



Full wwPDB NMR Structure Validation Report ⓘ

Nov 13, 2021 – 05:05 am GMT

PDB ID : 7NM5
Title : Solution structure of MLKL executioner domain in complex with a fragment
Authors : Ruebbelke, M.; Bauer, M.; Hamilton, J.; Binder, F.; Nar, H.; Zeeb, M.
Deposited on : 2021-02-23

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

MolProbity : 4.02b-467
Mogul : 1.8.4 (270009), CSD as541be (2020)
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.23.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

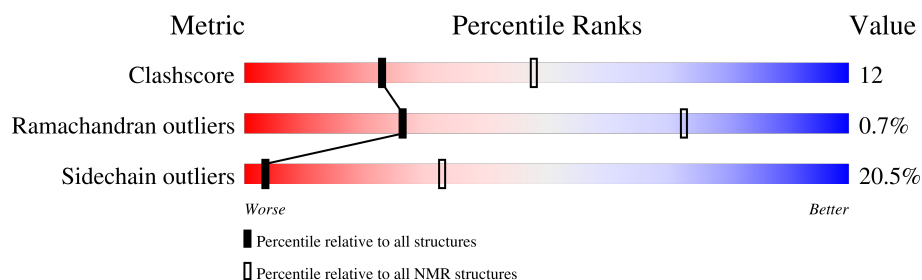
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 77%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	157	<div> <div></div> <div>62%</div> <div>23%</div> <div>•</div> <div>11%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 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:2-A:47, A:56-A:149 (140)	0.37	11

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. No single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2609 atoms, of which 1313 are hydrogens and 0 are deuteriums.

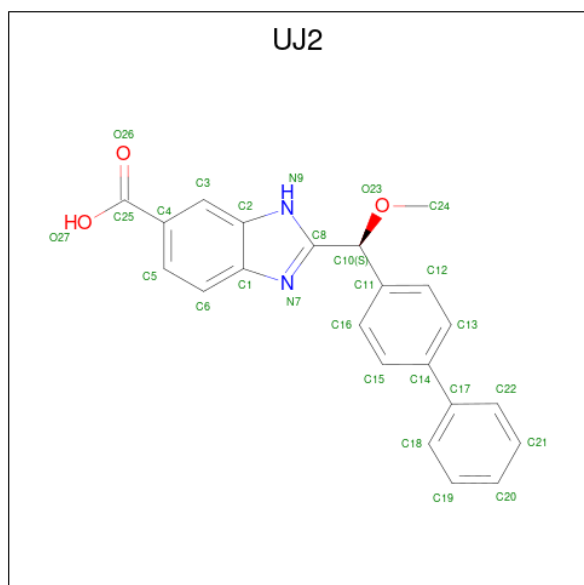
- Molecule 1 is a protein called Mixed lineage kinase domain-like protein.

Mol	Chain	Residues	Atoms						Trace
1	A	157	Total	C	H	N	O	S	0
			2564	786	1295	239	235	9	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q8NB16
A	-1	SER	-	expression tag	UNP Q8NB16
A	0	PRO	-	expression tag	UNP Q8NB16
A	1	GLY	-	expression tag	UNP Q8NB16

- Molecule 2 is 2-[(S)-methoxy-(4-phenylphenyl)methyl]-3H-benzimidazole-5-carboxylic acid (three-letter code: UJ2) (formula: C₂₂H₁₈N₂O₃) (labeled as "Ligand of Interest" by depositor).



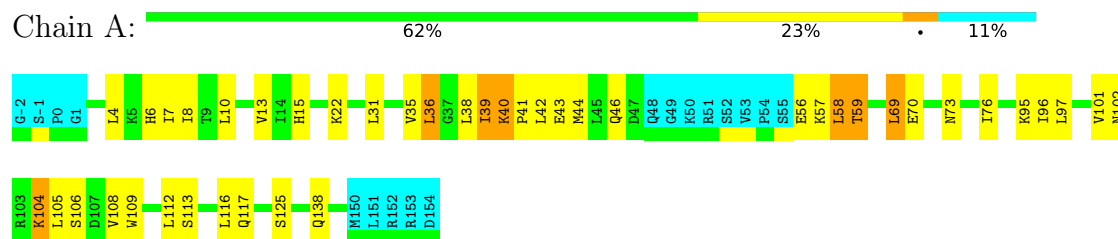
Mol	Chain	Residues	Atoms					
2	A	1	Total	C	H	N	O	
			45	22	18	2	3	

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: Mixed lineage kinase domain-like protein

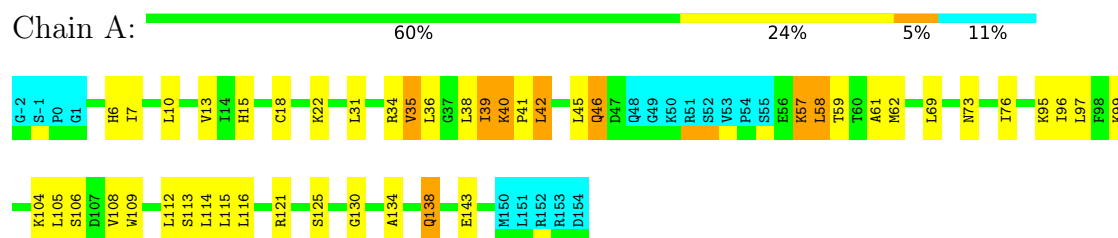


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

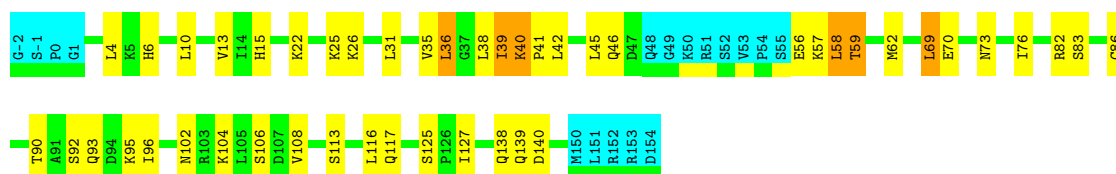
- Molecule 1: Mixed lineage kinase domain-like protein



4.2.2 Score per residue for model 2

- Molecule 1: Mixed lineage kinase domain-like protein

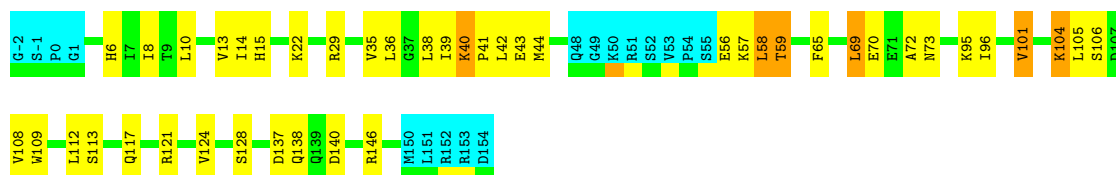




4.2.3 Score per residue for model 3

- Molecule 1: Mixed lineage kinase domain-like protein

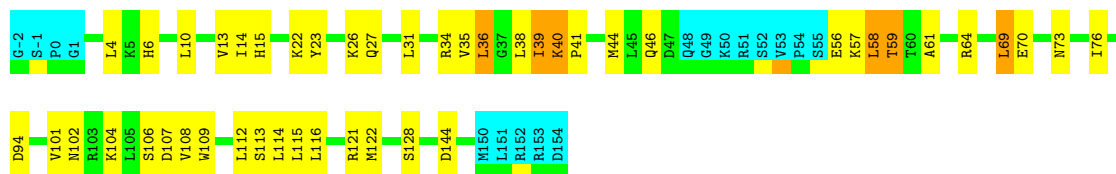
Chain A: 61% 24% 11%



4.2.4 Score per residue for model 4

- Molecule 1: Mixed lineage kinase domain-like protein

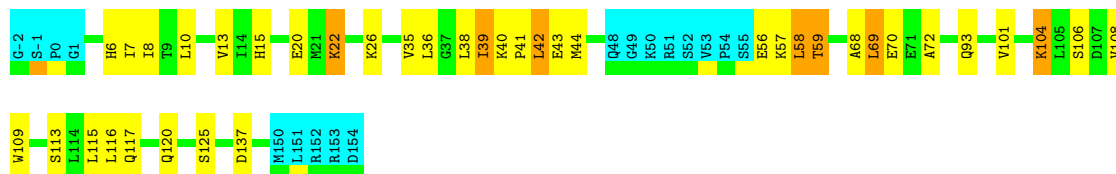
Chain A: 59% 26% 11%



4.2.5 Score per residue for model 5

- Molecule 1: Mixed lineage kinase domain-like protein

Chain A: 64% 20% 11%

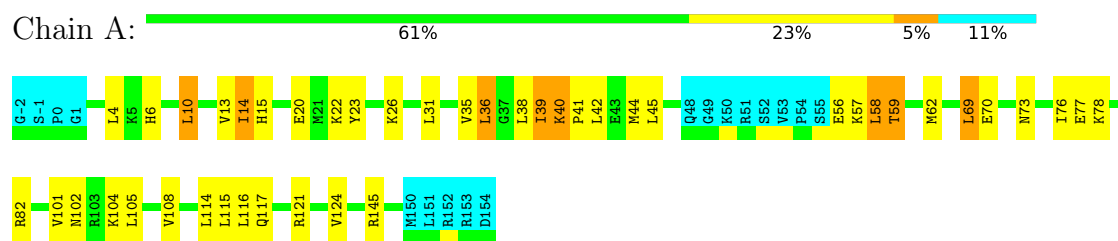


4.2.6 Score per residue for model 6

- Molecule 1: Mixed lineage kinase domain-like protein

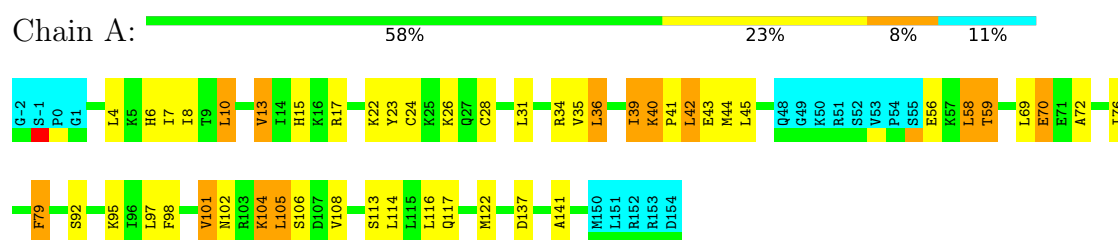
4.2.10 Score per residue for model 10

- Molecule 1: Mixed lineage kinase domain-like protein



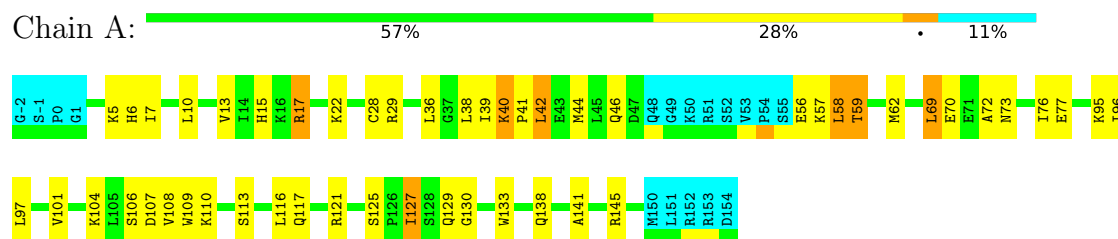
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Mixed lineage kinase domain-like protein



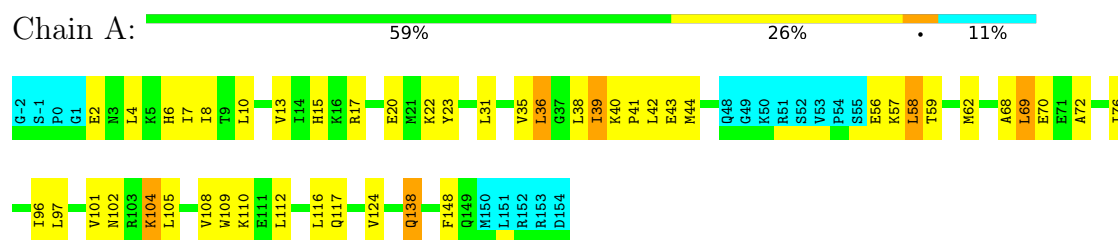
4.2.12 Score per residue for model 12

- Molecule 1: Mixed lineage kinase domain-like protein



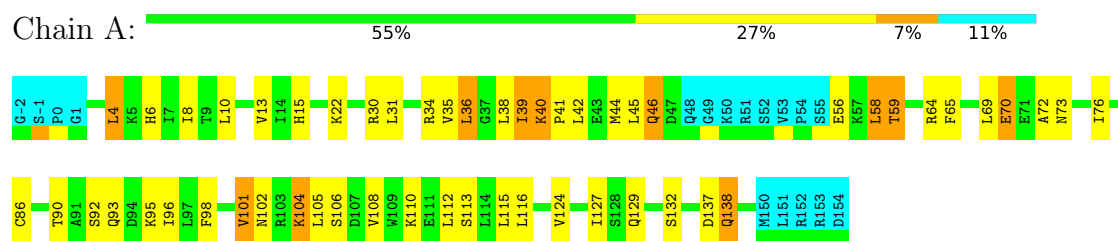
4.2.13 Score per residue for model 13

- Molecule 1: Mixed lineage kinase domain-like protein



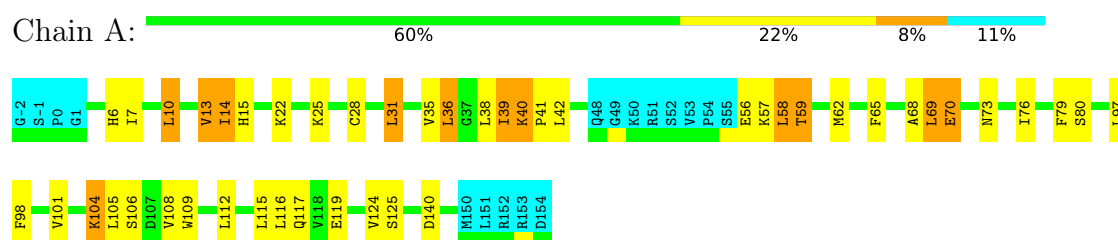
4.2.14 Score per residue for model 14

- Molecule 1: Mixed lineage kinase domain-like protein



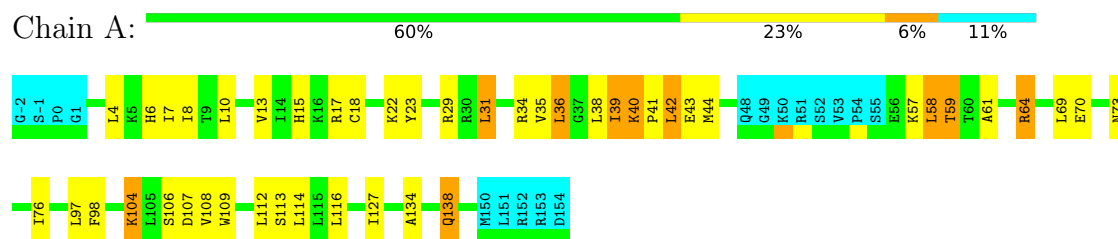
4.2.15 Score per residue for model 15

- Molecule 1: Mixed lineage kinase domain-like protein



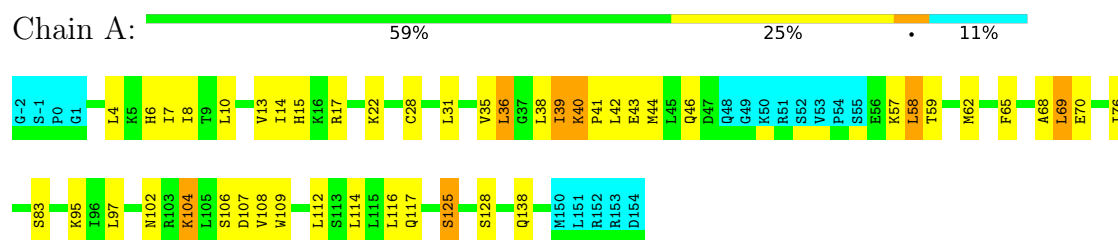
4.2.16 Score per residue for model 16

- Molecule 1: Mixed lineage kinase domain-like protein



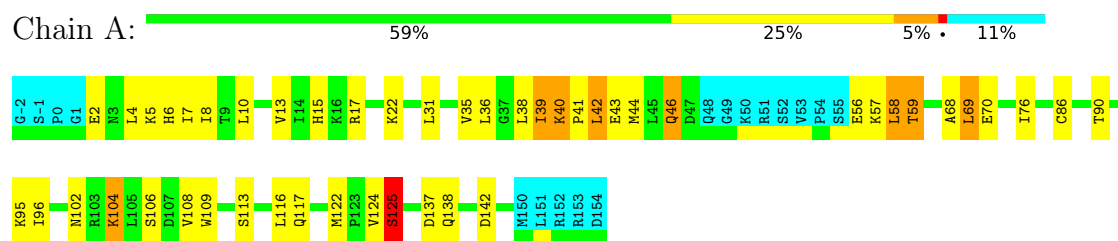
4.2.17 Score per residue for model 17

- Molecule 1: Mixed lineage kinase domain-like protein



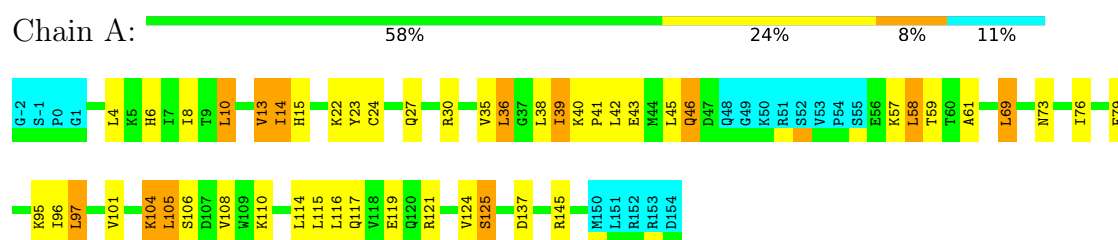
4.2.18 Score per residue for model 18

- Molecule 1: Mixed lineage kinase domain-like protein



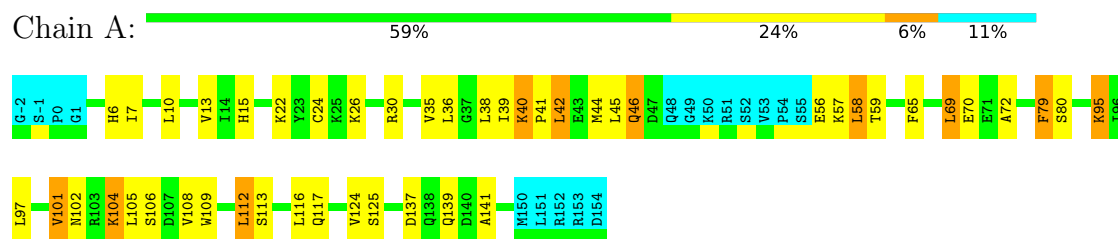
4.2.19 Score per residue for model 19

- Molecule 1: Mixed lineage kinase domain-like protein



4.2.20 Score per residue for model 20

- Molecule 1: Mixed lineage kinase domain-like protein



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	3.98.9

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	1738
Number of shifts mapped to atoms	1738
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UJ2

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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	1143	1164	1164	29±4
2	A	27	18	0	3±1
All	All	23400	23640	23280	583

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:ALA:HB2	1:A:115:LEU:HD21	0.91	1.41	4	1
1:A:58:LEU:HD13	1:A:59:THR:N	0.90	1.81	14	15
1:A:58:LEU:HD22	1:A:58:LEU:C	0.85	1.92	8	15
1:A:58:LEU:HD22	1:A:58:LEU:O	0.83	1.74	16	15
1:A:7:ILE:HG21	1:A:42:LEU:HD22	0.83	1.49	1	7
1:A:58:LEU:HD23	1:A:116:LEU:HD23	0.78	1.53	2	5
1:A:14:ILE:HD13	1:A:69:LEU:HD12	0.78	1.56	15	2
1:A:134:ALA:HB1	1:A:138:GLN:OE1	0.72	1.85	16	2
1:A:58:LEU:HD21	1:A:116:LEU:HD23	0.70	1.64	16	1
1:A:79:PHE:CE1	1:A:97:LEU:HD22	0.68	2.24	11	3
1:A:38:LEU:O	1:A:42:LEU:HD23	0.67	1.90	19	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:LEU:HD13	1:A:69:LEU:HD11	0.66	1.67	11	1
1:A:104:LYS:O	1:A:108:VAL:HG22	0.66	1.91	20	20
1:A:58:LEU:CD1	1:A:116:LEU:HD23	0.65	2.21	19	1
1:A:58:LEU:HA	1:A:115:LEU:HD13	0.65	1.69	4	1
1:A:36:LEU:HD13	1:A:39:ILE:CG2	0.64	2.22	14	16
1:A:95:LYS:O	1:A:96:ILE:HD13	0.64	1.93	14	3
1:A:10:LEU:HD23	1:A:69:LEU:HD11	0.63	1.71	7	11
1:A:58:LEU:HD12	1:A:116:LEU:HD12	0.63	1.69	6	4
1:A:116:LEU:HD23	1:A:122:MET:CE	0.63	2.24	4	2
1:A:8:ILE:HD12	1:A:43:GLU:CG	0.63	2.24	18	6
1:A:58:LEU:HD13	1:A:59:THR:H	0.63	1.53	8	13
1:A:6:HIS:NE2	1:A:10:LEU:HD22	0.62	2.10	13	15
1:A:58:LEU:HD12	1:A:116:LEU:CD1	0.62	2.24	6	3
1:A:69:LEU:CA	1:A:105:LEU:HD21	0.62	2.25	19	1
1:A:58:LEU:C	1:A:58:LEU:CD2	0.62	2.67	20	15
1:A:116:LEU:HD22	2:A:201:UJ2:C21	0.62	2.25	8	3
1:A:58:LEU:HD12	1:A:116:LEU:HD23	0.61	1.70	19	1
1:A:69:LEU:CB	1:A:105:LEU:HD21	0.61	2.25	19	3
1:A:61:ALA:CB	1:A:115:LEU:HD21	0.61	2.23	4	1
1:A:6:HIS:NE2	1:A:10:LEU:HD12	0.61	2.11	15	4
1:A:58:LEU:HD11	2:A:201:UJ2:C21	0.60	2.26	1	4
1:A:73:ASN:HA	1:A:76:ILE:HD12	0.60	1.73	10	11
1:A:10:LEU:O	1:A:13:VAL:HG12	0.60	1.96	16	12
1:A:38:LEU:HD22	1:A:109:TRP:CD1	0.60	2.31	17	3
1:A:116:LEU:HD22	2:A:201:UJ2:C20	0.60	2.25	20	7
1:A:7:ILE:CG2	1:A:42:LEU:HD22	0.60	2.26	8	6
1:A:8:ILE:HD12	1:A:43:GLU:HG2	0.59	1.74	7	3
1:A:10:LEU:HD21	1:A:70:GLU:CG	0.59	2.26	14	2
1:A:42:LEU:HD13	1:A:45:LEU:HD21	0.59	1.74	14	4
1:A:61:ALA:O	1:A:112:LEU:HD12	0.58	1.98	6	4
1:A:8:ILE:HD12	1:A:43:GLU:HG3	0.58	1.75	17	5
1:A:8:ILE:HG21	1:A:46:GLN:OE1	0.58	1.99	14	1
1:A:10:LEU:HD22	1:A:69:LEU:HD13	0.57	1.76	11	1
1:A:72:ALA:N	1:A:101:VAL:HG21	0.57	2.13	3	9
1:A:7:ILE:HD11	1:A:62:MET:HG2	0.57	1.76	17	5
1:A:99:LYS:HE2	1:A:134:ALA:HB2	0.57	1.73	1	1
1:A:116:LEU:HD23	1:A:122:MET:HE2	0.57	1.76	4	2
1:A:69:LEU:HB3	1:A:105:LEU:HD21	0.56	1.75	10	8
1:A:58:LEU:HD11	2:A:201:UJ2:C22	0.56	2.30	13	4
1:A:14:ILE:CD1	1:A:69:LEU:HD12	0.56	2.29	15	1
1:A:58:LEU:HD22	1:A:119:GLU:CD	0.56	2.20	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:ILE:HD11	1:A:138:GLN:HG2	0.55	1.77	13	7
1:A:58:LEU:HD11	2:A:201:UJ2:C18	0.55	2.31	19	1
1:A:31:LEU:HD13	1:A:102:ASN:OD1	0.55	2.02	10	5
1:A:61:ALA:C	1:A:112:LEU:HD12	0.55	2.22	16	4
1:A:59:THR:HG22	2:A:201:UJ2:C16	0.55	2.32	12	16
1:A:65:PHE:CE1	1:A:69:LEU:HD23	0.55	2.36	7	1
1:A:56:GLU:HA	1:A:59:THR:OG1	0.55	2.02	11	13
1:A:116:LEU:HD22	2:A:201:UJ2:C19	0.54	2.32	5	3
1:A:45:LEU:HD22	1:A:120:GLN:NE2	0.54	2.17	7	1
1:A:58:LEU:HD11	2:A:201:UJ2:C19	0.54	2.33	19	1
1:A:72:ALA:CA	1:A:101:VAL:HG21	0.53	2.33	9	7
1:A:101:VAL:HG23	1:A:104:LYS:HE2	0.53	1.78	4	2
1:A:65:PHE:O	1:A:69:LEU:HD23	0.53	2.03	6	1
1:A:10:LEU:HD13	1:A:69:LEU:CD1	0.53	2.33	11	1
1:A:62:MET:SD	1:A:116:LEU:HD11	0.53	2.44	1	1
1:A:115:LEU:HD12	1:A:116:LEU:N	0.53	2.18	4	1
1:A:68:ALA:CB	1:A:108:VAL:HG21	0.53	2.34	18	5
1:A:10:LEU:O	1:A:14:ILE:HD12	0.53	2.04	19	2
1:A:61:ALA:HB1	1:A:112:LEU:HB2	0.52	1.81	4	1
1:A:58:LEU:HD13	1:A:58:LEU:C	0.52	2.25	16	3
1:A:59:THR:HG22	2:A:201:UJ2:C15	0.52	2.33	12	10
1:A:45:LEU:HD12	1:A:46:GLN:N	0.52	2.19	19	7
1:A:8:ILE:HG23	1:A:43:GLU:HG2	0.52	1.82	11	3
1:A:114:LEU:HD23	1:A:117:GLN:OE1	0.52	2.05	8	1
1:A:14:ILE:HD11	1:A:69:LEU:O	0.52	2.05	19	1
1:A:4:LEU:HD11	1:A:45:LEU:CD1	0.51	2.34	11	1
1:A:69:LEU:HA	1:A:105:LEU:HD21	0.51	1.81	15	2
2:A:201:UJ2:C24	2:A:201:UJ2:C16	0.51	2.89	7	1
1:A:101:VAL:HG22	1:A:105:LEU:HD23	0.51	1.82	15	1
1:A:40:LYS:N	1:A:41:PRO:HD2	0.51	2.21	17	20
1:A:8:ILE:HG23	1:A:43:GLU:CG	0.51	2.35	17	6
1:A:58:LEU:HA	1:A:115:LEU:HD12	0.51	1.82	10	4
1:A:38:LEU:HD22	1:A:109:TRP:CD2	0.51	2.41	1	6
1:A:61:ALA:HB2	1:A:115:LEU:HD12	0.51	1.83	19	1
1:A:116:LEU:HD23	1:A:122:MET:SD	0.50	2.46	9	2
1:A:95:LYS:C	1:A:96:ILE:HD13	0.50	2.27	14	3
1:A:31:LEU:HD22	1:A:98:PHE:HB2	0.50	1.84	11	1
1:A:10:LEU:HG	1:A:69:LEU:HD12	0.50	1.83	12	2
1:A:7:ILE:HD11	1:A:62:MET:CG	0.49	2.37	8	5
1:A:10:LEU:HD21	1:A:70:GLU:HG3	0.49	1.83	7	2
1:A:4:LEU:HD22	1:A:46:GLN:HB2	0.49	1.84	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:LYS:O	1:A:141:ALA:HB1	0.49	2.06	12	3
1:A:13:VAL:HG22	1:A:17:ARG:NH1	0.49	2.23	16	1
1:A:109:TRP:CE3	1:A:112:LEU:HD22	0.49	2.42	7	1
1:A:38:LEU:HD23	1:A:125:SER:OG	0.49	2.06	19	1
1:A:4:LEU:O	1:A:4:LEU:HD23	0.49	2.07	4	1
1:A:4:LEU:HD12	1:A:4:LEU:O	0.49	2.07	16	1
1:A:79:PHE:CD1	1:A:97:LEU:HD23	0.48	2.43	19	1
2:A:201:UJ2:C16	2:A:201:UJ2:N7	0.48	2.75	19	1
1:A:17:ARG:HB3	1:A:76:ILE:HG21	0.48	1.86	13	4
1:A:96:ILE:HD11	1:A:138:GLN:OE1	0.48	2.09	3	1
1:A:58:LEU:CA	1:A:115:LEU:HD13	0.47	2.37	4	1
1:A:6:HIS:CD2	1:A:10:LEU:HD12	0.47	2.44	19	1
1:A:58:LEU:HD23	1:A:116:LEU:HD12	0.47	1.85	11	3
1:A:10:LEU:HD23	1:A:69:LEU:CD1	0.47	2.39	13	5
1:A:127:ILE:HD12	1:A:133:TRP:NE1	0.47	2.25	12	1
1:A:31:LEU:HD12	1:A:98:PHE:CG	0.47	2.45	16	2
1:A:65:PHE:HB2	1:A:112:LEU:HD12	0.47	1.87	20	1
2:A:201:UJ2:C16	2:A:201:UJ2:C24	0.46	2.93	19	1
1:A:69:LEU:HD12	1:A:70:GLU:N	0.46	2.25	11	1
1:A:109:TRP:CE3	1:A:112:LEU:HD23	0.46	2.46	13	3
1:A:7:ILE:HG21	1:A:42:LEU:CD2	0.46	2.40	20	2
1:A:115:LEU:HD12	1:A:115:LEU:C	0.46	2.31	4	1
1:A:58:LEU:CA	1:A:115:LEU:HD12	0.46	2.40	10	2
1:A:58:LEU:HD21	1:A:116:LEU:CD2	0.45	2.38	16	1
1:A:7:ILE:HG21	1:A:42:LEU:CD1	0.45	2.42	17	1
1:A:31:LEU:HD22	1:A:98:PHE:CB	0.45	2.40	11	1
1:A:58:LEU:CD1	1:A:59:THR:HG23	0.45	2.41	20	1
1:A:96:ILE:HG22	1:A:97:LEU:H	0.45	1.72	6	1
1:A:89:LEU:HD12	1:A:148:PHE:CD1	0.45	2.46	8	1
1:A:36:LEU:HD13	1:A:39:ILE:HG23	0.45	1.89	19	3
1:A:56:GLU:O	1:A:59:THR:OG1	0.45	2.29	20	1
1:A:124:VAL:CG2	1:A:125:SER:N	0.45	2.79	18	1
1:A:68:ALA:HB1	1:A:105:LEU:HA	0.45	1.88	13	1
1:A:101:VAL:O	1:A:105:LEU:HD12	0.44	2.13	11	2
1:A:4:LEU:HD12	1:A:46:GLN:HB2	0.44	1.89	14	1
1:A:38:LEU:HD22	1:A:109:TRP:CG	0.44	2.47	7	3
1:A:31:LEU:HD22	1:A:98:PHE:CD2	0.44	2.48	14	1
1:A:96:ILE:HG23	1:A:137:ASP:OD1	0.44	2.11	19	2
1:A:68:ALA:HB2	1:A:108:VAL:HG21	0.44	1.88	13	3
1:A:58:LEU:CD2	1:A:116:LEU:HD23	0.44	2.41	16	1
1:A:79:PHE:CD1	1:A:97:LEU:HD21	0.44	2.47	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LEU:HD13	1:A:102:ASN:ND2	0.44	2.28	9	1
1:A:38:LEU:HD23	1:A:125:SER:HB3	0.44	1.88	7	1
1:A:62:MET:HE3	1:A:116:LEU:HD21	0.44	1.89	12	1
1:A:38:LEU:O	1:A:42:LEU:HD13	0.44	2.12	18	1
1:A:58:LEU:HG	1:A:59:THR:N	0.43	2.26	19	2
1:A:62:MET:CE	1:A:116:LEU:HD21	0.43	2.44	12	3
1:A:65:PHE:CB	1:A:112:LEU:HD22	0.43	2.43	17	2
1:A:14:ILE:HD11	1:A:73:ASN:OD1	0.43	2.13	3	1
1:A:57:LYS:O	1:A:115:LEU:HD12	0.43	2.14	7	1
1:A:62:MET:SD	1:A:112:LEU:HD11	0.43	2.54	8	2
1:A:79:PHE:HE1	1:A:97:LEU:HD22	0.43	1.70	15	1
1:A:101:VAL:O	1:A:105:LEU:HD23	0.43	2.13	15	1
1:A:10:LEU:HD21	1:A:70:GLU:HG2	0.43	1.89	14	1
1:A:65:PHE:CB	1:A:112:LEU:HD12	0.43	2.43	20	1
1:A:36:LEU:HD13	1:A:39:ILE:HG21	0.42	1.89	18	5
1:A:38:LEU:HD22	1:A:109:TRP:CE2	0.42	2.49	3	1
1:A:40:LYS:CB	1:A:41:PRO:CD	0.42	2.96	7	16
1:A:65:PHE:HB2	1:A:112:LEU:HD22	0.42	1.89	14	2
1:A:35:VAL:CG2	1:A:105:LEU:HD13	0.42	2.44	1	1
1:A:58:LEU:CD2	1:A:116:LEU:HD12	0.42	2.45	7	1
1:A:124:VAL:O	1:A:125:SER:CB	0.42	2.66	18	1
1:A:112:LEU:HD12	1:A:116:LEU:HD13	0.42	1.91	13	2
1:A:57:LYS:HE2	1:A:115:LEU:HD13	0.41	1.93	1	1
1:A:58:LEU:HD23	1:A:116:LEU:CD2	0.41	2.35	2	1
1:A:31:LEU:C	1:A:31:LEU:HD13	0.41	2.36	7	1
1:A:14:ILE:HG12	1:A:72:ALA:HB3	0.41	1.92	3	1
1:A:10:LEU:HD22	1:A:69:LEU:CD1	0.41	2.44	11	1
1:A:86:CYS:O	1:A:90:THR:HG23	0.41	2.16	2	3
1:A:17:ARG:HB2	1:A:76:ILE:HG21	0.41	1.92	12	1
1:A:65:PHE:CG	1:A:112:LEU:HD22	0.41	2.51	15	1
1:A:40:LYS:N	1:A:41:PRO:CD	0.41	2.84	17	1
1:A:65:PHE:CG	1:A:112:LEU:HD12	0.41	2.51	20	1
1:A:10:LEU:HD11	1:A:70:GLU:HG3	0.40	1.93	15	1
1:A:65:PHE:HB2	1:A:112:LEU:HD13	0.40	1.92	7	1
1:A:64:ARG:NH2	1:A:108:VAL:HG12	0.40	2.31	16	1
1:A:65:PHE:CZ	1:A:69:LEU:HD22	0.40	2.51	6	1
1:A:114:LEU:O	1:A:118:VAL:HG12	0.40	2.16	7	1
1:A:115:LEU:HD23	1:A:115:LEU:N	0.40	2.31	7	1
1:A:116:LEU:HD23	2:A:201:UJ2:C21	0.40	2.47	7	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	140/157 (89%)	130±2 (93±2%)	9±2 (7±2%)	1±1 (1±1%)	26	73
All	All	2800/3140 (89%)	2593 (93%)	187 (7%)	20 (1%)	26	73

All 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	121	ARG	4
1	A	127	ILE	4
1	A	130	GLY	2
1	A	92	SER	2
1	A	93	GLN	2
1	A	129	GLN	2
1	A	125	SER	2
1	A	94	ASP	1
1	A	22	LYS	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	126/140 (90%)	100±3 (79±3%)	26±3 (21±3%)	3	33
All	All	2520/2800 (90%)	2003 (79%)	517 (21%)	3	33

All 75 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	15	HIS	20

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Mol	Chain	Res	Type	Models (Total)
1	A	22	LYS	20
1	A	39	ILE	20
1	A	58	LEU	20
1	A	35	VAL	19
1	A	57	LYS	18
1	A	106	SER	18
1	A	70	GLU	18
1	A	40	LYS	17
1	A	36	LEU	17
1	A	69	LEU	16
1	A	44	MET	15
1	A	104	LYS	15
1	A	113	SER	14
1	A	59	THR	14
1	A	117	GLN	12
1	A	13	VAL	11
1	A	125	SER	11
1	A	46	GLN	10
1	A	95	LYS	9
1	A	97	LEU	9
1	A	138	GLN	9
1	A	42	LEU	8
1	A	114	LEU	8
1	A	101	VAL	8
1	A	4	LEU	7
1	A	26	LYS	7
1	A	124	VAL	7
1	A	137	ASP	7
1	A	102	ASN	7
1	A	34	ARG	6
1	A	14	ILE	6
1	A	23	TYR	6
1	A	107	ASP	6
1	A	28	CYS	6
1	A	10	LEU	5
1	A	31	LEU	4
1	A	82	ARG	4
1	A	83	SER	4
1	A	64	ARG	4
1	A	30	ARG	4
1	A	24	CYS	4
1	A	110	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	25	LYS	3
1	A	139	GLN	3
1	A	140	ASP	3
1	A	29	ARG	3
1	A	121	ARG	3
1	A	128	SER	3
1	A	20	GLU	3
1	A	79	PHE	3
1	A	5	LYS	3
1	A	105	LEU	3
1	A	145	ARG	3
1	A	18	CYS	2
1	A	146	ARG	2
1	A	27	GLN	2
1	A	93	GLN	2
1	A	78	LYS	2
1	A	132	SER	2
1	A	77	GLU	2
1	A	2	GLU	2
1	A	80	SER	2
1	A	143	GLU	1
1	A	144	ASP	1
1	A	120	GLN	1
1	A	3	ASN	1
1	A	43	GLU	1
1	A	87	ARG	1
1	A	115	LEU	1
1	A	92	SER	1
1	A	17	ARG	1
1	A	119	GLU	1
1	A	142	ASP	1
1	A	112	LEU	1

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 [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 77% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *molecule_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	1738
Number of shifts mapped to atoms	1738
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

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	153	-0.50 ± 0.10	Should be applied
$^{13}\text{C}_\beta$	144	0.30 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	141	-0.09 ± 0.17	None needed (< 0.5 ppm)

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 77%, i.e. 1414 atoms were assigned a chemical shift out of a possible 1848. 22 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	530/694 (76%)	265/277 (96%)	136/280 (49%)	129/137 (94%)
Sidechain	818/1056 (77%)	507/622 (82%)	296/371 (80%)	15/63 (24%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	66/98 (67%)	33/53 (62%)	31/40 (78%)	2/5 (40%)
Overall	1414/1848 (77%)	805/952 (85%)	463/691 (67%)	146/205 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 1558 atoms were assigned a chemical shift out of a possible 2060. 24 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	588/775 (76%)	294/309 (95%)	153/314 (49%)	141/152 (93%)
Sidechain	904/1187 (76%)	562/702 (80%)	326/411 (79%)	16/74 (22%)
Aromatic	66/98 (67%)	33/53 (62%)	31/40 (78%)	2/5 (40%)
Overall	1558/2060 (76%)	889/1064 (84%)	510/765 (67%)	159/231 (69%)

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.

Random coil index (RCI) for chain A:

