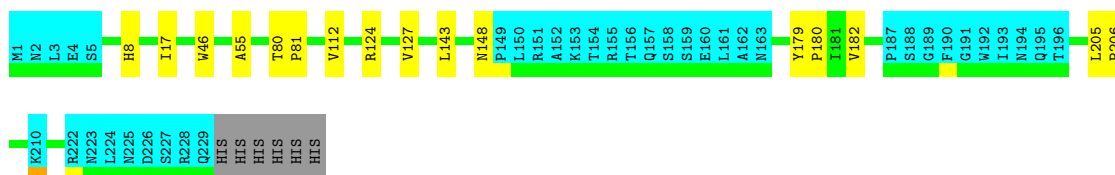


- Molecule 1: Bacteriorhodopsin



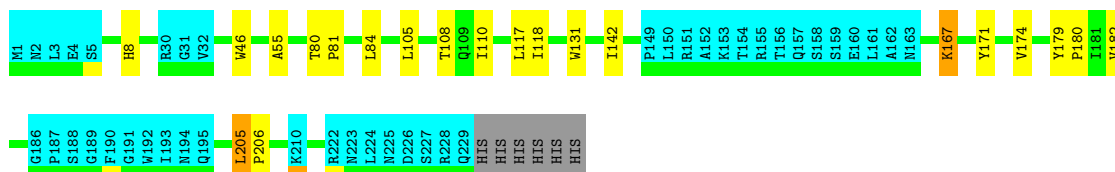
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.



• Molecule 1: Bacteriorhodopsin

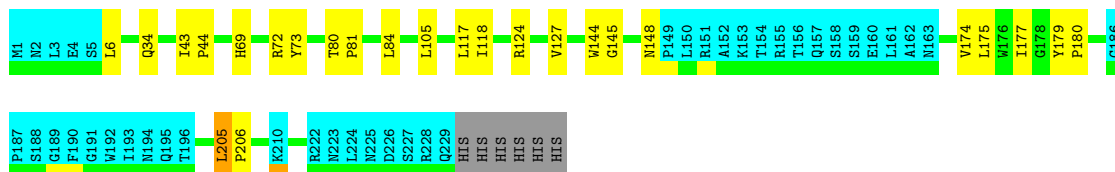
Chain C: 71% 8% 18%



4.2.3 Score per residue for model 3 (medoid)

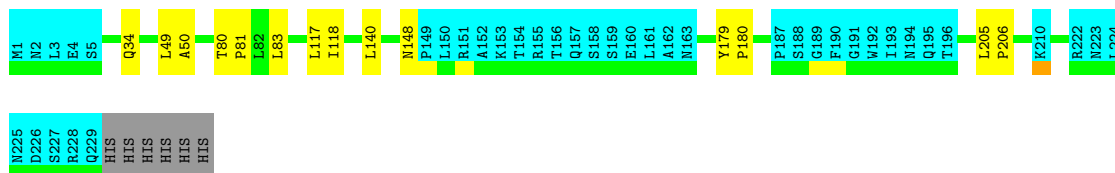
• Molecule 1: Bacteriorhodopsin

Chain A: 70% 10% 17%



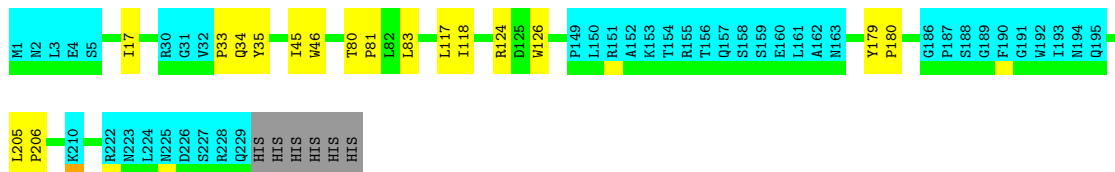
• Molecule 1: Bacteriorhodopsin

Chain B: 75% 6% 17%



• Molecule 1: Bacteriorhodopsin

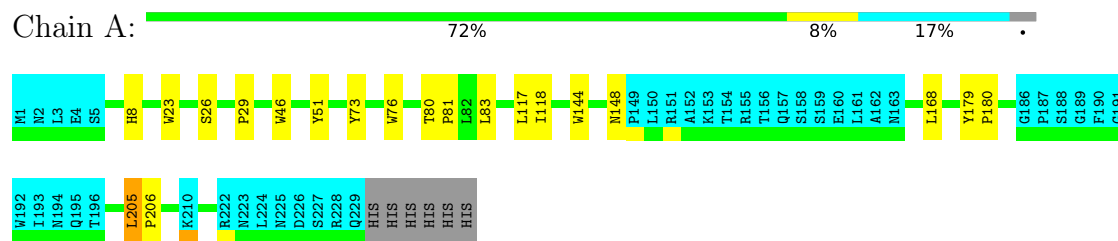
Chain C: 72% 7% 18%



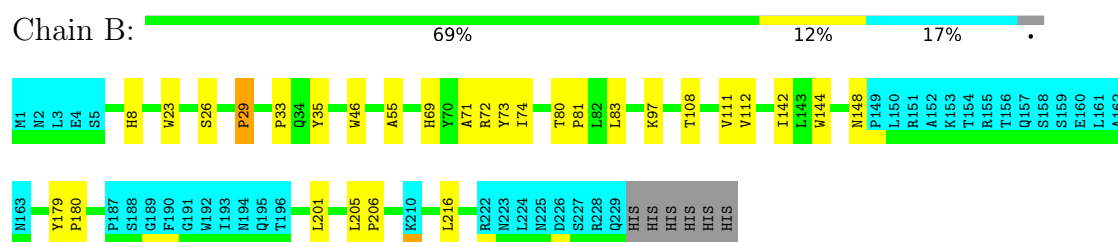


4.2.7 Score per residue for model 7

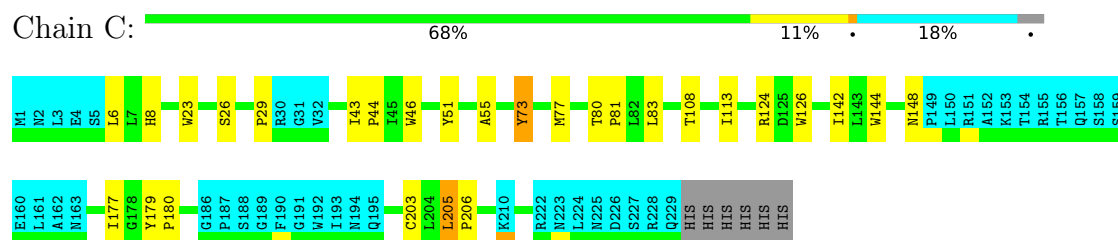
• Molecule 1: Bacteriorhodopsin



• Molecule 1: Bacteriorhodopsin

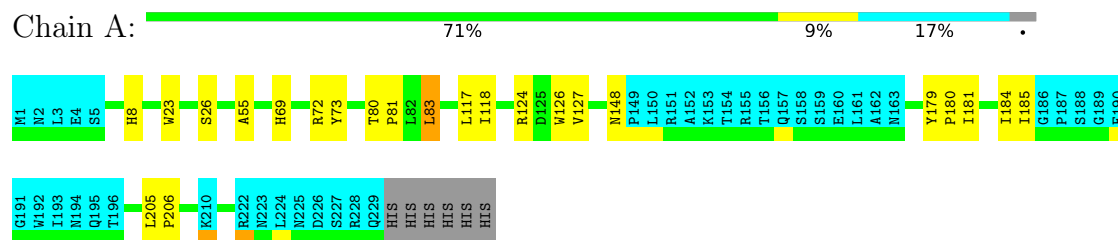


• Molecule 1: Bacteriorhodopsin



4.2.8 Score per residue for model 8

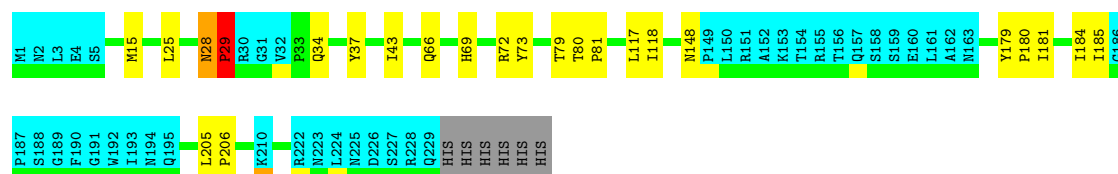
• Molecule 1: Bacteriorhodopsin



• Molecule 1: Bacteriorhodopsin

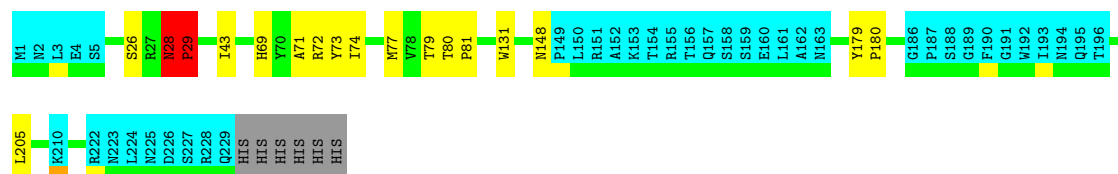


- Molecule 1: Bacteriorhodopsin

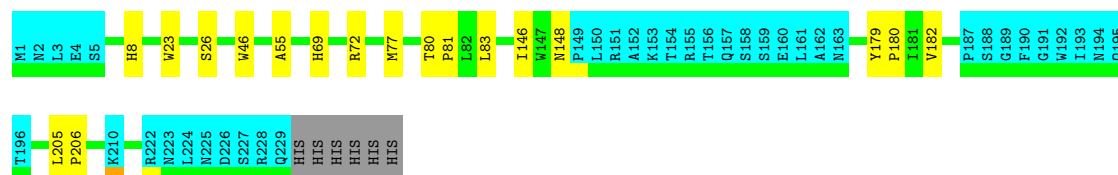


4.2.9 Score per residue for model 9

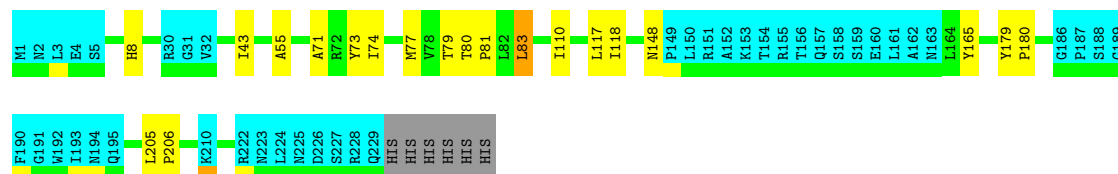
- Molecule 1: Bacteriorhodopsin



- Molecule 1: Bacteriorhodopsin

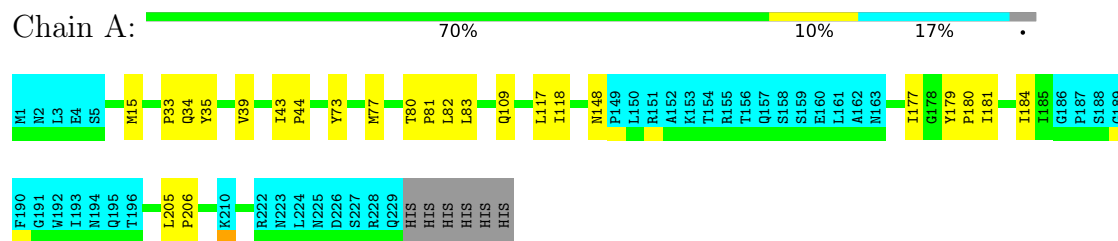


- Molecule 1: Bacteriorhodopsin

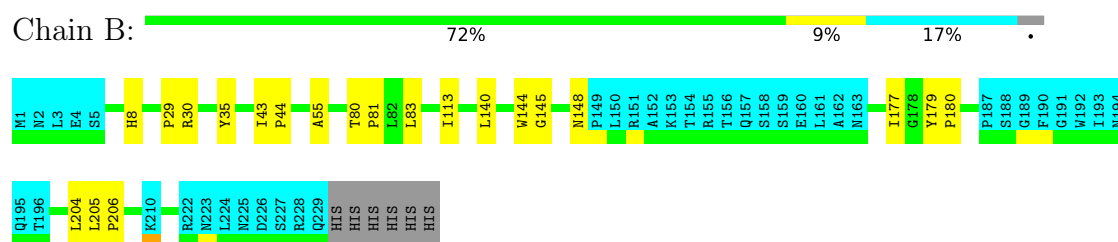


4.2.10 Score per residue for model 10

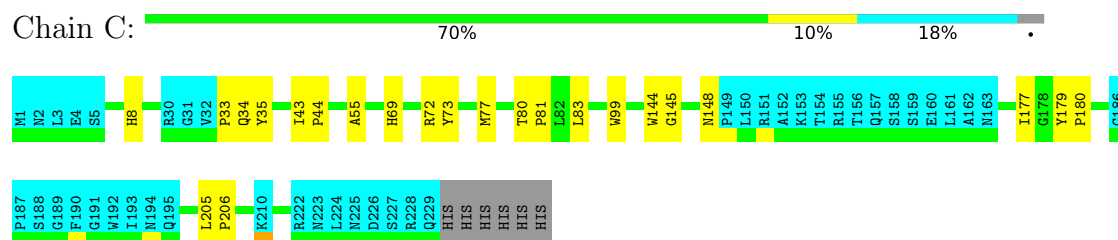
• Molecule 1: Bacteriorhodopsin



• Molecule 1: Bacteriorhodopsin



• Molecule 1: Bacteriorhodopsin



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 10 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
TopSpin	refinement	3.0
CNS	structure calculation	

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	2
Total number of shifts	1185
Number of shifts mapped to atoms	1185
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	12%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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	0.28±0.01	0±0/1609 (0.0± 0.0%)	0.63±0.01	0±0/2204 (0.0± 0.0%)
1	B	0.28±0.00	0±0/1613 (0.0± 0.0%)	0.64±0.01	0±0/2210 (0.0± 0.0%)
1	C	0.28±0.01	0±0/1594 (0.0± 0.0%)	0.63±0.01	0±0/2184 (0.0± 0.0%)
All	All	0.28	0/48160 (0.0%)	0.64	2/65980 (0.0%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	29	PRO	CA-N-CD	-5.52	104.27	112.00	8	1
1	A	29	PRO	CA-N-CD	-5.50	104.30	112.00	9	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1553	1515	1563	13±4
1	B	1557	1518	1566	10±3
1	C	1538	1497	1545	12±4
All	All	46480	45300	46740	342

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:GLY:HA2	1:A:148:ASN:ND2	1.27	1.44	2	3
1:C:145:GLY:HA2	1:C:148:ASN:ND2	1.23	1.48	10	1
1:B:145:GLY:HA2	1:B:148:ASN:ND2	1.22	1.45	10	2
1:B:145:GLY:HA2	1:B:148:ASN:HD21	1.01	1.14	8	2
1:B:145:GLY:CA	1:B:148:ASN:ND2	1.00	2.24	10	2
1:A:145:GLY:CA	1:A:148:ASN:ND2	0.97	2.26	2	3
1:C:145:GLY:CA	1:C:148:ASN:ND2	0.97	2.27	10	1
1:A:145:GLY:HA2	1:A:148:ASN:HD22	0.95	1.19	2	3
1:B:145:GLY:HA2	1:B:148:ASN:HD22	0.92	1.14	10	1
1:A:145:GLY:CA	1:A:148:ASN:HD22	0.90	1.80	2	3
1:B:145:GLY:CA	1:B:148:ASN:HD22	0.88	1.75	10	1
1:C:145:GLY:CA	1:C:148:ASN:HD22	0.83	1.83	10	1
1:C:145:GLY:HA2	1:C:148:ASN:HD22	0.83	1.23	10	1
1:A:145:GLY:HA2	1:A:148:ASN:HD21	0.82	1.32	2	2
1:C:145:GLY:HA2	1:C:148:ASN:HD21	0.77	1.37	10	1
1:A:144:TRP:O	1:A:148:ASN:ND2	0.75	2.20	7	5
1:C:144:TRP:O	1:C:148:ASN:ND2	0.71	2.23	7	4
1:C:28:ASN:CB	1:C:29:PRO:HD2	0.69	2.17	8	1
1:A:145:GLY:C	1:A:148:ASN:HD22	0.69	1.96	2	2
1:A:28:ASN:HB3	1:A:29:PRO:HD2	0.68	1.65	9	1
1:B:144:TRP:O	1:B:148:ASN:ND2	0.68	2.27	10	4
1:C:145:GLY:C	1:C:148:ASN:HD22	0.68	1.97	10	1
1:C:23:TRP:O	1:C:26:SER:OG	0.66	2.14	6	2
1:B:145:GLY:C	1:B:148:ASN:HD22	0.66	1.98	10	2
1:A:28:ASN:CB	1:A:29:PRO:HD2	0.65	2.21	9	1
1:A:23:TRP:O	1:A:26:SER:OG	0.64	2.14	8	4
1:C:28:ASN:HB3	1:C:29:PRO:HD2	0.61	1.70	8	1
1:B:145:GLY:C	1:B:148:ASN:ND2	0.60	2.60	8	1
1:B:23:TRP:O	1:B:26:SER:OG	0.59	2.16	9	2
1:C:22:PHE:O	1:C:26:SER:OG	0.57	2.21	4	1
1:C:179:TYR:O	1:C:182:VAL:HG22	0.56	2.01	6	2
1:A:205:LEU:HB3	1:A:206:PRO:HD3	0.54	1.79	1	7
1:A:80:THR:N	1:A:81:PRO:HD2	0.52	2.20	6	6
1:B:80:THR:N	1:B:81:PRO:HD2	0.52	2.20	9	5
1:B:205:LEU:HB3	1:B:206:PRO:HD3	0.52	1.82	5	10
1:B:179:TYR:O	1:B:182:VAL:HG22	0.52	2.05	6	4
1:C:108:THR:HG21	1:C:142:ILE:HG12	0.51	1.80	7	1
1:A:179:TYR:HB2	1:A:180:PRO:HD3	0.51	1.83	8	9

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ASN:O	1:A:29:PRO:C	0.51	2.53	9	1
1:A:43:ILE:HB	1:A:44:PRO:HD3	0.50	1.84	5	3
1:C:205:LEU:HB3	1:C:206:PRO:HD3	0.50	1.83	3	9
1:B:179:TYR:HB2	1:B:180:PRO:HD3	0.50	1.83	2	8
1:A:84:LEU:HD21	1:A:105:LEU:HB3	0.50	1.84	4	2
1:A:43:ILE:HG23	1:A:79:THR:HG23	0.50	1.83	6	2
1:C:179:TYR:HB2	1:C:180:PRO:HD3	0.49	1.83	3	8
1:C:80:THR:N	1:C:81:PRO:HD2	0.49	2.23	8	2
1:C:180:PRO:HA	1:C:183:TRP:NE1	0.49	2.22	5	1
1:C:28:ASN:O	1:C:29:PRO:C	0.48	2.56	8	1
1:C:28:ASN:CB	1:C:29:PRO:CD	0.48	2.91	8	1
1:C:124:ARG:HB2	1:C:127:VAL:HG12	0.48	1.85	5	1
1:A:127:VAL:HG11	1:C:58:GLN:NE2	0.48	2.24	6	1
1:B:22:PHE:O	1:B:26:SER:OG	0.48	2.31	4	1
1:C:8:HIS:HB2	1:C:55:ALA:HB2	0.48	1.86	6	6
1:A:179:TYR:O	1:A:182:VAL:HG22	0.47	2.08	6	4
1:C:80:THR:HB	1:C:81:PRO:HD3	0.47	1.84	3	8
1:A:28:ASN:CG	1:A:29:PRO:HD2	0.47	2.34	9	1
1:A:110:ILE:HG22	1:C:46:TRP:HE1	0.47	1.69	2	2
1:C:181:ILE:O	1:C:184:ILE:HG22	0.47	2.10	6	2
1:B:73:TYR:C	1:B:73:TYR:CD1	0.47	2.91	7	1
1:B:145:GLY:O	1:B:148:ASN:ND2	0.47	2.39	8	1
1:A:80:THR:HG22	1:A:109:GLN:NE2	0.47	2.24	10	1
1:B:69:HIS:HB3	1:B:72:ARG:HB2	0.46	1.86	9	2
1:A:184:ILE:HG13	1:A:185:ILE:HG23	0.46	1.87	8	1
1:C:205:LEU:N	1:C:206:PRO:HD2	0.46	2.25	4	1
1:B:8:HIS:HB2	1:B:55:ALA:HB2	0.46	1.87	10	6
1:A:8:HIS:HB2	1:A:55:ALA:HB2	0.46	1.86	8	2
1:A:108:THR:HG21	1:A:142:ILE:HG21	0.46	1.86	5	1
1:C:179:TYR:N	1:C:180:PRO:HD2	0.46	2.25	5	1
1:A:33:PRO:O	1:A:35:TYR:N	0.46	2.48	10	1
1:B:43:ILE:HB	1:B:44:PRO:HD3	0.46	1.85	8	1
1:C:117:LEU:HD12	1:C:118:ILE:N	0.46	2.26	8	6
1:B:84:LEU:HD22	1:B:109:GLN:HG3	0.46	1.88	1	1
1:B:145:GLY:CA	1:B:148:ASN:HD21	0.46	2.00	8	1
1:B:80:THR:HB	1:B:81:PRO:HD3	0.45	1.89	2	5
1:A:177:ILE:C	1:A:180:PRO:HD2	0.45	2.37	10	2
1:A:71:ALA:HA	1:A:74:ILE:HG22	0.45	1.88	9	1
1:B:29:PRO:HG3	1:B:33:PRO:HB3	0.45	1.88	7	1
1:B:108:THR:O	1:B:111:VAL:HG22	0.45	2.12	7	1
1:C:15:MET:HA	1:C:15:MET:HE2	0.45	1.87	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:205:LEU:N	1:A:206:PRO:HD2	0.45	2.26	7	1
1:B:43:ILE:HG23	1:B:79:THR:HG23	0.45	1.87	5	3
1:C:73:TYR:O	1:C:77:MET:HG3	0.44	2.12	10	2
1:B:19:ALA:HA	1:B:41:MET:HG3	0.44	1.90	6	1
1:B:124:ARG:HG2	1:B:126:TRP:H	0.44	1.72	4	1
1:C:184:ILE:HG23	1:C:185:ILE:HG23	0.44	1.89	8	1
1:B:84:LEU:HD13	1:B:109:GLN:NE2	0.44	2.27	6	1
1:C:43:ILE:HG23	1:C:79:THR:HG23	0.44	1.90	8	3
1:A:69:HIS:HB3	1:A:72:ARG:HB2	0.44	1.89	1	6
1:C:6:LEU:H	1:C:6:LEU:HD23	0.44	1.72	6	2
1:C:71:ALA:HA	1:C:74:ILE:HG22	0.44	1.89	9	2
1:A:117:LEU:HD12	1:A:118:ILE:N	0.44	2.28	8	5
1:A:181:ILE:O	1:A:184:ILE:HG12	0.44	2.13	8	1
1:B:75:ASP:O	1:B:79:THR:HG22	0.43	2.12	4	1
1:C:43:ILE:HB	1:C:44:PRO:HD3	0.43	1.88	7	1
1:C:45:ILE:HG23	1:C:46:TRP:N	0.43	2.28	4	2
1:A:39:VAL:HG23	1:A:82:LEU:HD12	0.43	1.90	10	1
1:C:84:LEU:HD21	1:C:105:LEU:HB3	0.43	1.90	2	1
1:C:77:MET:HG2	1:C:113:ILE:HG23	0.43	1.90	7	1
1:C:33:PRO:O	1:C:35:TYR:N	0.43	2.51	10	1
1:B:117:LEU:HD12	1:B:118:ILE:N	0.43	2.28	1	2
1:C:34:GLN:O	1:C:37:TYR:N	0.43	2.51	8	1
1:A:45:ILE:HG13	1:A:46:TRP:N	0.43	2.28	4	1
1:C:28:ASN:HB3	1:C:29:PRO:CD	0.43	2.42	8	1
1:C:203:CYS:C	1:C:206:PRO:HD2	0.43	2.39	7	1
1:B:43:ILE:N	1:B:44:PRO:HD2	0.43	2.29	10	1
1:A:130:LEU:N	1:A:130:LEU:HD22	0.43	2.29	4	2
1:A:84:LEU:HD21	1:A:109:GLN:HB3	0.43	1.90	6	1
1:A:80:THR:HB	1:A:81:PRO:HD3	0.43	1.91	2	4
1:C:216:LEU:C	1:C:216:LEU:HD13	0.43	2.39	5	1
1:C:25:LEU:O	1:C:28:ASN:HB2	0.43	2.14	8	1
1:B:71:ALA:HA	1:B:74:ILE:HD12	0.42	1.90	7	1
1:A:74:ILE:HG23	1:A:75:ASP:N	0.42	2.29	1	1
1:A:28:ASN:CB	1:A:29:PRO:CD	0.42	2.96	9	1
1:A:181:ILE:O	1:A:184:ILE:HG22	0.42	2.14	10	1
1:B:46:TRP:HE1	1:C:110:ILE:HG22	0.42	1.74	9	2
1:C:108:THR:HG21	1:C:142:ILE:HG21	0.42	1.90	2	1
1:A:8:HIS:HB3	1:A:51:TYR:O	0.42	2.13	7	1
1:C:43:ILE:N	1:C:44:PRO:HD2	0.42	2.29	10	2
1:A:124:ARG:HG2	1:A:126:TRP:H	0.42	1.74	2	2
1:B:207:PHE:O	1:B:211:VAL:HG22	0.42	2.14	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:177:ILE:C	1:C:180:PRO:HD2	0.42	2.39	10	2
1:A:77:MET:O	1:A:81:PRO:HG2	0.42	2.14	9	1
1:A:33:PRO:C	1:A:35:TYR:N	0.42	2.76	10	1
1:B:177:ILE:C	1:B:180:PRO:HD2	0.42	2.40	10	1
1:C:6:LEU:HD12	1:C:6:LEU:N	0.42	2.29	4	1
1:C:77:MET:HA	1:C:113:ILE:HD13	0.42	1.91	5	1
1:B:41:MET:C	1:B:44:PRO:HD2	0.42	2.40	6	1
1:A:117:LEU:HD12	1:A:118:ILE:HG13	0.42	1.92	7	1
1:C:145:GLY:C	1:C:148:ASN:ND2	0.42	2.71	10	1
1:A:110:ILE:HG22	1:C:46:TRP:NE1	0.42	2.30	2	1
1:C:34:GLN:H	1:C:34:GLN:NE2	0.42	2.13	8	1
1:A:41:MET:O	1:A:44:PRO:HD2	0.42	2.15	1	1
1:A:43:ILE:N	1:A:44:PRO:HD2	0.42	2.29	4	2
1:A:41:MET:C	1:A:44:PRO:HD2	0.42	2.40	6	1
1:C:181:ILE:O	1:C:184:ILE:HG12	0.42	2.15	1	1
1:C:124:ARG:HG2	1:C:126:TRP:H	0.42	1.74	7	2
1:A:26:SER:C	1:A:28:ASN:N	0.42	2.77	9	1
1:C:171:TYR:O	1:C:174:VAL:HG12	0.41	2.14	2	1
1:B:41:MET:O	1:B:44:PRO:HD2	0.41	2.15	8	1
1:A:175:LEU:HD13	1:A:209:SER:OG	0.41	2.15	1	1
1:B:81:PRO:HG3	1:B:113:ILE:HD11	0.41	1.91	10	1
1:A:73:TYR:O	1:A:77:MET:HG3	0.41	2.14	10	3
1:C:167:LYS:HB3	1:C:167:LYS:NZ	0.41	2.29	2	1
1:A:43:ILE:HD11	1:A:82:LEU:HB3	0.41	1.92	5	1
1:C:87:LEU:HB3	1:C:168:LEU:HD21	0.41	1.92	6	1
1:B:108:THR:O	1:B:112:VAL:HG23	0.41	2.16	7	1
1:A:170:THR:O	1:A:174:VAL:HG23	0.41	2.15	2	1
1:A:73:TYR:CD2	1:A:73:TYR:C	0.41	2.98	3	1
1:B:77:MET:O	1:B:81:PRO:HG3	0.41	2.15	5	1
1:A:73:TYR:CD1	1:A:73:TYR:C	0.41	2.97	8	1
1:B:106:MET:O	1:B:110:ILE:HG12	0.41	2.16	5	1
1:B:117:LEU:HD12	1:B:118:ILE:HG13	0.41	1.91	6	1
1:C:33:PRO:HB2	1:C:35:TYR:CD1	0.41	2.50	3	1
1:B:181:ILE:O	1:B:184:ILE:HG22	0.41	2.14	5	1
1:C:69:HIS:HB3	1:C:72:ARG:HB2	0.41	1.93	10	2
1:B:124:ARG:HB2	1:B:127:VAL:HG12	0.41	1.92	2	1
1:A:177:ILE:O	1:A:181:ILE:HG12	0.41	2.16	6	1
1:C:178:GLY:O	1:C:181:ILE:HG22	0.41	2.16	5	1
1:C:171:TYR:O	1:C:175:LEU:HD23	0.41	2.16	6	1
1:A:83:LEU:O	1:A:83:LEU:HD23	0.41	2.16	10	1
1:A:12:VAL:HG11	1:A:52:MET:HB3	0.41	1.92	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:84:LEU:HD21	1:B:105:LEU:HB3	0.41	1.92	1	1
1:A:6:LEU:N	1:A:6:LEU:HD22	0.41	2.31	3	1
1:B:179:TYR:N	1:B:180:PRO:HD2	0.41	2.31	4	1
1:C:81:PRO:HA	1:C:109:GLN:HG2	0.41	1.93	4	1
1:C:91:ALA:HB1	1:C:165:TYR:CE2	0.41	2.51	5	1
1:A:124:ARG:HB3	1:A:127:VAL:HG12	0.41	1.93	8	1
1:B:74:ILE:HG23	1:B:75:ASP:N	0.41	2.30	8	1
1:C:29:PRO:HG2	1:C:34:GLN:HG3	0.41	1.92	8	1
1:C:33:PRO:C	1:C:35:TYR:N	0.41	2.79	10	1
1:C:73:TYR:CD2	1:C:117:LEU:HB3	0.41	2.51	8	1
1:A:124:ARG:HB2	1:A:127:VAL:HG12	0.40	1.92	3	1
1:A:174:VAL:HG13	1:A:175:LEU:HD22	0.40	1.93	3	1
1:B:49:LEU:HD12	1:B:50:ALA:N	0.40	2.30	3	1
1:B:216:LEU:C	1:B:216:LEU:HD13	0.40	2.40	7	1
1:A:83:LEU:HD13	1:A:83:LEU:O	0.40	2.16	8	1
1:C:83:LEU:HD13	1:C:83:LEU:O	0.40	2.16	9	1
1:C:73:TYR:O	1:C:77:MET:HG2	0.40	2.15	9	1
1:A:6:LEU:HD23	1:A:6:LEU:N	0.40	2.32	1	1
1:A:9:TRP:O	1:A:12:VAL:HG12	0.40	2.17	5	1
1:B:141:ILE:HG13	1:B:142:ILE:N	0.40	2.31	5	1
1:B:108:THR:HB	1:B:142:ILE:HD13	0.40	1.93	7	1
1:C:8:HIS:HB3	1:C:51:TYR:O	0.40	2.17	7	1
1:A:15:MET:HA	1:A:15:MET:HE2	0.40	1.92	10	1
1:B:73:TYR:O	1:B:77:MET:HG3	0.40	2.17	8	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	189/235 (80%)	179±3 (95±1%)	9±2 (5±1%)	1±1 (0±0%)	37	78
1	B	190/235 (81%)	178±4 (94±2%)	11±3 (6±2%)	0±0 (0±0%)	49	83
1	C	187/235 (80%)	177±2 (95±1%)	9±2 (5±1%)	1±1 (0±0%)	37	78
All	All	5660/7050 (80%)	5351 (95%)	295 (5%)	14 (0%)	44	80

All 11 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	29	PRO	2
1	B	29	PRO	2
1	C	29	PRO	2
1	A	184	ILE	1
1	A	98	ASP	1
1	C	98	ASP	1
1	C	28	ASN	1
1	A	28	ASN	1
1	A	34	GLN	1
1	C	34	GLN	1
1	C	99	TRP	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	163/203 (80%)	160±1 (98±1%)	3±1 (2±1%)	52	92
1	B	163/203 (80%)	160±2 (98±1%)	3±2 (2±1%)	51	91
1	C	162/203 (80%)	159±1 (98±1%)	3±1 (2±1%)	48	91
All	All	4880/6090 (80%)	4790 (98%)	90 (2%)	51	91

All 52 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	C	83	LEU	8
1	A	83	LEU	4
1	A	205	LEU	4
1	B	83	LEU	4
1	B	140	LEU	4
1	A	34	GLN	3
1	C	17	ILE	3
1	C	205	LEU	3
1	A	46	TRP	3
1	B	46	TRP	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	C	73	TYR	3
1	C	140	LEU	2
1	A	165	TYR	2
1	A	17	ILE	2
1	B	73	TYR	2
1	C	46	TRP	2
1	C	165	TYR	2
1	B	35	TYR	2
1	A	15	MET	1
1	A	78	VAL	1
1	A	140	LEU	1
1	B	17	ILE	1
1	B	143	LEU	1
1	C	131	TRP	1
1	C	167	LYS	1
1	B	34	GLN	1
1	C	34	GLN	1
1	A	76	TRP	1
1	B	167	LYS	1
1	C	15	MET	1
1	C	38	LEU	1
1	B	66	GLN	1
1	B	87	LEU	1
1	B	165	TYR	1
1	A	182	VAL	1
1	B	41	MET	1
1	B	182	VAL	1
1	C	26	SER	1
1	C	54	MET	1
1	C	124	ARG	1
1	A	73	TYR	1
1	A	168	LEU	1
1	B	97	LYS	1
1	B	201	LEU	1
1	C	66	GLN	1
1	A	28	ASN	1
1	A	131	TRP	1
1	B	77	MET	1
1	A	179	TYR	1
1	B	179	TYR	1
1	B	204	LEU	1
1	C	179	TYR	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	LYR	A	210	1	27,29,30	1.34±0.01	3±0 (11±0%)
1	LYR	C	210	1	27,29,30	1.34±0.01	3±0 (12±1%)
1	LYR	B	210	1	27,29,30	1.34±0.01	3±0 (12±1%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	LYR	A	210	1	30,37,39	1.85±0.01	9±0 (30±0%)
1	LYR	C	210	1	30,37,39	1.85±0.02	9±0 (29±1%)
1	LYR	B	210	1	30,37,39	1.84±0.03	9±0 (29±1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LYR	C	210	1	-	0±0,22,40,42	0±0,1,1,1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LYR	A	210	1	-	0±0,22,40,42	0±0,1,1,1
1	LYR	B	210	1	-	0±0,22,40,42	0±0,1,1,1

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	210	LYR	C17-C11	3.91	1.58	1.53	2	10
1	B	210	LYR	C17-C11	3.88	1.58	1.53	3	10
1	C	210	LYR	C17-C11	3.88	1.58	1.53	4	10
1	B	210	LYR	C2-C3	3.30	1.41	1.33	6	10
1	A	210	LYR	C2-C3	3.26	1.41	1.33	4	10
1	C	210	LYR	C2-C3	3.23	1.41	1.33	7	10
1	B	210	LYR	C5-C3	2.33	1.41	1.46	10	10
1	C	210	LYR	C5-C3	2.32	1.41	1.46	8	10
1	A	210	LYR	C5-C3	2.32	1.41	1.46	1	10
1	B	210	LYR	C1-C2	2.02	1.37	1.47	9	3
1	C	210	LYR	C1-C2	2.01	1.37	1.47	3	4

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	210	LYR	C1-NZ-CE	5.00	123.00	112.85	1	10
1	C	210	LYR	C1-NZ-CE	5.00	122.99	112.85	7	10
1	B	210	LYR	C1-NZ-CE	4.98	122.95	112.85	1	10
1	B	210	LYR	C13-C12-C11	4.39	119.69	124.48	10	10
1	A	210	LYR	C13-C12-C11	4.34	119.75	124.48	5	10
1	C	210	LYR	C13-C12-C11	4.33	119.76	124.48	9	10
1	C	210	LYR	C6-C7-C80	3.47	122.41	127.28	10	10
1	A	210	LYR	C6-C7-C80	3.43	122.47	127.28	10	10
1	B	210	LYR	C6-C7-C80	3.39	122.53	127.28	6	10
1	B	210	LYR	C4-C3-C2	2.84	118.82	123.73	6	10
1	A	210	LYR	C4-C3-C2	2.78	118.92	123.73	6	10
1	C	210	LYR	C4-C3-C2	2.74	118.99	123.73	6	10
1	B	210	LYR	C10-C9-C80	2.60	122.38	126.23	6	10
1	C	210	LYR	C10-C9-C80	2.55	122.47	126.23	10	10
1	A	210	LYR	C10-C9-C80	2.53	122.49	126.23	3	10
1	B	210	LYR	C5-C3-C2	2.48	121.95	118.49	6	10
1	A	210	LYR	C5-C3-C2	2.47	121.93	118.49	10	10
1	C	210	LYR	C5-C3-C2	2.40	121.83	118.49	6	8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	210	LYR	C13-C12-C14	2.35	118.61	113.60	9	10
1	B	210	LYR	C13-C12-C14	2.35	118.60	113.60	7	10
1	A	210	LYR	C13-C12-C14	2.33	118.57	113.60	5	10
1	C	210	LYR	C8-C80-C7	2.31	119.07	122.82	5	10
1	A	210	LYR	C8-C80-C7	2.31	119.07	122.82	10	10
1	B	210	LYR	C8-C80-C7	2.30	119.09	122.82	9	9
1	B	210	LYR	C16-C17-C11	2.27	113.74	110.44	2	10
1	A	210	LYR	C16-C17-C11	2.27	113.74	110.44	4	10
1	C	210	LYR	C16-C17-C11	2.24	113.70	110.44	5	10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 12% for the well-defined parts and 11% 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	1142
Number of shifts mapped to atoms	1142
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	204	-1.33 ± 0.21	Should be checked
$^{13}\text{C}_\beta$	175	0.52 ± 0.09	Should be checked
$^{13}\text{C}'$	202	-0.43 ± 0.21	None needed (< 0.5 ppm)
^{15}N	204	1.39 ± 0.35	Should be applied

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 12%, i.e. 978 atoms were assigned a chemical shift out of a possible 8211. 0 out of 119 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	539/2833 (19%)	0/1153 (0%)	363/1132 (32%)	176/548 (32%)
Sidechain	371/4193 (9%)	0/2818 (0%)	366/1300 (28%)	5/75 (7%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Aromatic	68/1185 (6%)	0/576 (0%)	64/549 (12%)	4/60 (7%)
Overall	978/8211 (12%)	0/4547 (0%)	793/2981 (27%)	185/683 (27%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 1077 atoms were assigned a chemical shift out of a possible 9810. 0 out of 132 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	602/3420 (18%)	0/1392 (0%)	406/1368 (30%)	196/660 (30%)
Sidechain	407/5139 (8%)	0/3420 (0%)	402/1578 (25%)	5/141 (4%)
Aromatic	68/1251 (5%)	0/609 (0%)	64/579 (11%)	4/63 (6%)
Overall	1077/9810 (11%)	0/5421 (0%)	872/3525 (25%)	205/864 (24%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts ⓘ

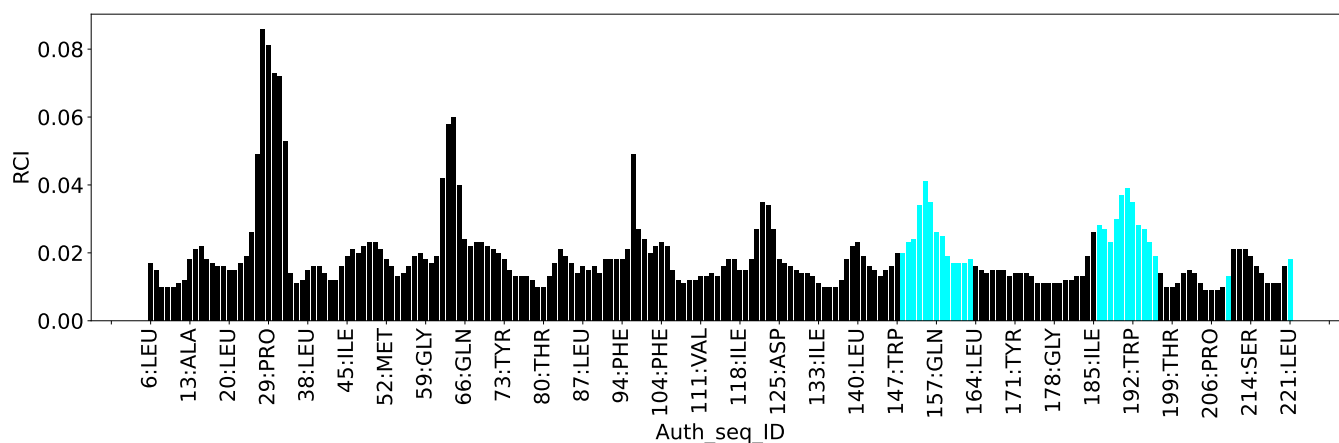
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	109	GLN	NE2	98.30	103.38 – 120.35	-8.0
1	B	128	ARG	CD	37.40	38.57 – 47.75	-6.3

7.1.5 Random Coil Index (RCI) plots ⓘ

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 B:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1_dup*

7.2.1 Bookkeeping [i](#)

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

Total number of shifts	43
Number of shifts mapped to atoms	43
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.2.2 Chemical shift referencing [i](#)

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

7.2.3 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 0%, i.e. 34 atoms were assigned a chemical shift out of a possible 8211. 0 out of 119 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	18/2833 (1%)	0/1153 (0%)	12/1132 (1%)	6/548 (1%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Sidechain	12/4193 (0%)	0/2818 (0%)	12/1300 (1%)	0/75 (0%)
Aromatic	4/1185 (0%)	0/576 (0%)	4/549 (1%)	0/60 (0%)
Overall	34/8211 (0%)	0/4547 (0%)	28/2981 (1%)	6/683 (1%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 41 atoms were assigned a chemical shift out of a possible 9810. 0 out of 132 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	24/3420 (1%)	0/1392 (0%)	16/1368 (1%)	8/660 (1%)
Sidechain	13/5139 (0%)	0/3420 (0%)	13/1578 (1%)	0/141 (0%)
Aromatic	4/1251 (0%)	0/609 (0%)	4/579 (1%)	0/63 (0%)
Overall	41/9810 (0%)	0/5421 (0%)	33/3525 (1%)	8/864 (1%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 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 B:

