Full wwPDB NMR Structure Validation Report (i)

Apr 20, 2024 – 11:23 AM EDT

PDB ID	:	2MS0
BMRB ID	:	25100
Title	:	Solution NMR structure pf tRNApro:MLV-Nucleocapsid (1:2) Complex
Authors	:	D'Souza, V.; Yildiz, Z.
Deposited on	:	2014-07-19

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 (i) symbol.

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

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

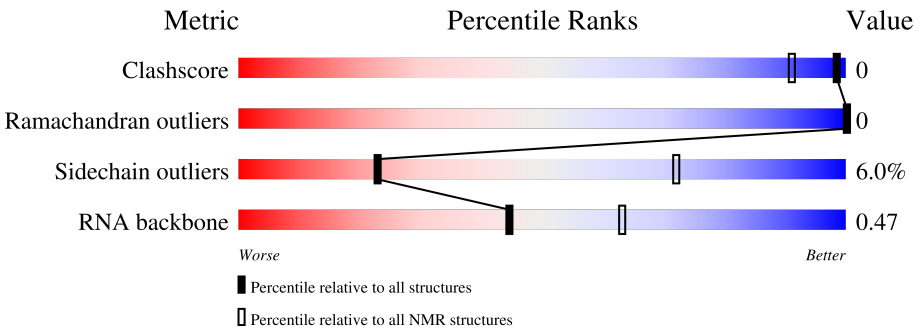
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 14%.

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
RNA backbone	4643	676

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

Mol	Chain	Length	Quality of chain
1	A	56	25% · 71% ·
1	C	56	29% 71%
2	B	71	21% 51% 24% ·

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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:25-A:39 (15)	0.18	5
2	C:125-C:140 (16)	0.25	6

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, 3, 4, 5, 6, 7, 8
2	9, 10
Single-model clusters	2

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4046 atoms, of which 1647 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Nucleocapsid protein p10.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	55	871	260	435	94	79	3	0
1	C	56	890	266	446	95	80	3	0

- Molecule 2 is a RNA chain called tRNApro.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	71	2283	676	766	270	501	70	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
3	A	1	1	1
3	C	1	1	1

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: Nucleocapsid protein p10

Chain A: 25% 71%

A1 T2 V3 V4 S5 G6 Q7 K8 Q9 D10 R11 Q12 G13 G14 E15 R16 R17 R18 S19 Q20 L21 D22 R23 D24 C29 P40 K41 K42 P43 R44 G45 P46 R47 G48 P49 R50 P51 Q52 T53 S54 L55 LEU

• Molecule 1: Nucleocapsid protein p10

Chain C: 29% 71%

A101 T102 V103 V104 S105 G106 Q107 K108 Q109 D110 R111 Q112 G113 G114 E115 R116 R117 R118 S119 Q120 L121 D122 R123 D124 K141 K142 P143 R144 G145 P146 R147 G148 P149 R150 P151 Q152 T153 S154 L155 L156

• Molecule 2: tRNApro

Chain B: 21% 51% 24%

G1 G2 C3 U4 C5 G6 U7 U8 G9 G10 U11 C12 U13 A14 G15 G16 G18 G19 U20 A21 U22 G23 A24 U25 U26 C27 U28 C29 G30 C31 U32 U33 A34 G35 G36 G37 U38 G39 C40 G41 A42 G43 A44 G45 G46 U47 C48 C49 C50 U54 U55 C56 A57 A58 A59 U60 C61 C62 C63

A66 C67 G68 A69 G70 C71 C72

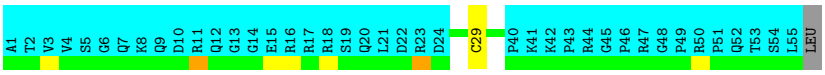
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

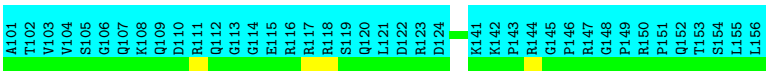
• Molecule 1: Nucleocapsid protein p10

Chain A: 25% 71%



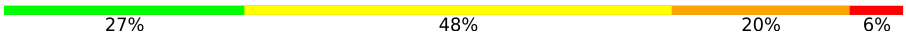
• Molecule 1: Nucleocapsid protein p10

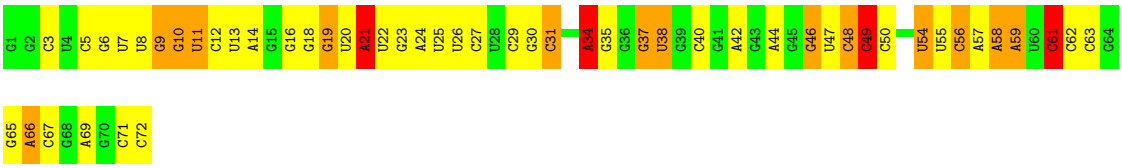
Chain C:



• Molecule 2: tRNApro

Chain B:

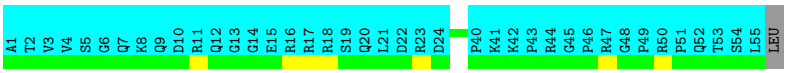




4.2.2 Score per residue for model 2

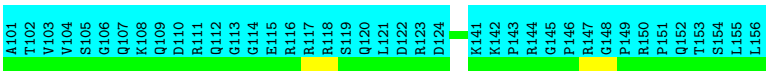
• Molecule 1: Nucleocapsid protein p10

Chain A:



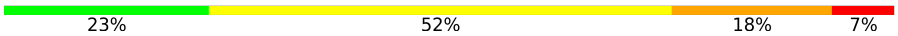
• Molecule 1: Nucleocapsid protein p10

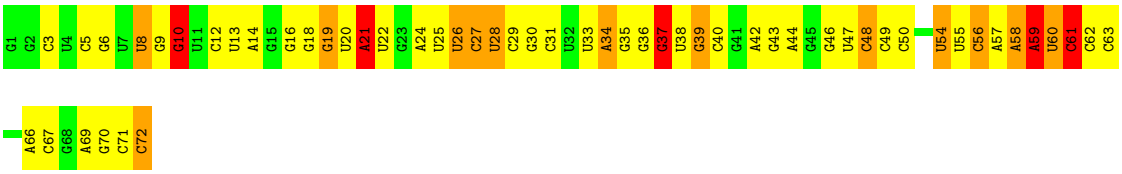
Chain C:



• Molecule 2: tRNApro

Chain B:





4.2.3 Score per residue for model 3

• Molecule 1: Nucleocapsid protein p10

Chain A: 25% • 71% •

A1 T2 V3 V4 S5 G6 Q7 K8 Q9 D10 R11 Q12 G13 G14 E15 R16 R17 R18 S19 Q20 L21 D22 R23 D24 C29 P40 K41 K42 P43 R44 G45 P46 R47 G48 P49 R50 P51 Q52 T53 S54 L55 LEU

• Molecule 1: Nucleocapsid protein p10

Chain C: 27% • 71%

A101 T102 V103 V104 S105 G106 Q107 K108 Q109 D110 R111 Q112 G113 G114 E115 R116 R117 R118 S119 Q120 L121 D122 R123 D124 Y128 K141 K142 P143 R144 G145 P146 R147 G148 P149 R150 P151 Q152 T153 S154 L155 L156

• Molecule 2: tRNApro

Chain B: 21% 38% 32% 8%

G1 G2 C3 U4 C5 G6 U7 U8 G9 G10 U11 C12 U13 A14 G15 G16 G18 G19 U20 A21 U22 G23 A24 U25 U26 C27 U28 C29 G30 C31 U32 U33 A34 G35 G36 G37 U38 G39 C40 G41 A42 G43 A44 G45 G46 U47 C48 C49 C50 U54 U55 C56 A57 A58 A59 U60 C61 C62 C63

A66 C67 G68 A69 G70 C71 C72

4.2.4 Score per residue for model 4

• Molecule 1: Nucleocapsid protein p10

Chain A: 23% • 71% •

A1 T2 V3 V4 S5 G6 Q7 K8 Q9 D10 R11 Q12 G13 G14 E15 R16 R17 R18 S19 Q20 L21 D22 R23 D24 C29 K32 P40 K41 K42 P43 R44 G45 P46 R47 G48 P49 R50 P51 Q52 T53 S54 L55 LEU

• Molecule 1: Nucleocapsid protein p10

Chain C: 27% • 71%

A101 T102 V103 V104 S105 G106 Q107 K108 Q109 D110 R111 Q112 G113 G114 E115 R116 R117 R118 S119 Q120 L121 D122 R123 D124 C129 K141 K142 P143 R144 G145 P146 R147 G148 P149 R150 P151 Q152 T153 S154 L155 L156

• Molecule 2: tRNApro

Chain B: 27% 39% 24% 10%

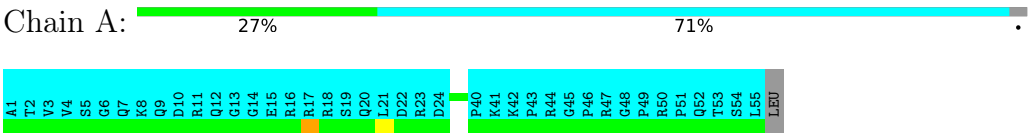
G1 G2 C3 U4 C5 G6 U7 U8 G9 G10 U11 C12 U13 A14 G15 G16 G18 G19 U20 A21 U22 G23 A24 U25 U26 C27 U28 C29 G30 C31 A34 G35 G36 G37 U38 G39 C40 G41 A42 G43 A44 G45 G46 U47 C48 C49 C50 U54 U55 C56 A57 A58 A59 U60 C61 C62 C63

A66 C67 G68 A69 G70 C71 C72

4.2.5 Score per residue for model 5

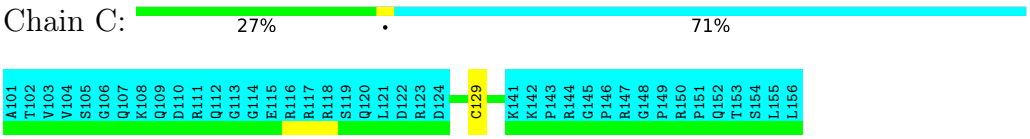
- Molecule 1: Nucleocapsid protein p10

Chain A:



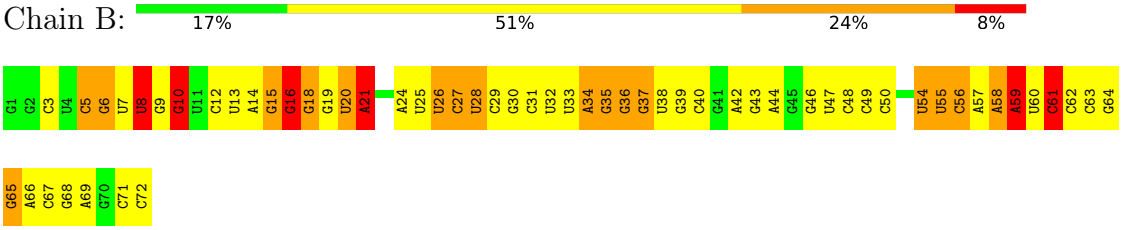
- Molecule 1: Nucleocapsid protein p10

Chain C:



- Molecule 2: tRNApro

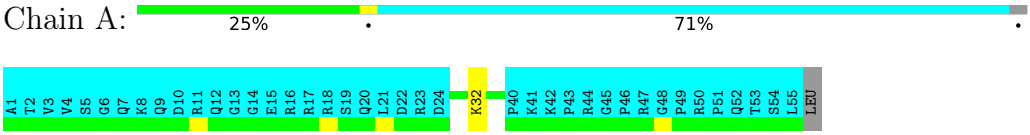
Chain B:



4.2.6 Score per residue for model 6 (medoid)

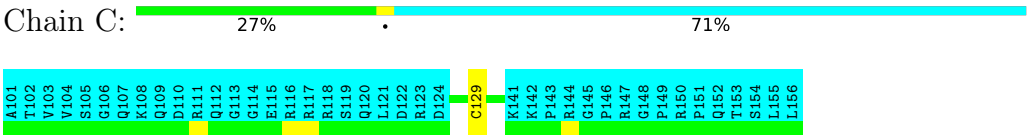
- Molecule 1: Nucleocapsid protein p10

Chain A:



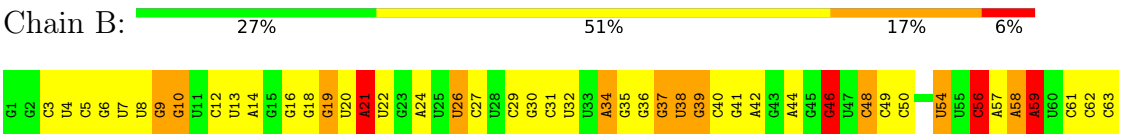
- Molecule 1: Nucleocapsid protein p10

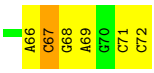
Chain C:



- Molecule 2: tRNApro

Chain B:

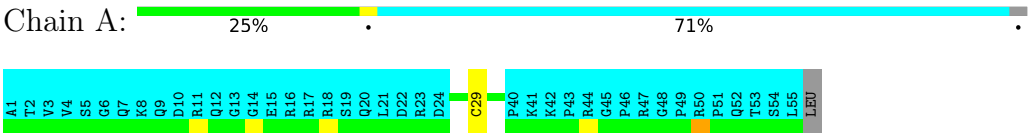




4.2.7 Score per residue for model 7

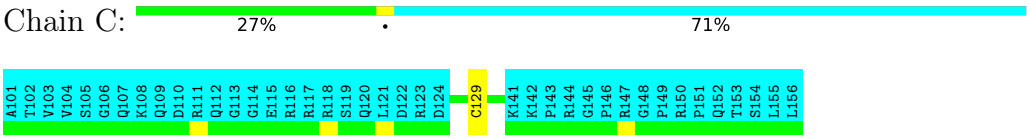
- Molecule 1: Nucleocapsid protein p10

Chain A:



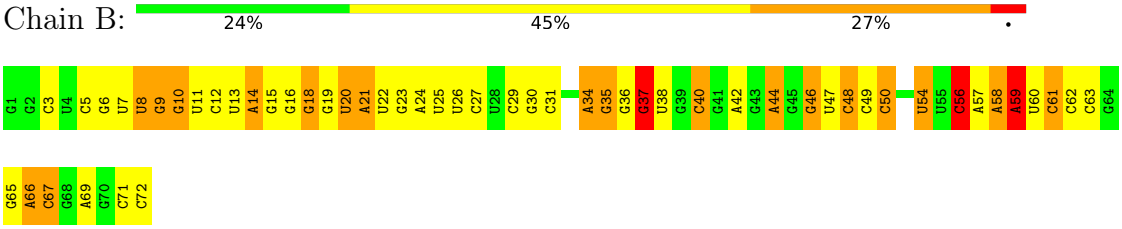
- Molecule 1: Nucleocapsid protein p10

Chain C:



- Molecule 2: tRNApro

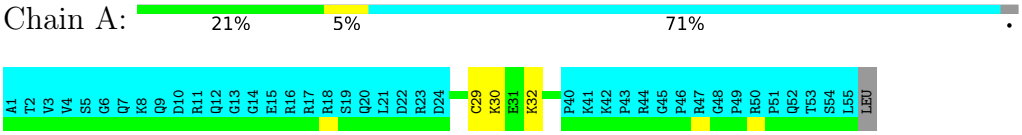
Chain B:



4.2.8 Score per residue for model 8

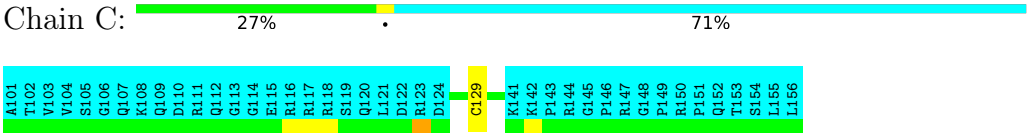
- Molecule 1: Nucleocapsid protein p10

Chain A:



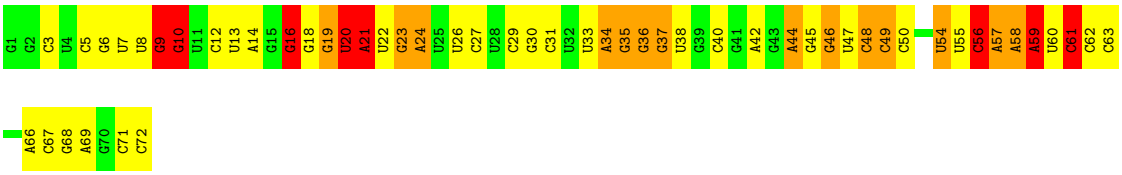
- Molecule 1: Nucleocapsid protein p10

Chain C:



- Molecule 2: tRNApro

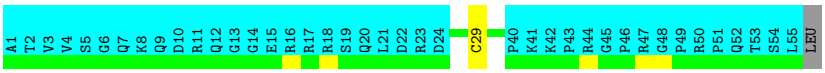
Chain B:



4.2.9 Score per residue for model 9

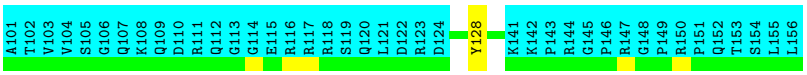
- Molecule 1: Nucleocapsid protein p10

Chain A:



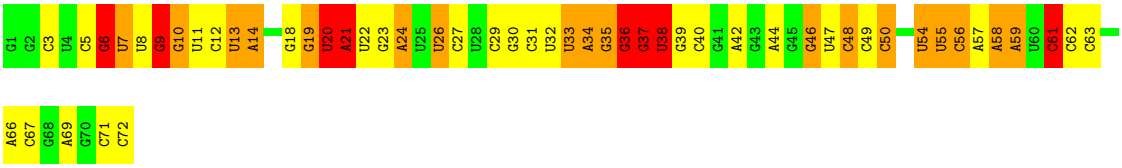
- Molecule 1: Nucleocapsid protein p10

Chain C:



- Molecule 2: tRNApro

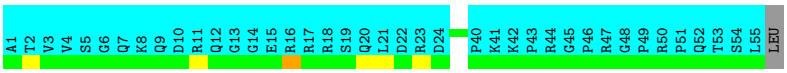
Chain B:



4.2.10 Score per residue for model 10

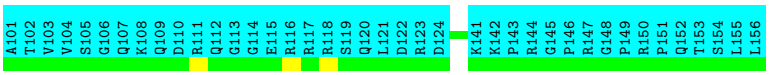
- Molecule 1: Nucleocapsid protein p10

Chain A:



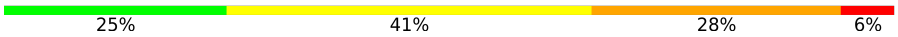
- Molecule 1: Nucleocapsid protein p10

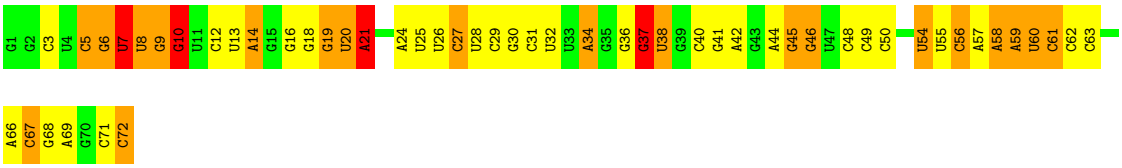
Chain C:



- Molecule 2: tRNApro

Chain B:


25%
41%
28%
6%


G1 G2 C3 U4 C5 G6 U7 U8 G9 G10 U11 C12 U13 A14 G15 G16 G18 G19 U20 A21 A24 U25 U26 C27 U28 C29 G30 C31 U32 U33 A34 G35 G36 G37 U38 G39 C40 G41 A42 G43 A44 G45 G46 U47 C48 C49 C50 U54 U55 C56 A57 A58 A59 U60 C61 C62 C63
A66 C67 G68 A69 G70 C71 C72

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry*.

Of the 20 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
Amber	refinement	
Amber	refinement	
Amber	refinement	
CYANA	refinement	

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	6
Total number of shifts	334
Number of shifts mapped to atoms	328
Number of unparsed shifts	0
Number of shifts with mapping errors	6
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	14%

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: ZN

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	0.77±0.01	0±0/125 (0.0± 0.0%)	1.06±0.03	0±0/168 (0.0± 0.0%)
1	C	0.77±0.01	0±0/133 (0.0± 0.0%)	1.06±0.04	0±0/179 (0.0± 0.0%)
2	B	1.42±0.01	0±0/1695 (0.0± 0.0%)	2.23±0.02	93±4/2643 (3.5± 0.2%)
All	All	1.36	2/19530 (0.0%)	2.13	932/29900 (3.1%)

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

Mol	Chain	Chirality	Planarity
1	C	0.0±0.0	0.2±0.4
2	B	0.0±0.0	13.8±3.3
All	All	0	140

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	37	G	C2-N2	-5.30	1.29	1.34	3	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	16	G	P-O3'-C3'	15.92	138.80	119.70	5	1
2	B	5	C	P-O3'-C3'	15.78	138.63	119.70	3	1
2	B	15	G	P-O3'-C3'	14.92	137.60	119.70	4	2
2	B	59	A	N1-C6-N6	-11.01	111.99	118.60	9	10
2	B	65	G	P-O3'-C3'	10.96	132.85	119.70	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	14	A	N1-C6-N6	-10.86	112.08	118.60	7	9
2	B	21	A	N1-C6-N6	-10.63	112.22	118.60	3	10
2	B	58	A	N1-C6-N6	-10.46	112.33	118.60	2	10
2	B	67	C	P-O3'-C3'	9.78	131.43	119.70	6	1
2	B	34	A	N1-C6-N6	-9.76	112.74	118.60	1	10
2	B	38	U	O4'-C1'-N1	9.53	115.82	108.20	4	5
2	B	59	A	O4'-C1'-N9	9.43	115.75	108.20	5	4
2	B	42	A	N1-C6-N6	-9.43	112.94	118.60	5	10
2	B	66	A	N1-C6-N6	-9.26	113.04	118.60	8	8
2	B	16	G	O4'-C1'-N9	9.22	115.58	108.20	8	2
2	B	57	A	N1-C6-N6	-9.09	113.15	118.60	7	10
2	B	14	A	C5-C6-N1	8.89	122.15	117.70	10	10
2	B	58	A	O4'-C1'-N9	8.59	115.07	108.20	10	8
2	B	56	C	O4'-C1'-N1	8.53	115.02	108.20	2	10
2	B	44	A	C5-C6-N1	8.43	121.91	117.70	3	10
2	B	69	A	N1-C6-N6	-8.27	113.64	118.60	1	10
2	B	48	C	N3-C2-O2	-8.23	116.14	121.90	2	10
2	B	44	A	N1-C6-N6	-8.22	113.67	118.60	8	10
2	B	34	A	C5-C6-N1	8.09	121.75	117.70	2	10
2	B	56	C	N3-C2-O2	-8.00	116.30	121.90	10	9
2	B	46	G	N3-C2-N2	-7.81	114.44	119.90	1	8
2	B	58	A	C5-C6-N1	7.76	121.58	117.70	7	10
2	B	66	A	C5-C6-N1	7.73	121.56	117.70	8	8
2	B	57	A	C5-C6-N1	7.70	121.55	117.70	10	9
2	B	14	A	C4-C5-C6	-7.67	113.16	117.00	10	10
2	B	24	A	N1-C6-N6	-7.66	114.01	118.60	2	10
2	B	67	C	N3-C2-O2	-7.65	116.55	121.90	5	9
2	B	59	A	C5-C6-N1	7.55	121.48	117.70	7	10
2	B	24	A	C5-C6-N1	7.53	121.46	117.70	6	10
2	B	9	G	N1-C6-O6	-7.44	115.44	119.90	10	10
2	B	40	C	N3-C2-O2	-7.38	116.74	121.90	8	10
2	B	49	C	N3-C2-O2	-7.32	116.77	121.90	5	10
2	B	29	C	N3-C2-O2	-7.32	116.78	121.90	7	10
2	B	31	C	N3-C2-O2	-7.30	116.79	121.90	2	10
2	B	21	A	C5-C6-N1	7.28	121.34	117.70	7	10
2	B	25	U	O4'-C1'-N1	7.26	114.01	108.20	7	6
2	B	58	A	C4-C5-C6	-7.25	113.37	117.00	5	10
2	B	72	C	N3-C2-O2	-7.24	116.83	121.90	9	10
2	B	69	A	C5-C6-N1	7.20	121.30	117.70	7	10
2	B	42	A	C5-C6-N1	7.19	121.30	117.70	10	10
2	B	37	G	N1-C6-O6	-7.18	115.59	119.90	10	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	38	U	C5'-C4'-O4'	7.14	117.66	109.10	3	1
2	B	5	C	N3-C2-O2	-7.13	116.91	121.90	10	10
2	B	63	C	N3-C2-O2	-7.07	116.95	121.90	6	10
2	B	61	C	N3-C2-O2	-7.05	116.96	121.90	9	10
2	B	50	C	N3-C2-O2	-7.05	116.97	121.90	10	10
2	B	62	C	N3-C2-O2	-7.04	116.97	121.90	10	10
2	B	48	C	N1-C2-O2	7.03	123.12	118.90	2	6
2	B	34	A	C4-C5-C6	-7.02	113.49	117.00	1	10
2	B	12	C	N3-C2-O2	-7.02	116.99	121.90	6	10
2	B	46	G	O4'-C1'-N9	7.01	113.81	108.20	4	1
2	B	27	C	N3-C2-O2	-7.01	116.99	121.90	10	10
2	B	42	A	C4-C5-C6	-7.00	113.50	117.00	5	10
2	B	71	C	N3-C2-O2	-6.97	117.02	121.90	4	10
2	B	3	C	N3-C2-O2	-6.97	117.02	121.90	5	10
2	B	57	A	C4-C5-C6	-6.81	113.60	117.00	10	9
2	B	7	U	O4'-C1'-N1	6.65	113.52	108.20	4	5
2	B	59	A	C4-C5-C6	-6.64	113.68	117.00	9	10
2	B	56	C	N1-C2-O2	6.64	122.88	118.90	10	9
2	B	22	U	O4'-C1'-N1	6.61	113.49	108.20	6	6
2	B	54	U	O4'-C1'-N1	6.58	113.47	108.20	9	3
2	B	9	G	O4'-C1'-N9	6.57	113.45	108.20	7	5
2	B	38	U	C1'-O4'-C4'	-6.57	104.65	109.90	3	2
2	B	12	C	O4'-C1'-N1	6.51	113.41	108.20	3	7
2	B	44	A	C4-C5-C6	-6.50	113.75	117.00	2	10
2	B	9	G	C3'-C2'-C1'	6.47	106.68	101.50	2	2
2	B	56	C	C5'-C4'-O4'	6.46	116.86	109.10	2	4
2	B	56	C	C1'-O4'-C4'	-6.42	104.77	109.90	5	2
2	B	19	G	C3'-C2'-C1'	6.41	106.63	101.50	10	7
2	B	34	A	P-O3'-C3'	6.37	127.35	119.70	6	2
2	B	54	U	C5-C6-N1	-6.34	119.53	122.70	4	10
2	B	29	C	O4'-C1'-N1	6.33	113.26	108.20	5	3
2	B	66	A	C4-C5-C6	-6.33	113.84	117.00	8	8
2	B	13	U	N3-C2-O2	-6.32	117.78	122.20	9	10
2	B	21	A	C4-C5-C6	-6.31	113.84	117.00	9	10
2	B	69	A	C4-C5-C6	-6.29	113.85	117.00	5	10
2	B	31	C	N1-C2-O2	6.26	122.66	118.90	3	9
2	B	5	C	O4'-C1'-N1	6.24	113.19	108.20	7	2
2	B	61	C	N1-C2-O2	6.17	122.60	118.90	9	8
2	B	35	G	O4'-C1'-N9	6.17	113.13	108.20	8	2
2	B	38	U	C4'-C3'-C2'	-6.04	96.56	102.60	3	3
2	B	6	G	O4'-C1'-N9	6.03	113.02	108.20	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	26	U	O4'-C1'-N1	6.01	113.01	108.20	2	8
2	B	49	C	N1-C2-O2	6.00	122.50	118.90	5	8
2	B	26	U	C5'-C4'-O4'	5.97	116.26	109.10	4	2
2	B	12	C	N1-C2-O2	5.96	122.47	118.90	6	9
2	B	10	G	O4'-C1'-N9	5.96	112.97	108.20	7	2
2	B	46	G	P-O3'-C3'	5.94	126.83	119.70	3	1
2	B	30	G	N1-C6-O6	-5.90	116.36	119.90	7	6
2	B	20	U	O4'-C1'-N1	5.89	112.91	108.20	4	1
2	B	37	G	N9-C4-C5	5.86	107.75	105.40	3	1
2	B	61	C	C5'-C4'-O4'	5.83	116.10	109.10	5	1
2	B	33	U	P-O3'-C3'	5.83	126.69	119.70	9	1
2	B	62	C	N1-C2-O2	5.80	122.38	118.90	3	10
2	B	67	C	N1-C2-O2	5.79	122.37	118.90	5	8
2	B	33	U	C3'-C2'-C1'	5.75	106.10	101.50	3	1
2	B	33	U	O4'-C1'-N1	5.74	112.79	108.20	5	1
2	B	28	U	O4'-C1'-N1	5.72	112.78	108.20	5	2
2	B	23	G	O4'-C1'-N9	5.71	112.77	108.20	8	3
2	B	8	U	N3-C2-O2	-5.69	118.22	122.20	5	4
2	B	35	G	P-O3'-C3'	5.65	126.48	119.70	5	2
2	B	32	U	O4'-C1'-N1	5.65	112.72	108.20	10	4
2	B	24	A	C4-C5-C6	-5.64	114.18	117.00	2	8
2	B	72	C	N1-C2-O2	5.62	122.27	118.90	9	10
2	B	4	U	O4'-C1'-N1	5.61	112.68	108.20	4	2
2	B	35	G	C4'-C3'-C2'	-5.60	97.00	102.60	3	1
2	B	7	U	C5'-C4'-O4'	5.60	115.82	109.10	10	1
2	B	50	C	N1-C2-O2	5.58	122.25	118.90	8	10
2	B	40	C	O4'-C1'-N1	5.57	112.65	108.20	10	1
2	B	46	G	N3-C4-C5	-5.54	125.83	128.60	4	2
2	B	66	A	O4'-C1'-N9	5.54	112.64	108.20	7	1
2	B	36	G	O4'-C1'-N9	5.54	112.63	108.20	8	2
2	B	11	U	O4'-C1'-N1	5.53	112.63	108.20	3	4
2	B	19	G	O4'-C1'-N9	5.52	112.62	108.20	4	2
2	B	5	C	N1-C2-O2	5.50	122.20	118.90	3	10
2	B	40	C	N1-C2-O2	5.50	122.20	118.90	8	9
2	B	61	C	O4'-C1'-N1	5.48	112.59	108.20	9	1
2	B	48	C	N3-C4-N4	-5.48	114.16	118.00	5	1
2	B	47	U	N3-C2-O2	-5.47	118.37	122.20	1	4
2	B	59	A	C6-C5-N7	5.46	136.12	132.30	9	1
2	B	10	G	C5-C6-N1	5.45	114.22	111.50	3	3
2	B	29	C	N1-C2-O2	5.45	122.17	118.90	7	9
2	B	48	C	N3-C4-C5	5.44	124.08	121.90	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	8	U	C1'-O4'-C4'	-5.42	105.56	109.90	4	1
2	B	19	G	N3-C4-C5	-5.41	125.90	128.60	10	1
2	B	59	A	C5'-C4'-O4'	5.40	115.58	109.10	5	1
2	B	27	C	N1-C2-O2	5.40	122.14	118.90	6	6
2	B	20	U	N3-C2-O2	-5.39	118.43	122.20	7	7
2	B	39	G	N1-C6-O6	-5.38	116.67	119.90	6	1
2	B	3	C	N1-C2-O2	5.38	122.13	118.90	5	10
2	B	35	G	N1-C6-O6	-5.38	116.67	119.90	8	2
2	B	14	A	O4'-C1'-N9	5.37	112.50	108.20	4	1
2	B	37	G	C5-C6-O6	5.37	131.82	128.60	10	2
2	B	25	U	N3-C2-O2	-5.37	118.44	122.20	10	1
2	B	48	C	O4'-C1'-N1	5.37	112.49	108.20	7	2
2	B	71	C	N1-C2-O2	5.36	122.12	118.90	4	9
2	B	63	C	N1-C2-O2	5.36	122.11	118.90	6	9
2	B	35	G	C5'-C4'-O4'	5.35	115.53	109.10	7	2
2	B	21	A	O4'-C1'-N9	5.35	112.48	108.20	1	1
2	B	55	U	P-O3'-C3'	5.34	126.11	119.70	3	2
2	B	25	U	C4'-C3'-C2'	-5.33	97.27	102.60	4	2
2	B	22	U	C4-C5-C6	5.32	122.89	119.70	2	2
2	B	22	U	C4'-C3'-C2'	-5.32	97.28	102.60	8	3
2	B	60	U	P-O3'-C3'	5.31	126.08	119.70	10	1
2	B	6	G	C2-N3-C4	-5.31	109.25	111.90	3	1
2	B	36	G	N3-C2-N2	-5.29	116.20	119.90	9	1
2	B	10	G	N1-C6-O6	-5.24	116.75	119.90	5	3
2	B	19	G	O4'-C4'-C3'	5.23	110.28	106.10	10	1
2	B	70	G	N1-C6-O6	-5.23	116.76	119.90	2	1
2	B	9	G	C4'-C3'-C2'	-5.21	97.39	102.60	3	1
2	B	42	A	C6-C5-N7	5.19	135.94	132.30	5	1
2	B	60	U	N3-C2-O2	-5.18	118.57	122.20	3	4
2	B	36	G	N3-C4-C5	-5.18	126.01	128.60	10	2
2	B	55	U	N3-C2-O2	-5.16	118.59	122.20	8	1
2	B	58	A	C6-C5-N7	5.16	135.91	132.30	9	2
2	B	66	A	C1'-O4'-C4'	-5.16	105.77	109.90	7	1
2	B	46	G	C6-N1-C2	-5.15	122.01	125.10	2	1
2	B	14	A	C6-C5-N7	5.13	135.89	132.30	7	2
2	B	38	U	N3-C2-O2	-5.12	118.62	122.20	1	2
2	B	50	C	O4'-C1'-N1	5.12	112.29	108.20	7	2
2	B	6	G	N3-C4-C5	-5.11	126.05	128.60	9	1
2	B	49	C	O4'-C1'-N1	5.10	112.28	108.20	8	1
2	B	64	G	O4'-C1'-N9	5.10	112.28	108.20	5	1
2	B	41	G	N1-C6-O6	-5.09	116.84	119.90	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	43	G	N1-C6-O6	-5.09	116.85	119.90	2	2
2	B	46	G	C8-N9-C4	-5.08	104.37	106.40	4	1
2	B	22	U	N1-C2-N3	5.07	117.94	114.90	1	1
2	B	39	G	N3-C4-C5	-5.06	126.07	128.60	2	2
2	B	45	G	N1-C6-O6	-5.05	116.87	119.90	10	1
2	B	19	G	N1-C6-O6	-5.04	116.87	119.90	4	1
2	B	36	G	C8-N9-C4	-5.04	104.38	106.40	8	1
2	B	20	U	C3'-C2'-C1'	5.04	105.53	101.50	4	1
2	B	61	C	C5'-C4'-C3'	-5.04	107.94	116.00	5	1
2	B	65	G	N1-C6-O6	-5.03	116.88	119.90	1	1
2	B	57	A	C5'-C4'-O4'	5.02	115.13	109.10	8	1
2	B	33	U	C2'-C3'-O3'	5.02	121.73	113.70	9	1
2	B	7	U	N3-C2-O2	-5.01	118.69	122.20	9	1
2	B	60	U	O4'-C1'-N1	5.00	112.20	108.20	5	1
2	B	12	C	N3-C4-N4	-5.00	114.50	118.00	7	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
2	B	18	G	Sidechain	10
2	B	54	U	Sidechain	10
2	B	21	A	Sidechain	8
2	B	10	G	Sidechain	8
2	B	59	A	Sidechain	7
2	B	46	G	Sidechain	6
2	B	61	C	Sidechain	6
2	B	26	U	Sidechain	6
2	B	6	G	Sidechain	5
2	B	55	U	Sidechain	4
2	B	37	G	Sidechain	4
2	B	39	G	Sidechain	4
2	B	72	C	Sidechain	4
2	B	27	C	Sidechain	3
2	B	28	U	Sidechain	3
2	B	23	G	Sidechain	3
2	B	36	G	Sidechain	3
2	B	15	G	Sidechain	3
2	B	30	G	Sidechain	3
2	B	56	C	Sidechain	3

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Mol	Chain	Res	Type	Group	Models (Total)
2	B	31	C	Sidechain	2
2	B	48	C	Sidechain	2
2	B	49	C	Sidechain	2
2	B	33	U	Sidechain	2
2	B	38	U	Sidechain	2
2	B	45	G	Sidechain	2
1	C	128	TYR	Sidechain	2
2	B	8	U	Sidechain	2
2	B	5	C	Sidechain	2
2	B	16	G	Sidechain	2
2	B	65	G	Sidechain	2
2	B	44	A	Sidechain	2
2	B	9	G	Sidechain	2
2	B	20	U	Sidechain	2
2	B	24	A	Sidechain	2
2	B	34	A	Sidechain	1
2	B	35	G	Sidechain	1
2	B	22	U	Sidechain	1
2	B	14	A	Sidechain	1
2	B	19	G	Sidechain	1
2	B	40	C	Sidechain	1
2	B	7	U	Sidechain	1

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	121	108	108	0±0
1	C	128	115	115	0±0
2	B	1517	766	766	0±0
All	All	17680	9890	9886	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:13:U:H2'	2:B:14:A:C8	0.42	2.49	3	2
2:B:14:A:N6	2:B:21:A:C2	0.40	2.89	10	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	15/56 (27%)	14±0 (97±3%)	0±0 (3±3%)	0±0 (0±0%)	100	100
1	C	16/56 (29%)	15±1 (96±4%)	1±1 (4±4%)	0±0 (0±0%)	100	100
All	All	310/1120 (28%)	299 (96%)	11 (4%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	12/47 (26%)	11±1 (92±7%)	1±1 (8±7%)	15	62
1	C	13/47 (28%)	12±0 (96±4%)	0±0 (4±4%)	36	84
All	All	250/940 (27%)	235 (94%)	15 (6%)	23	72

All 4 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	29	CYS	6
1	C	129	CYS	5
1	A	32	LYS	3
1	A	30	LYS	1

6.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	B	70/71 (99%)	20±3 (29±4%)	8±2 (11±4%)	0.47±0.03
All	All	700/710 (99%)	203 (29%)	77 (11%)	0.47

The overall RNA backbone suiteness is 0.47.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	10	G	10
2	B	20	U	10
2	B	21	A	10
2	B	34	A	10
2	B	38	U	10
2	B	58	A	10
2	B	59	A	10
2	B	16	G	9
2	B	19	G	9
2	B	61	C	9
2	B	6	G	9
2	B	56	C	9
2	B	8	U	8
2	B	37	G	8
2	B	9	G	7
2	B	36	G	7
2	B	35	G	7
2	B	48	C	6
2	B	47	U	5
2	B	7	U	5
2	B	45	G	4
2	B	60	U	4
2	B	68	G	4
2	B	66	A	3
2	B	46	G	3
2	B	50	C	3
2	B	49	C	2
2	B	14	A	2
2	B	18	G	2
2	B	55	U	2
2	B	67	C	2
2	B	11	U	1
2	B	33	U	1
2	B	39	G	1

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Mol	Chain	Res	Type	Models (Total)
2	B	57	A	1

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	20	U	10
2	B	19	G	9
2	B	37	G	8
2	B	6	G	5
2	B	60	U	5
2	B	59	A	4
2	B	34	A	4
2	B	8	U	3
2	B	58	A	3
2	B	10	G	2
2	B	56	C	2
2	B	33	U	2
2	B	35	G	2
2	B	36	G	2
2	B	46	G	2
2	B	47	U	2
2	B	16	G	2
2	B	55	U	2
2	B	67	C	2
2	B	9	G	2
2	B	5	C	1
2	B	38	U	1
2	B	15	G	1
2	B	45	G	1

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are 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 (i)

The completeness of assignment taking into account all chemical shift lists is 14% 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_2*

7.1.1 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	34
Number of shifts mapped to atoms	34
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 (i)

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

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 1%, i.e. 18 atoms were assigned a chemical shift out of a possible 1733. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	7/155 (5%)	7/63 (11%)	0/62 (0%)	0/30 (0%)
Sidechain	10/181 (6%)	10/114 (9%)	0/59 (0%)	0/8 (0%)
Aromatic	1/56 (2%)	1/28 (4%)	0/24 (0%)	0/4 (0%)
Sugar	0/781 (0%)	0/426 (0%)	0/355 (0%)	0/0 (—%)
Base	0/560 (0%)	0/347 (0%)	0/116 (0%)	0/97 (0%)
Overall	18/1733 (1%)	18/978 (2%)	0/616 (0%)	0/139 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure.

The overall completeness is 1%, i.e. 33 atoms were assigned a chemical shift out of a possible 2865. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	13/547 (2%)	13/224 (6%)	0/222 (0%)	0/101 (0%)
Sidechain	19/921 (2%)	19/579 (3%)	0/270 (0%)	0/72 (0%)
Aromatic	1/56 (2%)	1/28 (4%)	0/24 (0%)	0/4 (0%)
Sugar	0/781 (0%)	0/426 (0%)	0/355 (0%)	0/0 (—%)
Base	0/560 (0%)	0/347 (0%)	0/116 (0%)	0/97 (0%)
Overall	33/2865 (1%)	33/1604 (2%)	0/987 (0%)	0/274 (0%)

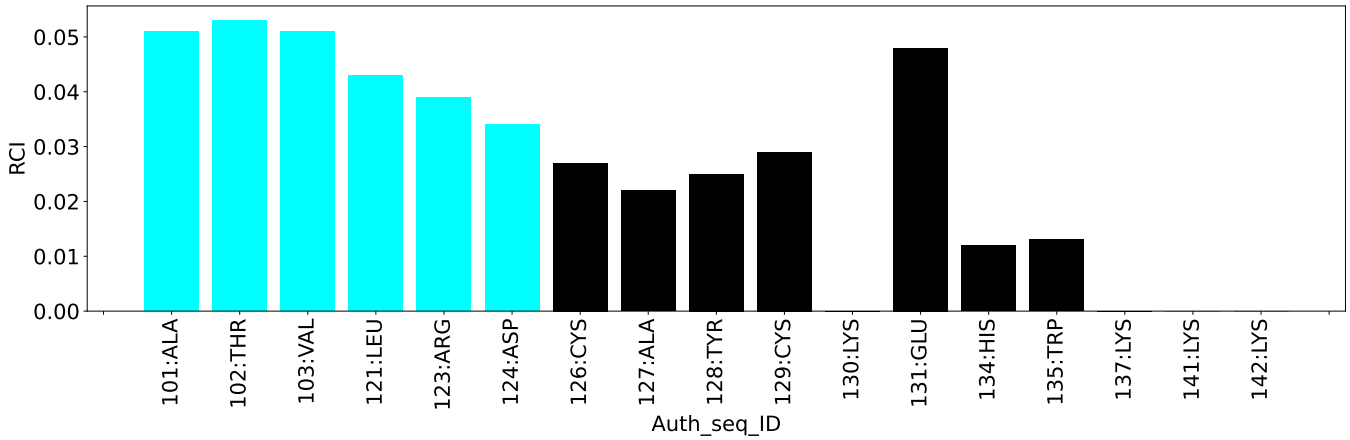
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain C:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2_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	74
Number of shifts mapped to atoms	74
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 2%, i.e. 34 atoms were assigned a chemical shift out of a possible 1733. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	10/155 (6%)	10/63 (16%)	0/62 (0%)	0/30 (0%)
Sidechain	14/181 (8%)	14/114 (12%)	0/59 (0%)	0/8 (0%)
Aromatic	10/56 (18%)	10/28 (36%)	0/24 (0%)	0/4 (0%)
Sugar	0/781 (0%)	0/426 (0%)	0/355 (0%)	0/0 (—%)
Base	0/560 (0%)	0/347 (0%)	0/116 (0%)	0/97 (0%)
Overall	34/1733 (2%)	34/978 (3%)	0/616 (0%)	0/139 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 74 atoms were assigned a chemical shift out of a possible 2865. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	27/547 (5%)	27/224 (12%)	0/222 (0%)	0/101 (0%)
Sidechain	37/921 (4%)	37/579 (6%)	0/270 (0%)	0/72 (0%)
Aromatic	10/56 (18%)	10/28 (36%)	0/24 (0%)	0/4 (0%)
Sugar	0/781 (0%)	0/426 (0%)	0/355 (0%)	0/0 (—%)
Base	0/560 (0%)	0/347 (0%)	0/116 (0%)	0/97 (0%)
Overall	74/2865 (3%)	74/1604 (5%)	0/987 (0%)	0/274 (0%)

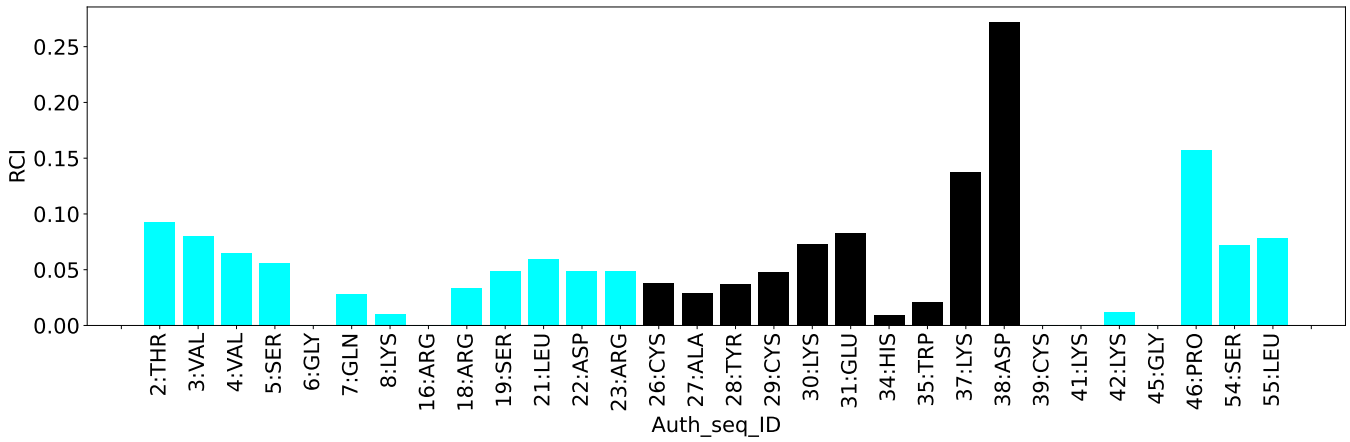
7.2.4 Statistically unusual chemical shifts (i)

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 A:



7.3 Chemical shift list 3

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2_dup_dup*

7.3.1 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	145
Number of shifts mapped to atoms	139
Number of unparsed shifts	0
Number of shifts with mapping errors	6
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. All 6 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3	B	74	C	H5	5.80568	0.0	1
3	B	74	C	H6	7.78857	0.0	1
3	B	75	C	H1'	5.66473	0.0	1
3	B	75	C	H6	7.753895	0.0	1
3	B	76	A	H1'	6.10641	0.0	1
3	B	76	A	H8	8.46201	0.0	1

7.3.2 Chemical shift referencing (i)

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

7.3.3 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 7%, i.e. 125 atoms were assigned a chemical shift out of a possible 1733. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/155 (0%)	0/63 (0%)	0/62 (0%)	0/30 (0%)
Sidechain	0/181 (0%)	0/114 (0%)	0/59 (0%)	0/8 (0%)
Aromatic	0/56 (0%)	0/28 (0%)	0/24 (0%)	0/4 (0%)
Sugar	50/781 (6%)	50/426 (12%)	0/355 (0%)	0/0 (—%)
Base	75/560 (13%)	75/347 (22%)	0/116 (0%)	0/97 (0%)
Overall	125/1733 (7%)	125/978 (13%)	0/616 (0%)	0/139 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 125 atoms were assigned a chemical shift out of a possible 2865. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/547 (0%)	0/224 (0%)	0/222 (0%)	0/101 (0%)
Sidechain	0/921 (0%)	0/579 (0%)	0/270 (0%)	0/72 (0%)
Aromatic	0/56 (0%)	0/28 (0%)	0/24 (0%)	0/4 (0%)
Sugar	50/781 (6%)	50/426 (12%)	0/355 (0%)	0/0 (—%)
Base	75/560 (13%)	75/347 (22%)	0/116 (0%)	0/97 (0%)
Overall	125/2865 (4%)	125/1604 (8%)	0/987 (0%)	0/274 (0%)

7.3.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.3.5 Random Coil Index (RCI) plots (i)

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins

7.4 Chemical shift list 4

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2_dup_dup_dup*

7.4.1 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	28
Number of shifts mapped to atoms	28
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

7.4.2 Chemical shift referencing (i)

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

7.4.3 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 2%, i.e. 26 atoms were assigned a chemical shift out of a possible 1733. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}**H**	^{13}**C**	^{15}**N**
Backbone	0/155 (0%)	0/63 (0%)	0/62 (0%)	0/30 (0%)
Sidechain	0/181 (0%)	0/114 (0%)	0/59 (0%)	0/8 (0%)
Aromatic	0/56 (0%)	0/28 (0%)	0/24 (0%)	0/4 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Sugar	22/781 (3%)	22/426 (5%)	0/355 (0%)	0/0 (—%)
Base	4/560 (1%)	4/347 (1%)	0/116 (0%)	0/97 (0%)
Overall	26/1733 (2%)	26/978 (3%)	0/616 (0%)	0/139 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 1%, i.e. 26 atoms were assigned a chemical shift out of a possible 2865. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/547 (0%)	0/224 (0%)	0/222 (0%)	0/101 (0%)
Sidechain	0/921 (0%)	0/579 (0%)	0/270 (0%)	0/72 (0%)
Aromatic	0/56 (0%)	0/28 (0%)	0/24 (0%)	0/4 (0%)
Sugar	22/781 (3%)	22/426 (5%)	0/355 (0%)	0/0 (—%)
Base	4/560 (1%)	4/347 (1%)	0/116 (0%)	0/97 (0%)
Overall	26/2865 (1%)	26/1604 (2%)	0/987 (0%)	0/274 (0%)

7.4.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.4.5 Random Coil Index (RCI) plots (i)

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins

7.5 Chemical shift list 5

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2_dup_dup_dup_dup*

7.5.1 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	33
Number of shifts mapped to atoms	33
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

7.5.2 Chemical shift referencing (i)

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

7.5.3 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 2%, i.e. 33 atoms were assigned a chemical shift out of a possible 1733. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}**H**	^{13}**C**	^{15}**N**
Backbone	0/155 (0%)	0/63 (0%)	0/62 (0%)	0/30 (0%)
Sidechain	0/181 (0%)	0/114 (0%)	0/59 (0%)	0/8 (0%)
Aromatic	0/56 (0%)	0/28 (0%)	0/24 (0%)	0/4 (0%)
Sugar	14/781 (2%)	0/426 (0%)	14/355 (4%)	0/0 (—%)
Base	19/560 (3%)	0/347 (0%)	19/116 (16%)	0/97 (0%)
Overall	33/1733 (2%)	0/978 (0%)	33/616 (5%)	0/139 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 1%, i.e. 33 atoms were assigned a chemical shift out of a possible 2865. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}**H**	^{13}**C**	^{15}**N**
Backbone	0/547 (0%)	0/224 (0%)	0/222 (0%)	0/101 (0%)
Sidechain	0/921 (0%)	0/579 (0%)	0/270 (0%)	0/72 (0%)
Aromatic	0/56 (0%)	0/28 (0%)	0/24 (0%)	0/4 (0%)
Sugar	14/781 (2%)	0/426 (0%)	14/355 (4%)	0/0 (—%)
Base	19/560 (3%)	0/347 (0%)	19/116 (16%)	0/97 (0%)
Overall	33/2865 (1%)	0/1604 (0%)	33/987 (3%)	0/274 (0%)

7.5.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.5.5 Random Coil Index (RCI) plots (i)

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins

7.6 Chemical shift list 6

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2_dup_dup_dup_dup_dup*

7.6.1 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	20
Number of shifts mapped to atoms	20
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

7.6.2 Chemical shift referencing (i)

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

7.6.3 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 1%, i.e. 20 atoms were assigned a chemical shift out of a possible 1733. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}**H**	^{13}**C**	^{15}**N**
Backbone	0/155 (0%)	0/63 (0%)	0/62 (0%)	0/30 (0%)
Sidechain	0/181 (0%)	0/114 (0%)	0/59 (0%)	0/8 (0%)
Aromatic	0/56 (0%)	0/28 (0%)	0/24 (0%)	0/4 (0%)
Sugar	15/781 (2%)	15/426 (4%)	0/355 (0%)	0/0 (—%)
Base	5/560 (1%)	5/347 (1%)	0/116 (0%)	0/97 (0%)
Overall	20/1733 (1%)	20/978 (2%)	0/616 (0%)	0/139 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 1%, i.e. 20 atoms were assigned a chemical shift out of a possible 2865. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}**H**	^{13}**C**	^{15}**N**
Backbone	0/547 (0%)	0/224 (0%)	0/222 (0%)	0/101 (0%)
Sidechain	0/921 (0%)	0/579 (0%)	0/270 (0%)	0/72 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/56 (0%)	0/28 (0%)	0/24 (0%)	0/4 (0%)
Sugar	15/781 (2%)	15/426 (4%)	0/355 (0%)	0/0 (—%)
Base	5/560 (1%)	5/347 (1%)	0/116 (0%)	0/97 (0%)
Overall	20/2865 (1%)	20/1604 (1%)	0/987 (0%)	0/274 (0%)

7.6.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.6.5 Random Coil Index (RCI) plots (i)

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins