



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:19 PM BST

PDB ID : 1K1G
Title : STRUCTURAL BASIS FOR RECOGNITION OF THE INTRON BRANCH
SITE RNA BY SPLICING FACTOR 1
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Deposited on : 2001-09-25

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
<http://wwpdb.org/validation/2016/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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

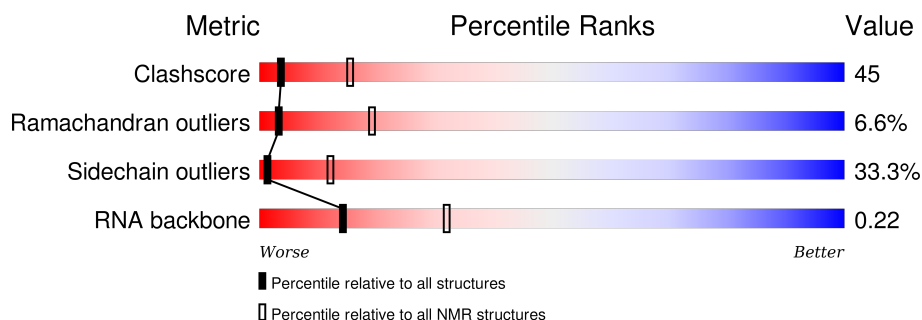
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958
RNA backbone	3027	600

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	B	11	<div> <div style="width: 27%; background-color: yellow;"></div> <div style="width: 73%; background-color: orange;"></div> </div> <div>27% 73%</div>
2	A	131	<div> <div style="width: 24%; background-color: green;"></div> <div style="width: 44%; background-color: yellow;"></div> <div style="width: 17%; background-color: orange;"></div> <div style="width: 8%; background-color: red;"></div> <div style="width: 7%; background-color: cyan;"></div> <div style="width: 7%; background-color: grey;"></div> </div> <div>24% 44% 17% • 8% 7%</div>

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:134-A:184, A:195-A:255 (112)	0.39	8

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 4 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2308 atoms, of which 1122 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'.

Mol	Chain	Residues	Atoms						Trace
1	B	11	Total	C	H	N	O	P	0
			349	105	120	42	72	10	

- Molecule 2 is a protein called SF1-Bo isoform.

Mol	Chain	Residues	Atoms						Trace
2	A	122	Total	C	H	N	O	S	0
			1959	591	1002	178	182	6	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	GLY	LYS	CLONING ARTIFACT	UNP Q15637
A	131	ALA	PRO	CLONING ARTIFACT	UNP Q15637
A	132	MET	PRO	CLONING ARTIFACT	UNP Q15637

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble


These plots are provided for all protein, RNA and DNA 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.

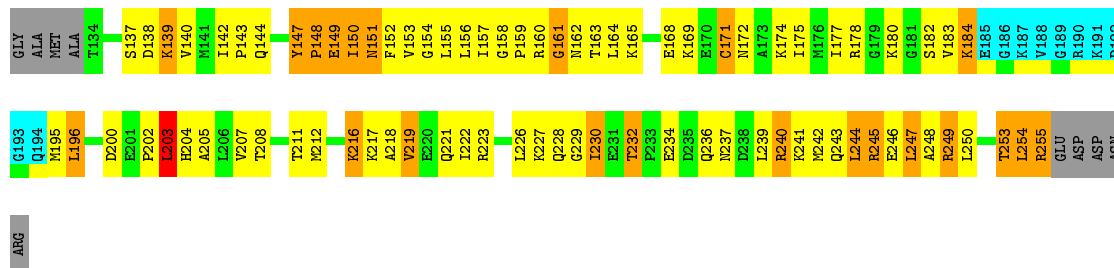
- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'

Chain B: 



- Molecule 2: SF1-Bo isoform

Chain A: 



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

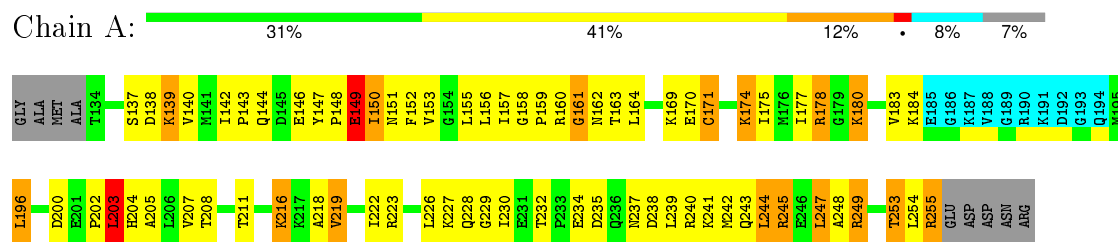
4.2.1 Score per residue for model 1

- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'

Chain B: 



- Molecule 2: SF1-Bo isoform

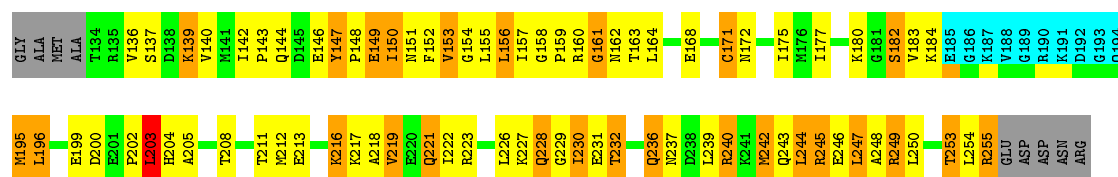
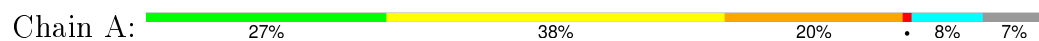


4.2.2 Score per residue for model 2

- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'



- Molecule 2: SF1-Bo isoform

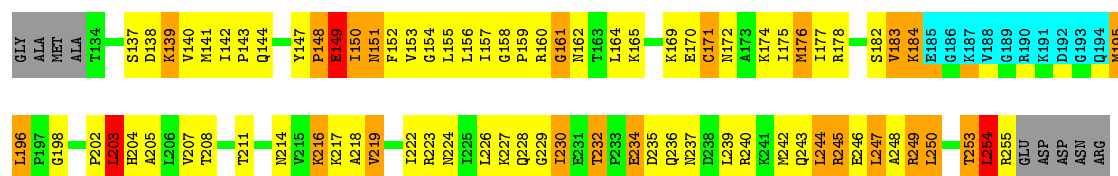


4.2.3 Score per residue for model 3

- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'



- Molecule 2: SF1-Bo isoform



4.2.4 Score per residue for model 4

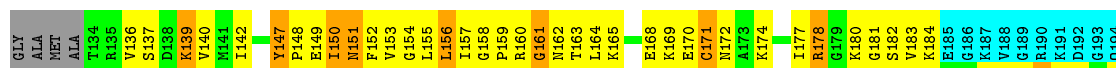
- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'

Chain B:  27% 73%



- Molecule 2: SF1-Bo isoform

Chain A:  29% 40% 15% 8% 7%



4.2.5 Score per residue for model 5

- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'

Chain B:  9% 9% 82%



- Molecule 2: SF1-Bo isoform

Chain A:  27% 41% 16% 8% 7%



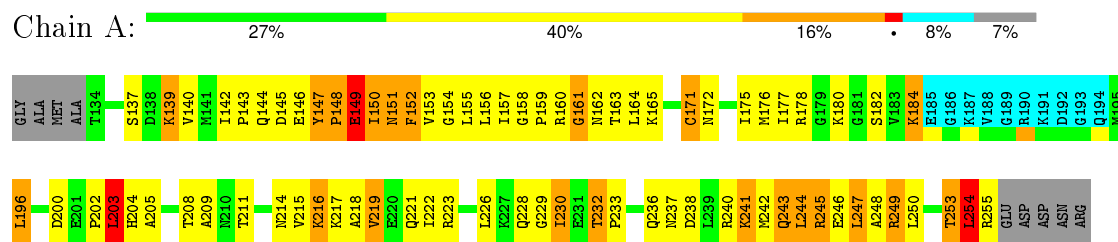
4.2.6 Score per residue for model 6

- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'

Chain B:  18% 82%



- Molecule 2: SF1-Bo isoform

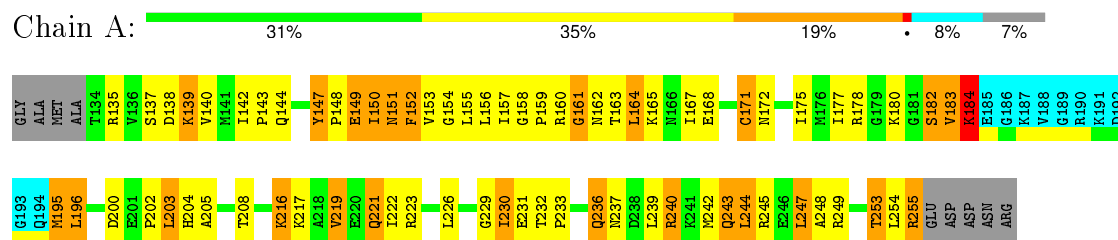


4.2.7 Score per residue for model 7

- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'



- Molecule 2: SF1-Bo isoform

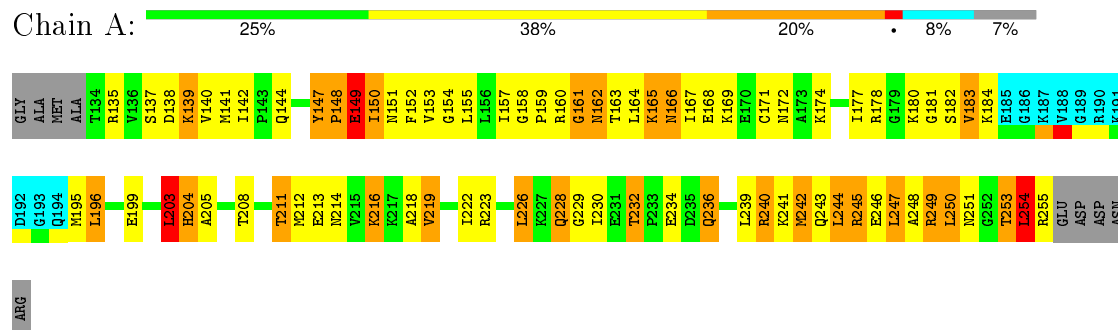


4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'



- Molecule 2: SF1-Bo isoform



4.2.9 Score per residue for model 9

- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'

Chain B: 



- Molecule 2: SF1-Bo isoform

Chain A: 



4.2.10 Score per residue for model 10

- Molecule 1: 5'-R(*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*A)-3'

Chain B: 



- Molecule 2: SF1-Bo isoform

Chain A: 



5 Refinement protocol and experimental data overview

The models were refined using the following method: *restrained molecular dynamics, simulated annealing*.

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *10 lowest energy structures consistent with experimental distance and dihedral angle restraints*.

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

Software name	Classification	Version
ARIA/CNS	structure solution	1.0
ARIA/CNS	refinement	1.0

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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	B	0.61±0.02	0±0/256 (0.0±0.1%)	0.88±0.03	0±0/396 (0.0±0.0%)
2	A	0.28±0.04	0±1/891 (0.0±0.1%)	0.39±0.01	0±0/1196 (0.0±0.0%)
All	All	0.38	5/11470 (0.0%)	0.55	0/15920 (0.0%)

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
2	A	147	TYR	CE2-CZ	-5.82	1.30	1.38	5	1
2	A	147	TYR	CE1-CZ	5.75	1.46	1.38	5	1
2	A	152	PHE	CE2-CZ	5.41	1.47	1.37	7	2
1	B	504	A	C2'-C1'	-5.16	1.47	1.53	7	1

There are no bond-angle outliers.

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	B	229	120	120	26±2
2	A	883	927	925	87±7
All	All	11120	10470	10450	967

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 45.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:507:A:C2	2:A:184:LYS:HG3	0.81	2.11	9	1
2:A:159:PRO:HD3	2:A:247:LEU:HB2	0.79	1.53	2	9
1:B:502:A:H2'	2:A:255:ARG:HA	0.75	1.58	8	7
2:A:151:ASN:HB2	2:A:155:LEU:HG	0.75	1.58	3	6
2:A:155:LEU:HD22	2:A:243:GLN:HB3	0.73	1.60	10	10
2:A:245:ARG:HD2	2:A:249:ARG:HB2	0.73	1.58	9	4
2:A:219:VAL:HA	2:A:222:ILE:HD12	0.72	1.61	4	10
2:A:142:ILE:HG13	2:A:226:LEU:HG	0.72	1.62	2	5
2:A:153:VAL:HG23	2:A:177:ILE:HD13	0.72	1.61	3	10
2:A:195:MET:HE2	2:A:196:LEU:HD23	0.71	1.62	8	4
2:A:195:MET:HE1	2:A:196:LEU:HD23	0.71	1.61	7	4
2:A:143:PRO:HD3	2:A:226:LEU:HD11	0.71	1.61	2	4
2:A:254:LEU:HD22	2:A:255:ARG:H	0.70	1.46	9	6
2:A:245:ARG:HD3	2:A:249:ARG:HB2	0.70	1.64	1	3
2:A:254:LEU:HD22	2:A:255:ARG:N	0.68	2.01	10	7
1:B:508:A:H2'	1:B:509:C:O4'	0.68	1.88	6	10
1:B:510:A:H2'	1:B:511:A:H3'	0.68	1.66	5	3
1:B:506:U:O4	2:A:151:ASN:HB3	0.68	1.89	7	3
2:A:245:ARG:HG2	2:A:254:LEU:HD23	0.67	1.66	7	9
2:A:228:GLN:HB3	2:A:232:THR:HB	0.67	1.65	9	6
1:B:506:U:C2	2:A:247:LEU:HD22	0.67	2.25	7	10
1:B:505:C:C2	2:A:244:LEU:HD11	0.66	2.25	2	10
2:A:139:LYS:HG3	2:A:204:HIS:HB2	0.66	1.68	8	9
1:B:508:A:H62	2:A:183:VAL:HG23	0.66	1.50	2	2
2:A:245:ARG:HD3	2:A:249:ARG:HB3	0.66	1.66	2	2
2:A:150:ILE:HD12	2:A:230:ILE:HD11	0.65	1.67	5	3
2:A:236:GLN:HB2	2:A:240:ARG:HB2	0.65	1.66	2	2
2:A:151:ASN:ND2	2:A:155:LEU:HD11	0.65	2.06	6	5
1:B:507:A:C4	2:A:184:LYS:HD3	0.64	2.27	3	2
1:B:505:C:H4'	1:B:506:U:O5'	0.64	1.92	8	4
2:A:236:GLN:HB2	2:A:239:LEU:HD12	0.63	1.70	8	1
2:A:157:ILE:HA	2:A:164:LEU:HG	0.63	1.70	10	10
2:A:142:ILE:HG13	2:A:226:LEU:HD11	0.63	1.69	5	4
2:A:161:GLY:HA3	2:A:164:LEU:HD12	0.62	1.69	3	10
2:A:140:VAL:CG1	2:A:205:ALA:HB3	0.62	2.24	9	9
2:A:147:TYR:CB	2:A:150:ILE:HD11	0.62	2.24	2	5
2:A:147:TYR:HB2	2:A:150:ILE:HD11	0.62	1.70	7	5
2:A:151:ASN:O	2:A:155:LEU:HG	0.62	1.93	1	10
1:B:506:U:O2	2:A:247:LEU:HD22	0.62	1.93	3	10
2:A:232:THR:HG21	2:A:240:ARG:HB3	0.62	1.70	2	1
2:A:151:ASN:ND2	2:A:155:LEU:HD21	0.62	2.09	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:157:ILE:HG23	2:A:164:LEU:HD11	0.62	1.70	4	10
1:B:507:A:H4'	1:B:508:A:O5'	0.61	1.95	9	10
2:A:147:TYR:HB3	2:A:150:ILE:HD11	0.61	1.73	8	4
2:A:177:ILE:HG22	2:A:182:SER:HB3	0.60	1.74	2	3
2:A:246:GLU:HG3	2:A:247:LEU:N	0.60	2.10	8	4
1:B:509:C:H2'	1:B:510:A:O4'	0.60	1.97	1	10
2:A:221:GLN:HG3	2:A:222:ILE:N	0.60	2.10	2	3
2:A:144:GLN:HA	2:A:147:TYR:O	0.59	1.97	1	9
1:B:507:A:H2'	2:A:184:LYS:HB2	0.59	1.73	2	7
2:A:244:LEU:HD23	2:A:247:LEU:CD2	0.59	2.27	10	10
2:A:151:ASN:HB2	2:A:155:LEU:CG	0.59	2.28	3	3
2:A:157:ILE:HG12	2:A:164:LEU:HD11	0.58	1.75	10	6
2:A:247:LEU:HG	2:A:248:ALA:N	0.58	2.13	9	10
2:A:143:PRO:HD2	2:A:226:LEU:HD21	0.58	1.76	6	3
2:A:152:PHE:HE1	2:A:229:GLY:HA3	0.58	1.59	2	6
1:B:511:A:N6	2:A:178:ARG:HA	0.57	2.13	5	4
2:A:216:LYS:O	2:A:219:VAL:HG12	0.57	1.99	10	9
2:A:151:ASN:OD1	2:A:155:LEU:HD11	0.57	2.00	3	1
2:A:157:ILE:HG22	2:A:158:GLY:O	0.57	2.00	8	10
1:B:507:A:N6	2:A:153:VAL:HG13	0.56	2.15	9	9
2:A:232:THR:OG1	2:A:237:ASN:HA	0.56	1.99	7	1
1:B:507:A:H2'	2:A:184:LYS:CB	0.56	2.30	3	2
2:A:164:LEU:HA	2:A:175:ILE:HG13	0.56	1.77	3	5
1:B:504:A:O2'	2:A:244:LEU:HD22	0.56	2.00	2	10
2:A:152:PHE:HB3	2:A:226:LEU:HG	0.56	1.76	5	2
1:B:502:A:H4'	1:B:503:U:H5	0.56	1.61	3	3
1:B:504:A:N7	2:A:255:ARG:HD2	0.55	2.15	7	1
2:A:228:GLN:HB2	2:A:232:THR:HB	0.55	1.77	8	1
2:A:177:ILE:HA	2:A:205:ALA:HA	0.55	1.77	7	9
2:A:232:THR:HG1	2:A:236:GLN:HG3	0.55	1.60	2	1
2:A:219:VAL:O	2:A:223:ARG:HG2	0.55	2.02	7	10
2:A:157:ILE:HA	2:A:164:LEU:CG	0.55	2.31	10	8
1:B:508:A:N7	2:A:183:VAL:HG12	0.55	2.17	9	2
2:A:159:PRO:HD2	2:A:162:ASN:HB2	0.55	1.78	7	7
1:B:510:A:H2'	1:B:511:A:H5"	0.55	1.80	3	1
2:A:248:ALA:HB1	2:A:253:THR:O	0.54	2.02	4	6
1:B:506:U:C4	2:A:154:GLY:HA3	0.54	2.37	3	9
2:A:151:ASN:HD22	2:A:155:LEU:HD21	0.54	1.60	9	2
2:A:155:LEU:HD13	2:A:243:GLN:CB	0.54	2.33	6	10
2:A:242:MET:O	2:A:245:ARG:HB2	0.54	2.03	10	1
1:B:511:A:H61	2:A:178:ARG:HA	0.54	1.63	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:157:ILE:HG12	2:A:164:LEU:HD21	0.54	1.80	4	6
2:A:152:PHE:CE1	2:A:229:GLY:HA3	0.54	2.38	2	3
2:A:162:ASN:HD22	2:A:250:LEU:HD13	0.54	1.61	4	1
2:A:244:LEU:HD23	2:A:247:LEU:HD23	0.54	1.80	8	10
1:B:505:C:H5''	1:B:506:U:H5'	0.54	1.80	1	2
1:B:510:A:N3	1:B:511:A:H8	0.53	2.01	5	6
2:A:152:PHE:O	2:A:156:LEU:HD23	0.53	2.03	4	2
2:A:142:ILE:HA	2:A:226:LEU:HD11	0.53	1.81	8	2
2:A:248:ALA:HB1	2:A:253:THR:C	0.53	2.24	4	10
2:A:142:ILE:HB	2:A:203:LEU:HB3	0.53	1.79	4	7
2:A:207:VAL:HG21	2:A:222:ILE:HD13	0.53	1.80	1	2
2:A:242:MET:HE1	2:A:245:ARG:HB3	0.53	1.81	3	1
2:A:230:ILE:O	2:A:240:ARG:HB2	0.53	2.03	8	3
2:A:140:VAL:HG12	2:A:205:ALA:HB3	0.52	1.82	6	6
1:B:510:A:C2	1:B:511:A:H2'	0.52	2.39	3	4
2:A:139:LYS:HG2	2:A:204:HIS:HB2	0.52	1.82	9	1
2:A:151:ASN:HD21	2:A:230:ILE:HG23	0.52	1.64	10	2
1:B:507:A:N3	2:A:184:LYS:HG2	0.52	2.20	6	2
1:B:507:A:C2	2:A:184:LYS:HD3	0.52	2.40	1	5
2:A:156:LEU:O	2:A:163:THR:HB	0.52	2.05	6	8
2:A:171:CYS:SG	2:A:218:ALA:HB2	0.51	2.44	6	5
1:B:502:A:H4'	1:B:503:U:C5	0.51	2.40	8	3
2:A:211:THR:HG23	2:A:214:ASN:HB2	0.51	1.82	8	1
2:A:175:ILE:N	2:A:175:ILE:HD12	0.51	2.20	6	1
1:B:511:A:N7	2:A:183:VAL:HG11	0.51	2.21	8	7
1:B:504:A:H4'	1:B:505:C:OP2	0.51	2.05	9	7
1:B:508:A:N3	2:A:164:LEU:HD13	0.51	2.20	7	7
2:A:156:LEU:HD23	2:A:222:ILE:HG23	0.51	1.82	9	2
2:A:156:LEU:HD11	2:A:222:ILE:HG12	0.51	1.83	3	2
2:A:155:LEU:HD22	2:A:243:GLN:CB	0.51	2.36	3	7
2:A:242:MET:HA	2:A:245:ARG:HB2	0.50	1.83	2	1
2:A:147:TYR:CD1	2:A:147:TYR:N	0.50	2.79	7	4
2:A:181:GLY:O	2:A:203:LEU:HD21	0.50	2.06	4	2
2:A:239:LEU:O	2:A:242:MET:HB3	0.50	2.06	3	6
2:A:254:LEU:C	2:A:254:LEU:HD22	0.50	2.27	3	2
1:B:508:A:H62	2:A:183:VAL:HG13	0.50	1.65	9	2
2:A:150:ILE:HG22	2:A:151:ASN:H	0.50	1.67	3	10
2:A:228:GLN:HA	2:A:232:THR:HA	0.50	1.84	9	5
2:A:155:LEU:HD13	2:A:243:GLN:HB3	0.50	1.84	2	7
2:A:242:MET:HE3	2:A:245:ARG:HB3	0.50	1.83	6	1
2:A:245:ARG:NH1	2:A:249:ARG:HG2	0.50	2.21	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:508:A:O3'	2:A:160:ARG:HD3	0.50	2.07	4	10
1:B:511:A:N1	2:A:178:ARG:HG3	0.50	2.22	4	2
1:B:510:A:N3	1:B:511:A:H2'	0.49	2.22	9	3
2:A:223:ARG:HH11	2:A:223:ARG:HA	0.49	1.67	5	1
2:A:144:GLN:HG2	2:A:148:PRO:O	0.49	2.07	8	5
2:A:142:ILE:HG13	2:A:226:LEU:CD1	0.49	2.37	9	1
2:A:156:LEU:CA	2:A:225:ILE:HG21	0.49	2.37	4	1
2:A:147:TYR:N	2:A:147:TYR:CD1	0.49	2.81	5	3
2:A:207:VAL:HG12	2:A:215:VAL:HG23	0.49	1.84	5	1
2:A:157:ILE:HG23	2:A:161:GLY:HA2	0.49	1.84	1	6
2:A:254:LEU:HD22	2:A:254:LEU:C	0.49	2.28	8	2
1:B:502:A:H1'	1:B:503:U:OP1	0.49	2.08	10	2
2:A:161:GLY:CA	2:A:164:LEU:HD12	0.49	2.38	1	9
1:B:511:A:C5	2:A:196:LEU:HD13	0.49	2.43	3	8
2:A:156:LEU:HD12	2:A:156:LEU:O	0.49	2.08	2	1
1:B:505:C:N3	2:A:244:LEU:HD11	0.49	2.23	8	9
2:A:156:LEU:HD22	2:A:156:LEU:O	0.49	2.08	1	1
2:A:234:GLU:HA	2:A:237:ASN:HD22	0.48	1.68	3	1
2:A:232:THR:HG1	2:A:237:ASN:HA	0.48	1.68	7	1
2:A:156:LEU:CD1	2:A:222:ILE:HG23	0.48	2.38	10	1
2:A:223:ARG:O	2:A:227:LYS:HB2	0.48	2.08	9	2
1:B:505:C:H1'	1:B:506:U:C5	0.48	2.42	2	6
1:B:507:A:N3	2:A:184:LYS:HB2	0.48	2.23	3	2
1:B:507:A:N3	2:A:184:LYS:HD3	0.48	2.24	3	1
2:A:245:ARG:NH1	2:A:254:LEU:HG	0.48	2.24	3	1
2:A:232:THR:HG23	2:A:240:ARG:HA	0.48	1.85	3	4
2:A:246:GLU:O	2:A:250:LEU:HB2	0.48	2.09	8	7
2:A:142:ILE:HD13	2:A:203:LEU:O	0.48	2.09	4	3
2:A:177:ILE:HB	2:A:182:SER:HB3	0.48	1.85	9	1
1:B:507:A:C2	2:A:184:LYS:HG2	0.48	2.44	6	1
2:A:230:ILE:N	2:A:230:ILE:HD13	0.47	2.24	2	3
2:A:149:GLU:O	2:A:150:ILE:O	0.47	2.32	6	6
1:B:511:A:N6	2:A:182:SER:HB2	0.47	2.24	9	1
1:B:507:A:H61	2:A:153:VAL:HG13	0.47	1.68	9	1
2:A:168:GLU:O	2:A:172:ASN:HA	0.47	2.09	7	5
1:B:508:A:H2'	1:B:509:C:C6	0.47	2.44	1	10
2:A:207:VAL:HG21	2:A:222:ILE:CD1	0.47	2.40	9	4
2:A:151:ASN:O	2:A:155:LEU:N	0.47	2.48	3	9
2:A:174:LYS:O	2:A:207:VAL:HA	0.47	2.09	3	3
2:A:245:ARG:HD3	2:A:254:LEU:HG	0.47	1.85	10	1
1:B:502:A:H4'	1:B:503:U:OP2	0.47	2.09	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:504:A:O2'	2:A:244:LEU:HB3	0.47	2.10	4	3
2:A:230:ILE:H	2:A:230:ILE:HD13	0.47	1.69	3	1
2:A:240:ARG:C	2:A:242:MET:H	0.47	2.13	2	1
2:A:195:MET:HG2	2:A:195:MET:O	0.47	2.09	7	1
2:A:165:LYS:O	2:A:169:LYS:HB3	0.47	2.10	8	1
2:A:157:ILE:HA	2:A:164:LEU:CD2	0.46	2.40	9	6
2:A:160:ARG:C	2:A:160:ARG:HD2	0.46	2.29	6	5
1:B:502:A:H4'	1:B:503:U:C6	0.46	2.46	2	1
2:A:150:ILE:HD12	2:A:152:PHE:CZ	0.46	2.45	9	2
2:A:151:ASN:CG	2:A:155:LEU:HD11	0.46	2.30	8	2
2:A:150:ILE:HG22	2:A:151:ASN:OD1	0.46	2.10	7	1
2:A:157:ILE:CG1	2:A:164:LEU:HD21	0.46	2.41	8	6
2:A:142:ILE:HG21	2:A:203:LEU:HD12	0.46	1.87	9	1
2:A:156:LEU:N	2:A:225:ILE:HG21	0.46	2.25	4	1
2:A:183:VAL:HG11	2:A:196:LEU:HD21	0.46	1.88	3	1
2:A:230:ILE:HD13	2:A:230:ILE:N	0.46	2.26	7	1
2:A:160:ARG:HD2	2:A:160:ARG:C	0.46	2.31	1	5
2:A:211:THR:HG23	2:A:214:ASN:H	0.46	1.71	6	3
2:A:151:ASN:O	2:A:152:PHE:C	0.45	2.55	2	5
1:B:506:U:O2'	1:B:507:A:H5'	0.45	2.11	2	1
2:A:149:GLU:HB3	2:A:203:LEU:HG	0.45	1.88	5	1
2:A:248:ALA:HB1	2:A:254:LEU:N	0.45	2.27	5	1
2:A:149:GLU:O	2:A:150:ILE:C	0.45	2.54	10	7
2:A:147:TYR:HE2	2:A:231:GLU:HB2	0.45	1.72	2	2
2:A:175:ILE:O	2:A:176:MET:HG3	0.45	2.12	3	2
2:A:139:LYS:HG3	2:A:204:HIS:CB	0.45	2.40	8	7
2:A:140:VAL:O	2:A:142:ILE:HD12	0.45	2.11	9	1
1:B:505:C:OP1	2:A:253:THR:HG21	0.45	2.12	8	1
2:A:243:GLN:O	2:A:246:GLU:HG2	0.45	2.12	4	1
2:A:223:ARG:HB3	2:A:227:LYS:HG3	0.45	1.88	5	2
2:A:242:MET:O	2:A:242:MET:HE3	0.45	2.12	8	1
1:B:502:A:H5'	1:B:503:U:H5	0.45	1.71	7	1
1:B:504:A:C5	2:A:255:ARG:HD2	0.45	2.47	8	1
2:A:156:LEU:O	2:A:156:LEU:HD12	0.45	2.12	4	1
2:A:163:THR:O	2:A:167:ILE:HG12	0.45	2.12	10	3
2:A:221:GLN:O	2:A:224:ASN:HB3	0.45	2.12	10	1
2:A:226:LEU:HD13	2:A:227:LYS:N	0.44	2.27	2	2
1:B:507:A:H2'	2:A:184:LYS:HD3	0.44	1.88	3	1
1:B:501:U:H2'	1:B:503:U:C5	0.44	2.47	3	1
1:B:505:C:C4'	1:B:506:U:H5'	0.44	2.42	1	2
2:A:240:ARG:HG3	2:A:241:LYS:N	0.44	2.27	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:136:VAL:HG21	2:A:212:MET:HA	0.44	1.90	4	2
2:A:162:ASN:ND2	2:A:250:LEU:HD13	0.44	2.27	4	1
2:A:151:ASN:CB	2:A:155:LEU:HG	0.44	2.42	1	1
2:A:164:LEU:O	2:A:168:GLU:HG3	0.44	2.13	2	1
2:A:155:LEU:CD2	2:A:243:GLN:HB3	0.44	2.39	2	3
1:B:505:C:C5'	1:B:506:U:H5'	0.44	2.42	1	1
2:A:226:LEU:O	2:A:227:LYS:C	0.43	2.56	9	2
1:B:502:A:H4'	1:B:503:U:H6	0.43	1.71	2	1
1:B:507:A:H3'	2:A:184:LYS:HZ2	0.43	1.73	5	1
2:A:155:LEU:HB3	2:A:243:GLN:HB3	0.43	1.89	5	1
1:B:502:A:H3'	2:A:255:ARG:NE	0.43	2.29	6	2
2:A:156:LEU:CD2	2:A:222:ILE:HG23	0.43	2.42	9	2
2:A:240:ARG:HD2	2:A:241:LYS:HD2	0.43	1.88	9	1
1:B:506:U:OP2	1:B:506:U:H6	0.43	1.96	8	2
2:A:217:LYS:HG3	2:A:218:ALA:N	0.43	2.28	2	1
2:A:157:ILE:HG23	2:A:164:LEU:CD1	0.43	2.43	10	5
1:B:501:U:O2'	1:B:503:U:H5'	0.43	2.13	6	2
2:A:240:ARG:HG3	2:A:241:LYS:H	0.43	1.72	9	2
2:A:254:LEU:HD22	2:A:255:ARG:HG2	0.43	1.90	5	2
2:A:254:LEU:O	2:A:255:ARG:HG3	0.43	2.13	8	1
2:A:139:LYS:CG	2:A:204:HIS:HB2	0.43	2.42	10	6
2:A:232:THR:CG2	2:A:240:ARG:HA	0.43	2.44	5	3
2:A:151:ASN:O	2:A:154:GLY:N	0.43	2.51	5	3
2:A:171:CYS:SG	2:A:217:LYS:HE2	0.43	2.53	6	3
2:A:156:LEU:HD11	2:A:177:ILE:HD11	0.43	1.89	4	1
2:A:159:PRO:HD2	2:A:162:ASN:ND2	0.43	2.27	4	1
1:B:507:A:H1'	1:B:508:A:C8	0.43	2.49	9	1
2:A:136:VAL:HG11	2:A:211:THR:C	0.43	2.34	9	1
2:A:135:ARG:HH12	2:A:174:LYS:HD2	0.43	1.72	9	1
2:A:166:ASN:O	2:A:169:LYS:HG2	0.43	2.14	8	1
2:A:209:ALA:HB3	2:A:215:VAL:HB	0.43	1.89	10	3
1:B:511:A:C6	2:A:196:LEU:HD13	0.43	2.49	5	1
2:A:157:ILE:O	2:A:163:THR:N	0.43	2.52	8	2
2:A:212:MET:HA	2:A:215:VAL:HG12	0.42	1.90	10	2
2:A:156:LEU:O	2:A:156:LEU:HD22	0.42	2.14	9	1
2:A:151:ASN:HB3	2:A:155:LEU:HG	0.42	1.91	1	1
2:A:254:LEU:HD13	2:A:255:ARG:H	0.42	1.75	3	1
2:A:140:VAL:O	2:A:204:HIS:HA	0.42	2.14	2	1
2:A:230:ILE:HD13	2:A:230:ILE:H	0.42	1.74	5	1
2:A:146:GLU:HB3	2:A:147:TYR:CD1	0.42	2.50	6	1
1:B:508:A:H62	2:A:183:VAL:HG12	0.42	1.75	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:214:ASN:O	2:A:217:LYS:HG2	0.42	2.14	6	1
2:A:176:MET:O	2:A:206:LEU:HB2	0.42	2.14	9	1
2:A:142:ILE:HB	2:A:203:LEU:O	0.42	2.14	5	2
2:A:144:GLN:HG3	2:A:203:LEU:HB2	0.42	1.92	9	2
2:A:245:ARG:HH11	2:A:249:ARG:HB2	0.42	1.74	3	1
1:B:505:C:H4'	1:B:506:U:H5'	0.42	1.92	1	2
2:A:228:GLN:HB3	2:A:232:THR:CB	0.41	2.46	1	2
2:A:157:ILE:HG22	2:A:158:GLY:N	0.41	2.29	2	3
2:A:255:ARG:H	2:A:255:ARG:HG2	0.41	1.37	5	1
2:A:137:SER:HB3	2:A:208:THR:HG23	0.41	1.92	10	1
2:A:151:ASN:OD1	2:A:230:ILE:HG23	0.41	2.16	3	1
2:A:236:GLN:HB2	2:A:239:LEU:HB2	0.41	1.91	3	1
1:B:511:A:N6	2:A:183:VAL:HG22	0.41	2.30	8	1
1:B:502:A:C2'	2:A:255:ARG:HA	0.41	2.44	7	1
2:A:150:ILE:HG22	2:A:151:ASN:N	0.41	2.30	7	3
2:A:218:ALA:O	2:A:222:ILE:HG13	0.41	2.16	10	2
1:B:502:A:O2'	2:A:255:ARG:HD2	0.41	2.16	9	1
1:B:502:A:N7	2:A:253:THR:HA	0.41	2.30	2	1
2:A:242:MET:HE2	2:A:242:MET:O	0.41	2.15	2	1
2:A:254:LEU:HD13	2:A:255:ARG:N	0.41	2.30	2	1
2:A:140:VAL:HG23	2:A:223:ARG:NE	0.41	2.30	3	1
2:A:147:TYR:HB2	2:A:152:PHE:HE2	0.41	1.76	8	1
2:A:228:GLN:O	2:A:229:GLY:C	0.41	2.60	8	1
2:A:149:GLU:HB3	2:A:203:LEU:CG	0.40	2.47	10	1
2:A:240:ARG:C	2:A:242:MET:N	0.40	2.75	2	1
2:A:224:ASN:O	2:A:228:GLN:HG3	0.40	2.16	3	1
2:A:184:LYS:CD	2:A:184:LYS:C	0.40	2.89	9	1
2:A:151:ASN:HB2	2:A:155:LEU:CD2	0.40	2.46	5	1
2:A:177:ILE:C	2:A:182:SER:HB3	0.40	2.37	10	1
2:A:195:MET:HE1	2:A:196:LEU:CD2	0.40	2.44	3	1
2:A:164:LEU:HB3	2:A:175:ILE:HB	0.40	1.94	7	1
2:A:150:ILE:CG2	2:A:151:ASN:H	0.40	2.28	2	1
2:A:159:PRO:HD2	2:A:162:ASN:CG	0.40	2.37	4	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	
2	A	110/131 (84%)	80±2 (73±2%)	22±2 (20±2%)	7±1 (7±1%)	3	19
All	All	1100/1310 (84%)	803 (73%)	224 (20%)	73 (7%)	3	19

All 17 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	A	203	LEU	10
2	A	150	ILE	10
2	A	148	PRO	10
2	A	161	GLY	10
2	A	202	PRO	8
2	A	149	GLU	5
2	A	254	LEU	4
2	A	233	PRO	3
2	A	184	LYS	2
2	A	198	GLY	2
2	A	236	GLN	2
2	A	180	LYS	2
2	A	197	PRO	1
2	A	237	ASN	1
2	A	199	GLU	1
2	A	232	THR	1
2	A	181	GLY	1

6.3.2 Protein sidechains ⓘ

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	
2	A	99/112 (88%)	66±3 (67±3%)	33±3 (33±3%)	1	12
All	All	990/1120 (88%)	660 (67%)	330 (33%)	1	12

All 72 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)
2	A	208	THR	10
2	A	139	LYS	10
2	A	203	LEU	10
2	A	253	THR	10
2	A	196	LEU	10
2	A	247	LEU	10
2	A	244	LEU	10
2	A	219	VAL	10
2	A	171	CYS	9
2	A	149	GLU	9
2	A	180	LYS	8
2	A	216	LYS	8
2	A	249	ARG	8
2	A	137	SER	8
2	A	245	ARG	8
2	A	147	TYR	8
2	A	182	SER	7
2	A	232	THR	7
2	A	230	ILE	7
2	A	165	LYS	6
2	A	151	ASN	6
2	A	250	LEU	6
2	A	241	LYS	6
2	A	195	MET	6
2	A	138	ASP	5
2	A	255	ARG	5
2	A	242	MET	5
2	A	200	ASP	5
2	A	211	THR	5
2	A	236	GLN	5
2	A	184	LYS	5
2	A	240	ARG	5
2	A	234	GLU	5
2	A	169	LYS	4
2	A	226	LEU	4
2	A	254	LEU	4
2	A	174	LYS	4
2	A	228	GLN	4
2	A	135	ARG	3
2	A	238	ASP	3
2	A	243	GLN	3
2	A	172	ASN	3
2	A	170	GLU	3

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Mol	Chain	Res	Type	Models (Total)
2	A	201	GLU	3
2	A	213	GLU	3
2	A	178	ARG	3
2	A	235	ASP	3
2	A	183	VAL	3
2	A	237	ASN	3
2	A	145	ASP	3
2	A	141	MET	3
2	A	227	LYS	2
2	A	166	ASN	2
2	A	168	GLU	2
2	A	221	GLN	2
2	A	239	LEU	2
2	A	156	LEU	2
2	A	251	ASN	2
2	A	146	GLU	2
2	A	144	GLN	1
2	A	199	GLU	1
2	A	246	GLU	1
2	A	212	MET	1
2	A	134	THR	1
2	A	164	LEU	1
2	A	153	VAL	1
2	A	206	LEU	1
2	A	162	ASN	1
2	A	175	ILE	1
2	A	204	HIS	1
2	A	217	LYS	1
2	A	176	MET	1

6.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	B	11/11 (100%)	8±1 (70±7%)	3±1 (23±9%)	0.22±0.12
All	All	104/110 (95%)	77 (74%)	25 (24%)	0.21

The overall RNA backbone suiteness is 0.22.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	508	A	10

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Mol	Chain	Res	Type	Models (Total)
1	B	502	A	10
1	B	511	A	10
1	B	507	A	10
1	B	503	U	10
1	B	506	U	10
1	B	504	A	10
1	B	510	A	4
1	B	505	C	2
1	B	509	C	1

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	507	A	10
1	B	505	C	7
1	B	501	U	4
1	B	503	U	2
1	B	502	A	2

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 carbohydrates 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

No chemical shift data were provided