Full wwPDB NMR Structure Validation Report (i)

Mar 6, 2022 – 02:18 PM EST

PDB ID	:	2P89
Title	:	Solution structure of the 3' pseudouridyation pocket of U65 snoRNA with bound substrate
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Deposited on	:	2007-03-22

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

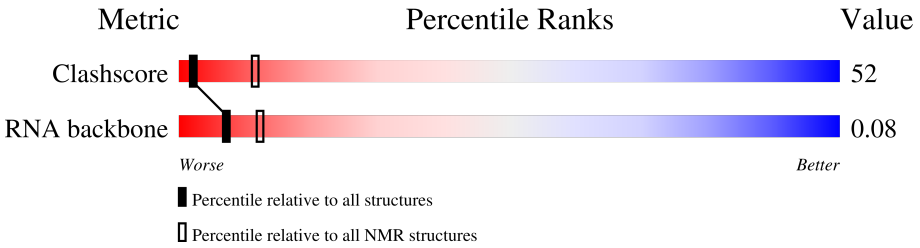
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 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	158937	12864
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	34	44% 44% 12%
2	B	14	36% 57% 7%

2 Ensemble composition and analysis (i)

This entry contains 20 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1530 atoms, of which 519 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called U65 H/ACA snoRNA.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	34	1095	325	369	133	235	33	0

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	14	435	129	150	42	101	13	0

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: U65 H/ACA snoRNA

Chain A: 44% 44% 12%

G1 G2 C3 C4 U5 U6 A7 G8 G9 A10 A11 A12 C13 A14 G15 U16 U17 C18 G19 C20 U21 G22 U23 G24 C25 C26 G27 A28 A29 A30 G31 G32 U33 C34

• Molecule 2: 28S rRNA

Chain B: 36% 57% 7%

U35 U36 C37 G38 G39 C40 U41 C42 U43 U44 C45 C46 U47 A48

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: U65 H/ACA snoRNA

Chain A: 6% 41% 32% 21%

G1 G2 C3 C4 U5 U6 A7 G8 G9 A10 A11 A12 C13 A14 G15 U16 U17 C18 G19 C20 U21 G22 U23 G24 C25 C26 G27 A28 A29 A30 G31 G32 U33 C34

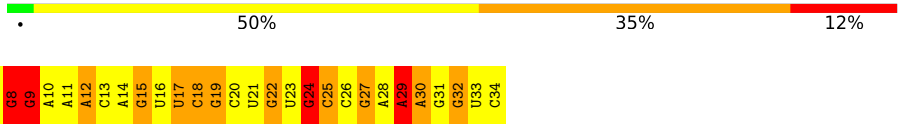
• Molecule 2: 28S rRNA

Chain B: 14% 14% 50% 21%

U35 U36 C37 G38 G39 C40 U41 C42 U43 U44 C45 C46 U47 A48

4.2.2 Score per residue for model 2

- Molecule 1: U65 H/ACA snoRNA

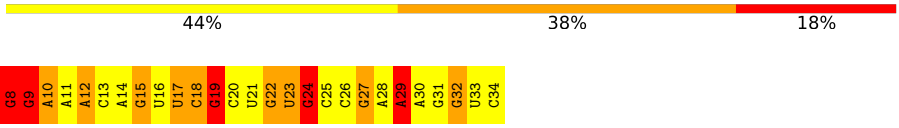
Chain A: 

- Molecule 2: 28S rRNA

Chain B:

4.2.3 Score per residue for model 3

- Molecule 1: U65 H/ACA snoRNA

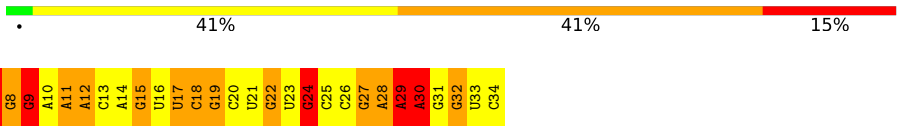
Chain A: 

- Molecule 2: 28S rRNA

Chain B:

4.2.4 Score per residue for model 4

- Molecule 1: U65 H/ACA snoRNA

Chain A: 

- Molecule 2: 28S rRNA

Chain B:

4.2.5 Score per residue for model 5

- Molecule 1: U65 H/ACA snoRNA

Chain A: 38% 44% 15%

- Molecule 2: 28S rRNA

Chain B: 14% 36% 36% 14%

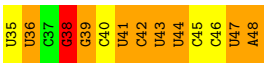
4.2.6 Score per residue for model 6

- Molecule 1: U65 H/ACA snoRNA

Chain A: 6% 41% 41% 12%

- Molecule 2: 28S rRNA

Chain B: 7% 29% 57% 7%



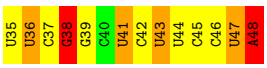
4.2.7 Score per residue for model 7

- Molecule 1: U65 H/ACA snoRNA

Chain A: 47% 41% 12%

- Molecule 2: 28S rRNA

Chain B: 7% 50% 29% 14%



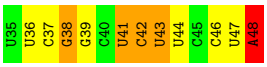
4.2.8 Score per residue for model 8

- Molecule 1: U65 H/ACA snoRNA

Chain A: 50% 35% 15%

- Molecule 2: 28S rRNA

Chain B: 21% 43% 29% 7%



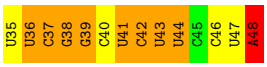
4.2.9 Score per residue for model 9

- Molecule 1: U65 H/ACA snoRNA

Chain A: 47% 38% 15%

- Molecule 2: 28S rRNA

Chain B: 7% 29% 57% 7%



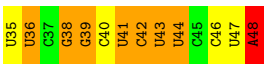
4.2.10 Score per residue for model 10

- Molecule 1: U65 H/ACA snoRNA

Chain A: 47% 35% 15%

- Molecule 2: 28S rRNA

Chain B: 14% 29% 50% 7%



4.2.11 Score per residue for model 11

- Molecule 1: U65 H/ACA snoRNA

Chain A: 44% 38% 15%

- Molecule 2: 28S rRNA

Chain B: 43% 43% 14%

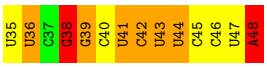
4.2.12 Score per residue for model 12

- Molecule 1: U65 H/ACA snoRNA

Chain A: 38% 47% 12%

- Molecule 2: 28S rRNA

Chain B: 7% 36% 43% 14%



4.2.13 Score per residue for model 13

- Molecule 1: U65 H/ACA snoRNA

Chain A: 38% 50% 12%

- Molecule 2: 28S rRNA

Chain B: 14% 43% 29% 14%

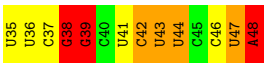
4.2.14 Score per residue for model 14

- Molecule 1: U65 H/ACA snoRNA

Chain A: 44% 38% 15%

- Molecule 2: 28S rRNA

Chain B: 14% 36% 29% 21%



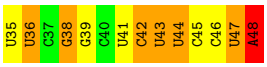
4.2.15 Score per residue for model 15

- Molecule 1: U65 H/ACA snoRNA

Chain A: 47% 41% 9%

- Molecule 2: 28S rRNA

Chain B: 14% 36% 43% 7%



4.2.16 Score per residue for model 16

- Molecule 1: U65 H/ACA snoRNA

Chain A: 6% 35% 47% 12%

- Molecule 2: 28S rRNA

Chain B: 7% 71% 14% 7%

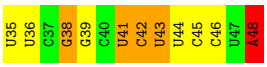
4.2.17 Score per residue for model 17

- Molecule 1: U65 H/ACA snoRNA

Chain A:

- Molecule 2: 28S rRNA

Chain B:

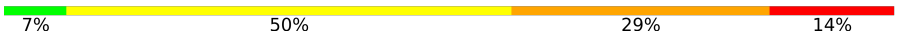


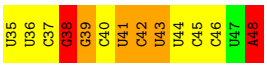
4.2.18 Score per residue for model 18

- Molecule 1: U65 H/ACA snoRNA

Chain A:

- Molecule 2: 28S rRNA

Chain B: 



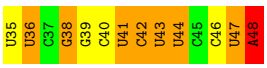
4.2.19 Score per residue for model 19

- Molecule 1: U65 H/ACA snoRNA

Chain A:

- Molecule 2: 28S rRNA

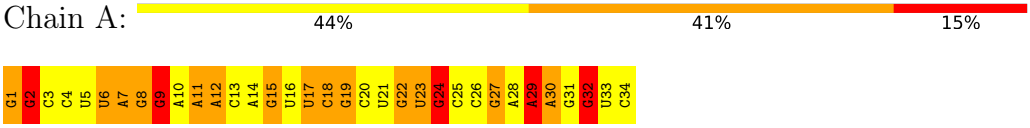
Chain B:



4.2.20 Score per residue for model 20

- Molecule 1: U65 H/ACA snoRNA

Chain A:



- Molecule 2: 28S rRNA

Chain B:

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
X-PLOR	refinement	NIH

No chemical shift data was provided.

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	A	1.11±0.00	0±0/812 (0.0± 0.0%)	1.98±0.00	47±1/1265 (3.7± 0.1%)
2	B	1.04±0.00	0±0/315 (0.0± 0.0%)	1.68±0.01	7±1/487 (1.5± 0.1%)
All	All	1.09	0/22540 (0.0%)	1.90	1093/35040 (3.1%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	19	G	N7-C8-N9	9.41	117.80	113.10	8	20
1	A	9	G	N7-C8-N9	9.37	117.79	113.10	14	20
1	A	22	G	N7-C8-N9	9.36	117.78	113.10	3	20
1	A	2	G	N7-C8-N9	9.34	117.77	113.10	5	20
1	A	31	G	N7-C8-N9	9.34	117.77	113.10	11	20
1	A	15	G	N7-C8-N9	9.34	117.77	113.10	6	20
1	A	32	G	N7-C8-N9	9.27	117.73	113.10	3	20
1	A	1	G	N7-C8-N9	9.24	117.72	113.10	16	20
1	A	8	G	N7-C8-N9	9.21	117.71	113.10	15	20
2	B	39	G	N7-C8-N9	9.20	117.70	113.10	20	20
1	A	27	G	N7-C8-N9	9.17	117.68	113.10	3	20
1	A	24	G	N7-C8-N9	9.16	117.68	113.10	2	20
2	B	38	G	N7-C8-N9	9.11	117.66	113.10	5	20
1	A	12	A	N7-C8-N9	7.93	117.76	113.80	3	20
1	A	30	A	N7-C8-N9	7.68	117.64	113.80	20	20
1	A	14	A	N7-C8-N9	7.66	117.63	113.80	8	20
1	A	7	A	N7-C8-N9	7.64	117.62	113.80	6	20
1	A	10	A	N7-C8-N9	7.64	117.62	113.80	18	20
1	A	29	A	N7-C8-N9	7.64	117.62	113.80	11	20
2	B	48	A	N7-C8-N9	7.56	117.58	113.80	18	20
1	A	11	A	N7-C8-N9	7.54	117.57	113.80	9	20
1	A	28	A	N7-C8-N9	7.54	117.57	113.80	10	20
1	A	2	G	C8-N9-C4	-6.90	103.64	106.40	5	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	32	G	C8-N9-C4	-6.87	103.65	106.40	3	20
1	A	15	G	C8-N9-C4	-6.85	103.66	106.40	15	20
1	A	27	G	C8-N9-C4	-6.85	103.66	106.40	3	20
1	A	1	G	C8-N9-C4	-6.82	103.67	106.40	11	20
1	A	31	G	C8-N9-C4	-6.78	103.69	106.40	11	20
1	A	19	G	C8-N9-C4	-6.75	103.70	106.40	8	20
1	A	22	G	C8-N9-C4	-6.75	103.70	106.40	4	20
1	A	9	G	C8-N9-C4	-6.75	103.70	106.40	16	20
1	A	8	G	C8-N9-C4	-6.71	103.72	106.40	1	20
2	B	39	G	C8-N9-C4	-6.68	103.73	106.40	10	20
1	A	24	G	C8-N9-C4	-6.67	103.73	106.40	17	20
2	B	38	G	C8-N9-C4	-6.63	103.75	106.40	10	20
1	A	14	A	C8-N9-C4	-5.96	103.42	105.80	15	20
1	A	11	A	C8-N9-C4	-5.82	103.47	105.80	15	20
1	A	30	A	C8-N9-C4	-5.80	103.48	105.80	10	20
1	A	10	A	C8-N9-C4	-5.71	103.52	105.80	20	20
1	A	7	A	C8-N9-C4	-5.70	103.52	105.80	6	20
1	A	28	A	C8-N9-C4	-5.67	103.53	105.80	17	20
2	B	48	A	C8-N9-C4	-5.65	103.54	105.80	17	20
1	A	29	A	C8-N9-C4	-5.62	103.55	105.80	2	20
1	A	12	A	C8-N9-C4	-5.43	103.63	105.80	8	19
1	A	22	G	C5-N7-C8	-5.33	101.64	104.30	3	20
1	A	19	G	C5-N7-C8	-5.30	101.65	104.30	8	19
1	A	15	G	C5-N7-C8	-5.29	101.65	104.30	6	19
1	A	9	G	C5-N7-C8	-5.26	101.67	104.30	14	17
1	A	8	G	C5-N7-C8	-5.25	101.67	104.30	17	18
1	A	2	G	C5-N7-C8	-5.24	101.68	104.30	1	14
2	B	38	G	C5-N7-C8	-5.24	101.68	104.30	13	14
1	A	1	G	C5-N7-C8	-5.23	101.68	104.30	20	15
1	A	31	G	C5-N7-C8	-5.22	101.69	104.30	7	16
2	B	39	G	C5-N7-C8	-5.21	101.69	104.30	17	14
1	A	32	G	C5-N7-C8	-5.18	101.71	104.30	14	14
1	A	24	G	C5-N7-C8	-5.18	101.71	104.30	19	17
1	A	27	G	C5-N7-C8	-5.17	101.72	104.30	2	14
1	A	12	A	C5-N7-C8	-5.11	101.34	103.90	3	3

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	726	369	369	62±5
2	B	285	150	150	19±4
All	All	20220	10380	10380	1588

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 52.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:G:H2'	1:A:20:C:O4'	0.98	1.58	11	20
1:A:25:C:O2'	1:A:26:C:H5'	0.97	1.59	1	11
2:B:42:C:H5"	2:B:43:U:OP2	0.92	1.64	8	10
2:B:35:U:HO5'	2:B:35:U:H6	0.92	0.96	19	6
2:B:40:C:H2'	2:B:42:C:OP2	0.90	1.67	13	1
2:B:35:U:H6	2:B:35:U:HO5'	0.89	0.92	9	4
1:A:26:C:H2'	1:A:27:G:O4'	0.85	1.71	7	17
1:A:21:U:H2'	1:A:22:G:O4'	0.81	1.75	1	20
1:A:19:G:O2'	1:A:20:C:H5'	0.81	1.75	20	20
1:A:4:C:O5'	1:A:4:C:H6	0.77	1.62	7	19
2:B:36:U:H6	2:B:36:U:O5'	0.77	1.62	19	20
1:A:23:U:H5"	1:A:24:G:OP2	0.75	1.82	20	1
1:A:32:G:C5	1:A:33:U:C5	0.74	2.76	1	18
1:A:24:G:H8	1:A:24:G:O5'	0.74	1.64	12	6
2:B:35:U:H6	2:B:35:U:O5'	0.74	1.65	13	7
1:A:17:U:H6	1:A:17:U:O5'	0.74	1.65	15	10
1:A:15:G:C6	1:A:16:U:C4	0.74	2.76	4	20
2:B:42:C:H6	2:B:42:C:O5'	0.74	1.65	12	12
1:A:9:G:H8	1:A:9:G:O5'	0.74	1.66	4	20
2:B:43:U:O5'	2:B:43:U:H6	0.73	1.64	14	7
1:A:33:U:O2'	1:A:34:C:H5'	0.73	1.83	19	2
1:A:2:G:C6	1:A:3:C:C4	0.73	2.77	20	20
1:A:17:U:O2'	1:A:18:C:H5'	0.73	1.84	2	16
1:A:20:C:O5'	1:A:20:C:H6	0.73	1.67	20	20
1:A:32:G:C5	1:A:33:U:C4	0.73	2.77	12	18
1:A:2:G:C5	1:A:3:C:C5	0.72	2.77	5	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:G:C6	1:A:25:C:N4	0.72	2.58	18	9
1:A:32:G:N7	1:A:33:U:C5	0.72	2.58	15	17
1:A:24:G:C6	1:A:25:C:C4	0.72	2.78	18	8
1:A:15:G:C6	1:A:16:U:N3	0.72	2.58	7	20
1:A:16:U:C4	1:A:18:C:N4	0.71	2.58	17	11
1:A:24:G:H4'	1:A:24:G:OP1	0.71	1.84	20	3
1:A:19:G:N2	1:A:20:C:C4	0.71	2.59	19	20
1:A:1:G:C2	1:A:2:G:C8	0.71	2.79	16	6
1:A:16:U:O2'	1:A:17:U:C5	0.70	2.45	5	20
1:A:11:A:C6	1:A:12:A:C4	0.70	2.79	10	9
2:B:42:C:O2'	2:B:43:U:P	0.70	2.48	9	2
1:A:16:U:O2'	1:A:17:U:C6	0.70	2.45	3	20
2:B:40:C:HO2'	2:B:41:U:H5	0.69	1.27	6	1
1:A:24:G:O6	2:B:43:U:H5"	0.69	1.87	8	5
2:B:46:C:H6	2:B:46:C:O5'	0.69	1.70	1	20
1:A:30:A:C2	1:A:31:G:C8	0.68	2.81	5	7
1:A:5:U:H5"	1:A:6:U:OP1	0.68	1.87	8	2
2:B:41:U:H6	2:B:41:U:O5'	0.68	1.72	3	9
1:A:26:C:O5'	1:A:26:C:H6	0.68	1.72	11	11
1:A:24:G:N2	2:B:42:C:N3	0.68	2.40	12	2
1:A:24:G:H8	1:A:24:G:OP2	0.68	1.71	14	1
1:A:16:U:C5	1:A:18:C:N4	0.68	2.62	17	8
2:B:43:U:OP2	2:B:43:U:H6	0.68	1.72	17	1
1:A:11:A:N6	1:A:12:A:C6	0.67	2.62	10	2
1:A:15:G:C5	1:A:16:U:C5	0.67	2.82	11	20
2:B:48:A:H8	2:B:48:A:O5'	0.67	1.73	7	20
1:A:1:G:O5'	1:A:1:G:C8	0.67	2.46	3	2
1:A:11:A:C6	1:A:12:A:C5	0.67	2.82	10	3
1:A:5:U:H4'	1:A:6:U:OP1	0.66	1.90	13	2
1:A:32:G:C6	1:A:33:U:C4	0.66	2.83	13	18
1:A:18:C:H4'	1:A:19:G:O5'	0.66	1.90	17	15
1:A:19:G:N2	1:A:20:C:C5	0.66	2.64	1	17
1:A:2:G:C6	1:A:3:C:N4	0.65	2.63	9	14
1:A:2:G:C5	1:A:3:C:C4	0.65	2.85	3	15
1:A:32:G:N7	1:A:33:U:C4	0.65	2.65	16	9
1:A:29:A:H8	1:A:29:A:O5'	0.64	1.74	12	20
1:A:17:U:O2'	1:A:18:C:C5'	0.64	2.45	17	16
1:A:32:G:C8	1:A:33:U:C5	0.64	2.85	16	16
1:A:33:U:N3	1:A:34:C:C5	0.64	2.65	19	3
1:A:18:C:O4'	1:A:19:G:C2	0.64	2.51	1	20
2:B:44:U:H6	2:B:44:U:O5'	0.64	1.74	2	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:G:C5	1:A:25:C:C5	0.63	2.86	18	7
1:A:15:G:N1	1:A:16:U:C2	0.63	2.67	9	20
1:A:20:C:O5'	1:A:20:C:C6	0.62	2.53	3	20
2:B:43:U:OP1	2:B:43:U:C6	0.62	2.53	2	6
2:B:42:C:O5'	2:B:42:C:C6	0.62	2.53	12	6
1:A:9:G:O5'	1:A:9:G:C8	0.62	2.53	2	20
2:B:40:C:C5	2:B:42:C:OP2	0.62	2.53	16	1
2:B:40:C:O2	2:B:42:C:C5	0.61	2.53	19	2
1:A:30:A:C6	1:A:31:G:N7	0.61	2.68	6	2
1:A:30:A:H8	1:A:30:A:O5'	0.61	1.78	8	6
2:B:40:C:O2'	2:B:41:U:H5	0.61	1.79	6	1
2:B:45:C:O2'	2:B:46:C:C5'	0.60	2.49	16	4
2:B:43:U:OP2	2:B:43:U:C6	0.60	2.54	17	1
1:A:24:G:O6	1:A:25:C:N4	0.60	2.34	5	7
1:A:5:U:H5"	1:A:6:U:OP2	0.60	1.96	16	1
2:B:39:G:C6	2:B:40:C:N4	0.60	2.70	1	3
2:B:43:U:C6	2:B:43:U:OP2	0.60	2.54	16	1
1:A:16:U:C4	1:A:18:C:C4	0.60	2.89	11	8
1:A:16:U:N3	1:A:18:C:C4	0.60	2.69	19	9
1:A:1:G:O5'	1:A:1:G:H8	0.60	1.79	3	3
1:A:24:G:N2	2:B:42:C:C4	0.60	2.70	14	4
1:A:2:G:O6	1:A:3:C:N4	0.60	2.34	8	14
1:A:24:G:O5'	1:A:24:G:C8	0.60	2.54	12	4
1:A:33:U:O4	1:A:34:C:N4	0.60	2.35	19	2
1:A:1:G:C2	1:A:2:G:N7	0.59	2.70	11	3
1:A:17:U:O2	1:A:19:G:N7	0.59	2.35	13	6
2:B:47:U:H6	2:B:47:U:O5'	0.59	1.81	2	18
1:A:25:C:H6	1:A:25:C:O5'	0.59	1.81	3	7
2:B:43:U:O2'	2:B:44:U:O5'	0.59	2.21	6	6
2:B:45:C:O2'	2:B:46:C:O4'	0.59	2.21	11	12
1:A:5:U:O2'	2:B:35:U:O5'	0.59	2.18	9	1
1:A:20:C:O2'	1:A:21:U:H5'	0.58	1.98	18	16
2:B:40:C:O2	2:B:42:C:N4	0.58	2.35	4	3
1:A:1:G:C8	1:A:1:G:O5'	0.58	2.50	4	3
1:A:15:G:H2'	1:A:16:U:O4'	0.58	1.99	17	20
1:A:17:U:O5'	1:A:17:U:C6	0.58	2.55	15	7
1:A:32:G:C6	1:A:33:U:N3	0.58	2.71	16	10
2:B:41:U:O5'	2:B:41:U:C6	0.58	2.56	3	2
2:B:35:U:O2'	2:B:36:U:O4'	0.58	2.22	7	11
1:A:6:U:H2'	1:A:7:A:O4'	0.58	1.98	19	2
2:B:42:C:C5'	2:B:43:U:OP2	0.58	2.52	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:43:U:O2'	2:B:44:U:O4'	0.57	2.21	10	10
1:A:17:U:O2'	1:A:18:C:O5'	0.57	2.22	9	8
1:A:29:A:O5'	1:A:29:A:C8	0.57	2.57	12	20
1:A:15:G:C5	1:A:16:U:C4	0.57	2.93	4	20
1:A:24:G:C6	1:A:25:C:C5	0.57	2.92	1	2
1:A:4:C:O5'	1:A:4:C:C6	0.57	2.54	13	6
1:A:24:G:C5	2:B:43:U:OP1	0.57	2.58	17	2
2:B:38:G:H8	2:B:38:G:O5'	0.57	1.83	12	19
2:B:43:U:HO2'	2:B:44:U:H6	0.57	1.39	1	2
2:B:39:G:C6	2:B:40:C:C4	0.56	2.93	1	3
2:B:41:U:H5'	2:B:42:C:OP2	0.56	2.01	9	2
1:A:26:C:O2'	1:A:27:G:C5'	0.56	2.54	18	3
2:B:42:C:C2'	2:B:43:U:OP1	0.56	2.54	13	1
1:A:19:G:C2	1:A:20:C:C5	0.56	2.94	1	9
1:A:21:U:C4	1:A:22:G:N7	0.56	2.74	17	3
1:A:26:C:C2'	1:A:27:G:O4'	0.56	2.53	20	6
1:A:18:C:O4'	1:A:19:G:N2	0.56	2.39	5	16
1:A:24:G:OP1	1:A:24:G:C4'	0.55	2.54	2	3
2:B:39:G:H8	2:B:39:G:O5'	0.55	1.85	11	6
1:A:5:U:C4'	1:A:6:U:OP1	0.55	2.53	13	1
1:A:24:G:C6	2:B:43:U:OP1	0.55	2.60	14	3
2:B:43:U:O5'	2:B:43:U:C6	0.55	2.55	14	3
1:A:18:C:H6	1:A:18:C:O5'	0.55	1.84	11	1
2:B:36:U:O5'	2:B:36:U:C6	0.55	2.54	2	6
1:A:6:U:O2'	1:A:7:A:C8	0.55	2.57	14	6
1:A:26:C:O2'	1:A:27:G:H5'	0.55	2.02	18	1
1:A:13:C:H6	1:A:13:C:O5'	0.54	1.86	3	14
2:B:42:C:O2'	2:B:43:U:OP2	0.54	2.20	9	1
2:B:42:C:H4'	2:B:43:U:OP2	0.53	2.03	9	1
1:A:30:A:O5'	1:A:30:A:C8	0.53	2.60	8	2
2:B:48:A:O5'	2:B:48:A:C8	0.53	2.59	7	19
1:A:6:U:O2'	1:A:7:A:H5'	0.53	2.04	20	1
2:B:39:G:O2'	2:B:40:C:H5'	0.53	2.04	10	5
1:A:33:U:C4	1:A:34:C:C5	0.52	2.97	19	2
1:A:6:U:O2'	1:A:7:A:O4'	0.52	2.28	18	3
1:A:11:A:C5	1:A:12:A:C8	0.51	2.98	10	1
1:A:11:A:C5	1:A:12:A:C5	0.51	2.98	10	1
1:A:21:U:C2	1:A:22:G:C8	0.51	2.99	17	2
2:B:40:C:O2	2:B:42:C:C4	0.51	2.64	2	2
1:A:15:G:C6	1:A:16:U:C2	0.51	2.99	11	20
1:A:15:G:C2	1:A:16:U:C2	0.51	2.99	18	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:G:C2	1:A:20:C:C4	0.51	2.99	1	10
2:B:40:C:O2	2:B:42:C:H5	0.51	1.88	13	2
1:A:2:G:C4	1:A:3:C:C5	0.50	2.99	9	11
1:A:11:A:H8	1:A:11:A:O5'	0.50	1.89	17	3
1:A:11:A:C4	1:A:12:A:C8	0.49	3.00	10	2
1:A:12:A:H2'	1:A:13:C:C6	0.49	2.42	5	20
1:A:24:G:OP2	1:A:24:G:C8	0.49	2.61	14	1
1:A:24:G:C4	1:A:25:C:C5	0.49	3.01	18	4
1:A:30:A:O2'	1:A:31:G:H5'	0.49	2.08	5	4
1:A:15:G:N7	1:A:16:U:C5	0.48	2.81	11	4
1:A:7:A:O5'	1:A:7:A:C8	0.48	2.66	10	2
1:A:23:U:H5"	1:A:24:G:OP1	0.48	2.09	9	1
2:B:38:G:O5'	2:B:38:G:C8	0.47	2.68	7	12
2:B:39:G:O5'	2:B:39:G:C8	0.47	2.65	1	2
1:A:7:A:O5'	1:A:7:A:H8	0.47	1.93	10	1
2:B:43:U:H2'	2:B:44:U:C6	0.47	2.45	1	11
2:B:45:C:O2'	2:B:46:C:C4'	0.47	2.63	16	1
1:A:15:G:O6	1:A:16:U:C4	0.47	2.68	5	10
1:A:6:U:H2'	1:A:7:A:C8	0.46	2.46	15	11
2:B:42:C:H2'	2:B:43:U:OP1	0.46	2.10	13	1
1:A:2:G:N7	1:A:3:C:C5	0.46	2.84	12	4
2:B:43:U:O2'	2:B:44:U:C6	0.46	2.67	20	2
2:B:44:U:O5'	2:B:44:U:H6	0.46	1.93	7	2
1:A:13:C:O5'	1:A:13:C:C6	0.46	2.68	3	2
2:B:40:C:C4	2:B:42:C:OP2	0.46	2.69	16	1
1:A:24:G:C4	2:B:43:U:OP1	0.46	2.69	13	1
1:A:33:U:N3	1:A:34:C:C4	0.46	2.84	7	2
1:A:24:G:N3	2:B:42:C:H2'	0.45	2.26	6	2
1:A:24:G:O6	2:B:43:U:C5'	0.45	2.64	3	1
1:A:18:C:O5'	1:A:18:C:H6	0.45	1.94	9	1
2:B:39:G:O6	2:B:40:C:N4	0.45	2.50	12	3
1:A:33:U:H2'	1:A:34:C:C6	0.45	2.47	10	15
1:A:22:G:H2'	1:A:23:U:C6	0.44	2.48	3	18
1:A:19:G:O2'	1:A:20:C:C5'	0.44	2.58	20	1
2:B:40:C:C2'	2:B:41:U:O5'	0.44	2.64	18	2
1:A:8:G:H2'	1:A:9:G:C8	0.44	2.47	12	12
1:A:11:A:H2'	1:A:12:A:O4'	0.44	2.13	20	3
1:A:33:U:C4	1:A:34:C:N4	0.43	2.86	7	2
1:A:19:G:C2'	1:A:20:C:O4'	0.43	2.52	20	1
1:A:24:G:N1	1:A:25:C:C4	0.43	2.86	1	1
1:A:11:A:O5'	1:A:11:A:C8	0.43	2.71	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:G:C4	1:A:16:U:C6	0.43	3.06	4	17
1:A:33:U:C2	1:A:34:C:C5	0.43	3.06	11	3
1:A:15:G:C5	1:A:16:U:C6	0.43	3.06	11	1
1:A:24:G:O6	2:B:43:U:OP1	0.43	2.36	14	1
2:B:42:C:C4'	2:B:43:U:OP2	0.43	2.66	9	1
1:A:1:G:N1	1:A:2:G:N7	0.43	2.65	11	2
1:A:11:A:C5	1:A:12:A:N7	0.43	2.87	10	1
2:B:45:C:HO2'	2:B:46:C:C4'	0.43	2.27	16	1
1:A:21:U:C2'	1:A:22:G:O4'	0.43	2.63	12	2
1:A:5:U:C2'	2:B:35:U:O5'	0.43	2.67	9	1
1:A:28:A:H2'	1:A:29:A:C8	0.42	2.49	13	6
2:B:37:C:H6	2:B:37:C:O5'	0.42	1.97	20	6
1:A:3:C:H2'	1:A:4:C:C6	0.42	2.50	7	5
1:A:18:C:O4'	1:A:19:G:N3	0.42	2.51	1	1
1:A:2:G:C6	1:A:3:C:C5	0.42	3.08	14	1
1:A:6:U:OP2	2:B:35:U:C5'	0.42	2.68	15	1
1:A:6:U:C2'	1:A:7:A:C8	0.41	3.03	4	2
2:B:40:C:O2'	2:B:41:U:C5	0.41	2.62	6	1
1:A:11:A:C2	1:A:12:A:H1'	0.41	2.50	4	5
1:A:32:G:O6	1:A:33:U:C4	0.41	2.74	14	1
1:A:2:G:C8	1:A:3:C:C5	0.41	3.08	12	3
1:A:19:G:N3	1:A:19:G:H3'	0.41	2.30	13	1
1:A:3:C:O2'	1:A:4:C:O4'	0.41	2.37	7	1
1:A:26:C:O5'	1:A:26:C:C6	0.41	2.62	11	1
1:A:31:G:O2'	1:A:32:G:O4'	0.41	2.35	17	1
1:A:32:G:C5	1:A:33:U:C6	0.41	3.09	1	1
1:A:5:U:C5'	1:A:6:U:OP1	0.41	2.69	13	1
2:B:37:C:H2'	2:B:38:G:C8	0.41	2.51	18	1
1:A:5:U:HO2'	2:B:35:U:C5'	0.41	2.27	9	1
1:A:24:G:H2'	1:A:25:C:C6	0.41	2.51	8	1
2:B:37:C:O5'	2:B:37:C:H6	0.40	1.99	14	1
1:A:4:C:H6	1:A:4:C:O5'	0.40	1.98	15	1
1:A:7:A:H8	1:A:7:A:O5'	0.40	1.99	17	1
2:B:35:U:HO2'	2:B:36:U:C4'	0.40	2.28	18	1
2:B:41:U:C5	2:B:42:C:N4	0.40	2.89	6	1
1:A:11:A:N6	1:A:12:A:C5	0.40	2.86	10	1
2:B:40:C:H2'	2:B:41:U:O5'	0.40	2.16	18	1
2:B:43:U:C2'	2:B:44:U:C6	0.40	3.05	20	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

There are no protein molecules in this entry.

6.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

6.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	34/34 (100%)	10±2 (28±5%)	0±0 (1±1%)	0.10±0.02
2	B	13/14 (93%)	7±2 (52±14%)	0±1 (2±4%)	0.04±0.02
All	All	924/960 (96%)	326 (35%)	11 (1%)	0.08

The overall RNA backbone suiteness is 0.08.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	9	G	20
1	A	17	U	20
1	A	18	C	20
1	A	24	G	20
1	A	29	A	20
2	B	41	U	20
2	B	43	U	20
1	A	6	U	18
2	B	42	C	18
2	B	48	A	18
1	A	7	A	15
1	A	30	A	15
2	B	36	U	12
2	B	44	U	12
2	B	47	U	12
2	B	38	G	10
1	A	8	G	9
1	A	5	U	6
1	A	23	U	6
1	A	19	G	5
2	B	46	C	4

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Mol	Chain	Res	Type	Models (Total)
1	A	4	C	4
2	B	37	C	4
1	A	11	A	4
2	B	39	G	3
2	B	40	C	2
1	A	25	C	2
1	A	10	A	2
1	A	2	G	2
1	A	27	G	1
1	A	21	U	1
1	A	32	G	1

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	1	G	4
2	B	42	C	4
1	A	5	U	2
2	B	41	U	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)

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 (i)

No chemical shift data were provided