Full wwPDB NMR Structure Validation Report (i)

Feb 26, 2022 – 12:16 PM EST

PDB ID	:	2ADT
Title	:	NMR structure of a 30 kDa GAAA tetraloop-receptor complex.
Authors	:	Davis, J.H.; Tonelli, M.; Scott, L.G.; Jaeger, L.; Williamson, J.R.; Butcher, S.E.
Deposited on	:	2005-07-20

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

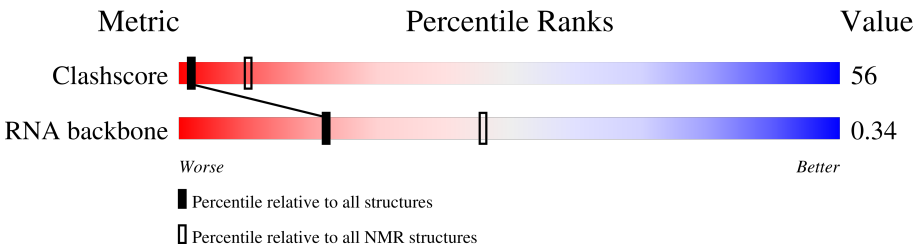
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	43	19% 60% 21%
1	B	43	21% 58% 21%

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 is only 1 type of molecule in this entry. The entry contains 2763 atoms, of which 927 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 43-MER.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	43	1381	411	463	166	299	42	0
1	B	43	1382	411	464	166	299	42	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: 43-MER

Chain A: 19% 60% 21%

G1 G2 G3 A4 U5 A6 U7 G8 G9 C15 C16 G17 G18 G19 G20 A21 A22 A23 C24 U25 U26 G27 G28 U29 U30 C31 U32 U33 C34 C35 U36 A37 A38 G39 U40 C41 C42 U43

• Molecule 1: 43-MER

Chain B: 21% 58% 21%

G44 G45 U48 A49 U50 G51 G52 C58 C59 G60 G61 G62 G63 A64 A65 A66 C67 U68 U69 G70 G71 U72 U73 C74 U75 U76 C77 C78 U79 A80 A81 G82 U83 C84 C85 U86

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: 43-MER

Chain A: 26% 51% 23%

G1 G2 G3 A4 U5 A6 U7 G8 G9 G12 A13 A14 C15 C16 G17 G18 G19 G20 A21 A22 A23 C24 U25 U26 G27 C35 U36 A37 A38 G39 U40 C41 C42 U43

• Molecule 1: 43-MER

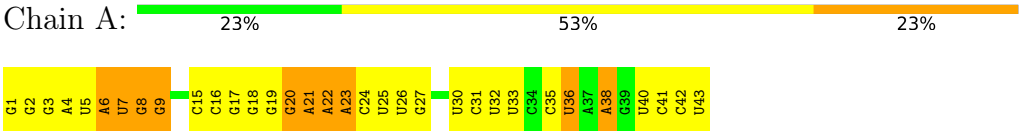
Chain B: 26% 56% 19%

G44 G45 G46 A47 U48 A49 U50 G51 G52 C58 C59 G60 G61 G62 G63 A64 A65 A66 C67 U68 U69 G70 G71 U72 U73 C74 U75 C78 U79 A80 A81 G82 U83 C84 C85 U86

4.2.2 Score per residue for model 2

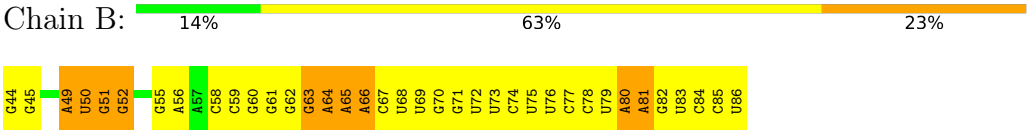
- Molecule 1: 43-MER

Chain A:



- Molecule 1: 43-MER

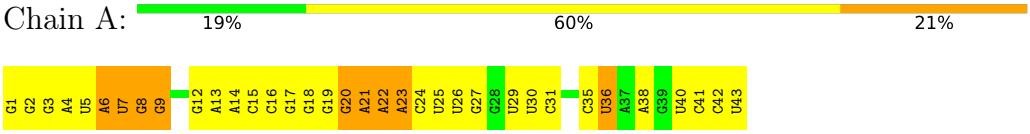
Chain B:



4.2.3 Score per residue for model 3

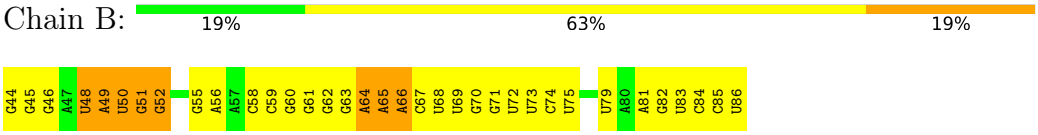
- Molecule 1: 43-MER

Chain A:



- Molecule 1: 43-MER

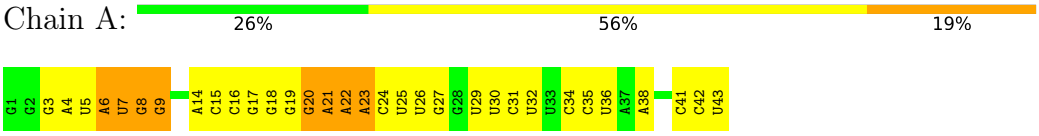
Chain B:



4.2.4 Score per residue for model 4

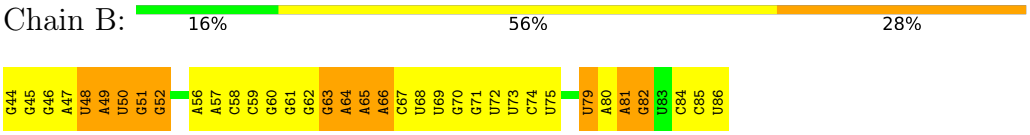
- Molecule 1: 43-MER

Chain A:



- Molecule 1: 43-MER

Chain B:



4.2.5 Score per residue for model 5

- Molecule 1: 43-MER

Chain A: 16% 56% 28%

- Molecule 1: 43-MER

Chain B: 33% 47% 21%

4.2.6 Score per residue for model 6

- Molecule 1: 43-MER

Chain A: 21% 60% 19%

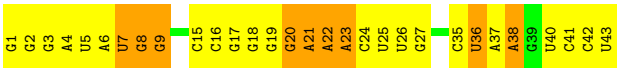
- Molecule 1: 43-MER

Chain B: 12% 65% 23%

4.2.7 Score per residue for model 7

- Molecule 1: 43-MER

Chain A: 30% 49% 21%



- Molecule 1: 43-MER

Chain B: 26% 51% 23%

4.2.8 Score per residue for model 8

- Molecule 1: 43-MER

Chain A: 16% 67% 16%

G1 G2 G3 A4 U5 A6 U7 G8 G9 C15 C16 G17 G18 G19 G20 A21 A22 A23 C24 U25 U26 G27 G28 U29 U30 C31 U32 U33 U36 A37 A38 G39 U40 C41 C42 U43

- Molecule 1: 43-MER

Chain B: 21% 56% 23%

G44 U48 A49 U50 G51 G52 A53 A54 G55 A56 A57 C58 C59 G60 G61 G62 G63 A64 A65 A66 C67 U68 U69 G70 G71 U72 U73 C74 U79 A80 A81 G82 U83 C84 C85 U86

4.2.9 Score per residue for model 9

- Molecule 1: 43-MER

Chain A: 12% 70% 19%

G1 G2 G3 A4 U5 A6 U7 G8 G9 A10 A11 A14 C15 C16 G17 G18 G19 G20 A21 A22 A23 C24 U25 U26 G27 G28 U29 U30 C31 U32 U33 C34 C35 U36 A37 A38 G39 U40 C41 C42 U43

- Molecule 1: 43-MER

Chain B: 26% 56% 19%

G44 G45 G46 A47 U48 A49 U50 G51 G52 C58 C59 G60 G61 G62 G63 A64 A65 A66 C67 U68 U69 G70 G71 U72 U73 C74 C78 U79 A80 A81 G82 U83 C84 C85 U86

4.2.10 Score per residue for model 10

- Molecule 1: 43-MER

Chain A: 14% 65% 21%

G1 G2 G3 A4 U5 A6 U7 G8 G9 A10 A11 G12 A13 A14 C15 C16 G17 G18 G19 G20 A21 A22 A23 C24 U25 U26 G27 U30 C31 U36 A37 A38 G39 U40 C41 C42 U43

- Molecule 1: 43-MER

Chain B: 21% 65% 14%

G44 G45 G46 A47 U48 A49 U50 G51 G52 G55 A56 A57 C58 C59 G60 G61 G62 G63 A64 A65 A66 C67 U68 U69 G70 G71 C74 U75 U79 A80 A81 G82 U83 C84 C85 U86

4.2.11 Score per residue for model 11

- Molecule 1: 43-MER

Chain A: 12% 65% 23%

- Molecule 1: 43-MER

Chain B: 26% 53% 21%

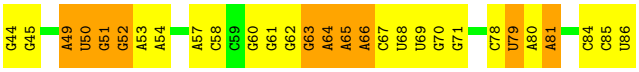
4.2.12 Score per residue for model 12

- Molecule 1: 43-MER

Chain A: 21% 58% 21%

- Molecule 1: 43-MER

Chain B: 33% 44% 23%



4.2.13 Score per residue for model 13

- Molecule 1: 43-MER

Chain A: 14% 63% 23%

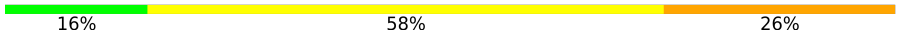
- Molecule 1: 43-MER

Chain B: 21% 60% 19%

4.2.14 Score per residue for model 14

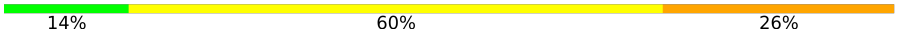
- Molecule 1: 43-MER

Chain A:



- Molecule 1: 43-MER

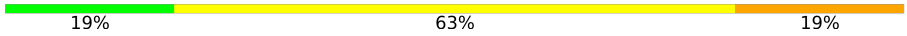
Chain B:



4.2.15 Score per residue for model 15

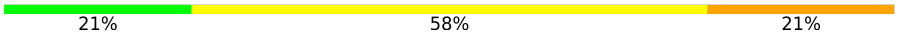
- Molecule 1: 43-MER

Chain A:



- Molecule 1: 43-MER

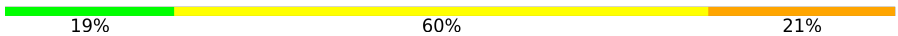
Chain B:



4.2.16 Score per residue for model 16

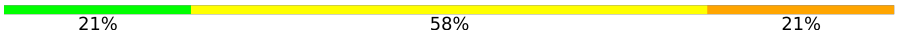
- Molecule 1: 43-MER

Chain A:



- Molecule 1: 43-MER

Chain B:



4.2.17 Score per residue for model 17

- Molecule 1: 43-MER

Chain A: 23% 56% 21%

- Molecule 1: 43-MER

Chain B: 28% 44% 28%

4.2.18 Score per residue for model 18

- Molecule 1: 43-MER

Chain A: 19% 60% 21%

- Molecule 1: 43-MER

Chain B: 19% 56% 26%

4.2.19 Score per residue for model 19

- Molecule 1: 43-MER

Chain A: 26% 51% 23%

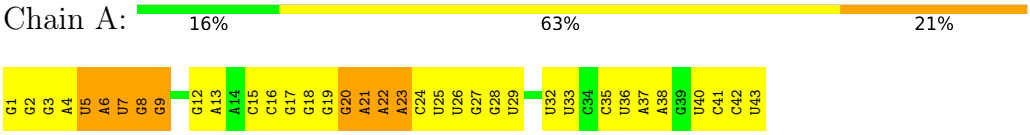
- Molecule 1: 43-MER

Chain B: 16% 53% 30%

4.2.20 Score per residue for model 20

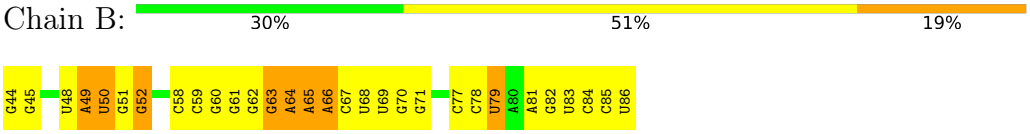
- Molecule 1: 43-MER

Chain A:



- Molecule 1: 43-MER

Chain B:



5 Refinement protocol and experimental data overview (i)

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
CNS	structure solution	1.0
X-PLOR-NIH	structure solution	2.11
X-PLOR-NIH	refinement	2.11

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (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	918	463	464	86±6
1	B	918	464	464	76±9
All	All	36720	18540	18560	3117

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 56.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:U:O2'	1:A:8:G:H5'	1.05	1.51	2	13
1:B:48:U:O2'	1:B:49:A:H5'	1.04	1.52	14	2
1:A:29:U:O2'	1:A:30:U:H5'	0.98	1.56	8	11
1:A:24:C:O2'	1:A:25:U:H5'	0.96	1.59	17	20
1:B:60:G:O2'	1:B:61:G:H5'	0.96	1.58	3	19
1:A:3:G:O2'	1:A:4:A:H5'	0.95	1.61	7	18
1:B:85:C:O2'	1:B:86:U:H5'	0.95	1.61	15	20
1:B:46:G:O2'	1:B:47:A:H5'	0.95	1.61	19	7
1:A:42:C:O2'	1:A:43:U:H5'	0.95	1.60	11	20
1:A:18:G:O2'	1:A:19:G:H5'	0.95	1.59	19	20
1:A:41:C:O2'	1:A:42:C:H5'	0.93	1.64	1	19
1:B:84:C:O2'	1:B:85:C:H5'	0.93	1.63	3	20
1:A:21:A:H3'	1:A:21:A:OP1	0.93	1.64	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:69:U:O2'	1:B:70:G:H5'	0.91	1.64	7	20
1:A:17:G:O2'	1:A:18:G:H5'	0.91	1.66	2	20
1:A:26:U:O2'	1:A:27:G:H5'	0.90	1.66	9	20
1:B:67:C:O2'	1:B:68:U:H5'	0.90	1.66	13	19
1:B:49:A:O2'	1:B:50:U:H5"	0.89	1.67	8	2
1:A:4:A:O2'	1:A:5:U:H5'	0.88	1.68	16	19
1:B:50:U:O2'	1:B:51:G:H8	0.88	1.52	11	3
1:B:50:U:HO2'	1:B:51:G:H8	0.87	0.95	16	2
1:B:53:A:O2'	1:B:54:A:H5'	0.87	1.68	13	7
1:A:25:U:O2'	1:A:26:U:H5'	0.87	1.69	14	20
1:A:6:A:O2'	1:A:7:U:H5"	0.86	1.68	9	3
1:B:49:A:O2'	1:B:50:U:H2'	0.86	1.69	11	5
1:A:8:G:H2'	1:A:9:G:O4'	0.85	1.72	1	18
1:B:61:G:O2'	1:B:62:G:H5'	0.84	1.72	17	20
1:B:51:G:H2'	1:B:52:G:O4'	0.84	1.72	19	10
1:B:62:G:H2'	1:B:63:G:O4'	0.83	1.72	20	14
1:B:73:U:O2'	1:B:74:C:H5'	0.83	1.72	18	12
1:B:66:A:H2'	1:B:67:C:O4'	0.83	1.73	2	20
1:B:49:A:N3	1:B:50:U:H6	0.82	1.72	8	9
1:B:68:U:O2'	1:B:69:U:H5'	0.81	1.76	5	19
1:B:50:U:H1'	1:B:51:G:OP1	0.81	1.75	5	5
1:A:7:U:HO2'	1:A:8:G:C5'	0.80	1.89	18	7
1:B:49:A:H1'	1:B:50:U:O5'	0.80	1.76	14	3
1:A:5:U:H5"	1:A:6:A:OP2	0.80	1.77	13	1
1:B:49:A:H1'	1:B:50:U:OP1	0.79	1.78	3	3
1:B:55:G:O2'	1:B:56:A:H5'	0.79	1.78	10	9
1:A:36:U:O2'	1:A:37:A:H5'	0.78	1.76	12	1
1:A:1:G:O2'	1:A:2:G:H5'	0.78	1.76	16	18
1:B:58:C:O2'	1:B:59:C:H5'	0.78	1.78	2	5
1:B:64:A:H8	1:B:64:A:O5'	0.78	1.62	8	18
1:B:80:A:H4'	1:B:81:A:OP1	0.78	1.77	6	4
1:B:48:U:HO2'	1:B:49:A:H5'	0.77	1.37	14	2
1:A:21:A:H8	1:A:21:A:O5'	0.77	1.63	12	19
1:B:72:U:O2'	1:B:73:U:H5'	0.77	1.78	19	9
1:B:44:G:O2'	1:B:45:G:H5'	0.76	1.80	10	19
1:B:50:U:C6	1:B:51:G:N7	0.76	2.54	20	3
1:B:77:C:O2'	1:B:78:C:P	0.76	2.44	19	2
1:B:46:G:HO2'	1:B:47:A:H5'	0.76	1.36	19	1
1:A:23:A:H2'	1:A:24:C:O4'	0.75	1.81	5	17
1:B:50:U:O2'	1:B:51:G:P	0.75	2.45	5	5
1:B:65:A:N1	1:B:66:A:C2	0.75	2.55	6	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:64:A:H2'	1:B:65:A:O4'	0.74	1.82	6	6
1:A:7:U:C6	1:A:8:G:N7	0.74	2.55	14	1
1:A:2:G:O2'	1:A:3:G:H5'	0.74	1.80	8	10
1:A:22:A:N1	1:A:23:A:C2	0.74	2.56	11	20
1:A:22:A:C6	1:A:23:A:C6	0.74	2.76	16	19
1:A:15:C:C4	1:A:16:C:C4	0.74	2.76	18	20
1:A:22:A:C2	1:A:23:A:C2	0.73	2.76	12	19
1:B:49:A:C4	1:B:51:G:C8	0.73	2.76	8	13
1:A:22:A:OP2	1:A:22:A:H8	0.73	1.67	16	1
1:A:6:A:C2	1:A:8:G:C8	0.73	2.77	11	13
1:B:65:A:C2	1:B:66:A:C2	0.73	2.77	7	17
1:B:65:A:C6	1:B:66:A:C6	0.72	2.76	5	20
1:B:45:G:O2'	1:B:46:G:H5'	0.72	1.84	18	5
1:A:5:U:O2'	1:A:6:A:H5'	0.72	1.84	17	3
1:A:6:A:N3	1:A:7:U:C6	0.72	2.58	11	15
1:A:21:A:H1'	1:B:81:A:O4'	0.72	1.85	17	5
1:B:65:A:N6	1:B:66:A:C6	0.72	2.58	11	3
1:B:58:C:C4	1:B:59:C:C4	0.72	2.77	1	15
1:B:50:U:O2'	1:B:51:G:C8	0.72	2.42	11	3
1:B:51:G:C6	1:B:52:G:N7	0.72	2.57	20	6
1:B:48:U:O2'	1:B:49:A:P	0.72	2.48	16	7
1:A:6:A:H1'	1:A:7:U:OP1	0.72	1.84	15	3
1:A:8:G:C6	1:A:9:G:C5	0.72	2.77	11	13
1:B:58:C:H2'	1:B:59:C:O4'	0.72	1.84	1	5
1:B:60:G:HO2'	1:B:61:G:H5'	0.72	1.45	13	5
1:A:6:A:C4	1:A:8:G:N7	0.72	2.57	12	18
1:B:64:A:N6	1:B:65:A:C6	0.72	2.58	7	17
1:A:21:A:N6	1:A:22:A:C6	0.71	2.58	4	17
1:B:49:A:C4	1:B:51:G:N7	0.71	2.58	3	13
1:A:8:G:C5	1:A:9:G:C8	0.71	2.78	18	11
1:A:19:G:N7	1:A:20:G:C5	0.71	2.58	13	16
1:B:49:A:N3	1:B:50:U:C6	0.71	2.59	8	11
1:A:6:A:N3	1:A:7:U:H6	0.71	1.84	2	13
1:A:22:A:N1	1:A:23:A:N1	0.71	2.39	16	18
1:A:22:A:C6	1:A:23:A:N1	0.71	2.59	16	20
1:A:32:U:O2'	1:A:33:U:H5'	0.71	1.86	11	10
1:A:6:A:H4'	1:A:7:U:OP1	0.71	1.85	8	3
1:B:49:A:O2'	1:B:50:U:P	0.70	2.49	15	7
1:A:5:U:O2'	1:A:6:A:P	0.70	2.49	18	4
1:A:21:A:P	1:A:21:A:C8	0.70	2.85	16	1
1:A:23:A:H8	1:A:23:A:O5'	0.70	1.69	16	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:60:G:C6	1:B:70:G:N2	0.70	2.59	19	13
1:B:65:A:N1	1:B:66:A:N1	0.70	2.40	16	17
1:B:44:G:HO5'	1:B:44:G:H8	0.70	1.28	14	2
1:B:50:U:O2'	1:B:51:G:H5'	0.70	1.86	1	11
1:A:8:G:C5	1:A:9:G:N7	0.70	2.60	7	9
1:B:65:A:N6	1:B:66:A:N1	0.70	2.39	11	3
1:B:49:A:O2'	1:B:50:U:C6	0.70	2.45	14	3
1:B:64:A:C6	1:B:65:A:C6	0.70	2.79	20	14
1:B:64:A:O2'	1:B:65:A:P	0.70	2.49	6	1
1:B:79:U:O2'	1:B:80:A:P	0.69	2.49	17	1
1:B:65:A:C6	1:B:66:A:N1	0.69	2.60	9	20
1:A:6:A:N3	1:A:8:G:C8	0.69	2.60	20	12
1:A:37:A:H4'	1:A:38:A:OP1	0.69	1.85	15	3
1:B:64:A:N6	1:B:65:A:N1	0.69	2.40	14	15
1:B:83:U:H6	1:B:83:U:O5'	0.69	1.70	16	13
1:A:38:A:O5'	1:B:64:A:H1'	0.69	1.87	1	1
1:A:21:A:N7	1:A:22:A:N7	0.69	2.41	12	9
1:A:5:U:H4'	1:A:6:A:OP1	0.69	1.87	14	1
1:A:15:C:C4	1:A:16:C:N4	0.68	2.61	20	17
1:A:6:A:C5	1:A:8:G:C5	0.68	2.82	19	14
1:B:50:U:OP1	1:B:50:U:H2'	0.68	1.88	3	2
1:A:15:C:N4	1:A:16:C:N4	0.68	2.41	17	18
1:B:62:G:N7	1:B:63:G:C5	0.68	2.61	20	11
1:A:6:A:O2'	1:A:7:U:P	0.68	2.52	19	10
1:A:40:U:O2'	1:A:41:C:H5'	0.68	1.88	8	5
1:A:6:A:O2'	1:A:7:U:C6	0.68	2.44	14	1
1:A:6:A:C4	1:A:8:G:C8	0.68	2.82	6	16
1:B:85:C:HO2'	1:B:86:U:H5'	0.67	1.48	2	6
1:B:51:G:C6	1:B:52:G:C5	0.67	2.82	5	8
1:A:12:G:O2'	1:A:13:A:H5'	0.67	1.89	10	9
1:A:7:U:H1'	1:A:8:G:OP1	0.67	1.89	7	1
1:B:62:G:C5	1:B:63:G:C5	0.67	2.83	11	12
1:B:60:G:C6	1:B:70:G:C2	0.67	2.82	19	18
1:A:14:A:C6	1:A:15:C:N4	0.67	2.63	10	8
1:A:17:G:C6	1:A:27:G:N2	0.67	2.63	13	16
1:A:7:U:HO2'	1:A:8:G:H8	0.67	1.29	7	1
1:A:42:C:HO2'	1:A:43:U:H5'	0.67	1.50	5	8
1:A:6:A:N3	1:A:7:U:C5	0.67	2.62	20	4
1:A:8:G:O2'	1:B:65:A:N6	0.67	2.27	6	3
1:B:51:G:C5	1:B:52:G:N7	0.67	2.63	18	8
1:A:7:U:O2'	1:A:8:G:P	0.67	2.52	9	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:G:C6	1:A:27:G:C2	0.66	2.83	11	18
1:B:49:A:O2'	1:B:50:U:H3'	0.66	1.90	1	2
1:B:58:C:N4	1:B:59:C:N4	0.66	2.43	9	7
1:B:62:G:C8	1:B:63:G:C8	0.66	2.83	12	8
1:B:64:A:C5	1:B:65:A:C5	0.66	2.83	19	17
1:B:50:U:O2'	1:B:51:G:C5'	0.66	2.43	4	13
1:B:49:A:C2	1:B:51:G:C8	0.66	2.84	18	10
1:B:77:C:O2'	1:B:78:C:H5'	0.66	1.90	18	1
1:B:49:A:C6	1:B:51:G:C8	0.66	2.83	14	2
1:A:6:A:N9	1:A:8:G:N7	0.66	2.44	17	4
1:B:49:A:C5	1:B:51:G:N7	0.66	2.64	14	3
1:A:15:C:C5	1:A:16:C:C4	0.66	2.84	8	14
1:A:21:A:H2'	1:A:22:A:O4'	0.66	1.90	15	13
1:B:69:U:O2'	1:B:70:G:C5'	0.66	2.44	9	18
1:B:50:U:HO2'	1:B:51:G:C5'	0.66	2.04	3	6
1:A:21:A:N1	1:B:49:A:N1	0.66	2.44	2	2
1:B:74:C:H2'	1:B:75:U:O4'	0.65	1.92	4	12
1:A:19:G:C8	1:A:20:G:N7	0.65	2.65	16	15
1:A:9:G:OP1	1:A:9:G:H4'	0.65	1.92	6	2
1:B:52:G:H4'	1:B:52:G:OP1	0.65	1.91	1	3
1:B:85:C:O2'	1:B:86:U:C5'	0.65	2.45	3	17
1:B:50:U:H4'	1:B:51:G:OP1	0.65	1.89	10	1
1:B:57:A:C6	1:B:58:C:N4	0.65	2.64	13	2
1:A:15:C:C5	1:A:16:C:N4	0.65	2.65	20	11
1:A:18:G:O2'	1:A:19:G:C5'	0.65	2.45	12	19
1:A:26:U:O2'	1:A:27:G:C5'	0.65	2.44	10	20
1:A:41:C:O2'	1:A:42:C:C5'	0.65	2.45	17	15
1:A:42:C:O2'	1:A:43:U:C5'	0.65	2.45	4	20
1:A:7:U:O2'	1:A:8:G:C5'	0.64	2.45	1	14
1:A:19:G:C5	1:A:20:G:C5	0.64	2.86	9	18
1:B:49:A:O2'	1:B:50:U:C2'	0.64	2.45	11	4
1:A:21:A:H2	1:B:80:A:O4'	0.64	1.75	10	1
1:B:57:A:N6	1:B:58:C:N4	0.64	2.45	13	1
1:A:3:G:O2'	1:A:4:A:C5'	0.64	2.46	16	8
1:B:62:G:N7	1:B:63:G:N7	0.64	2.45	12	5
1:B:64:A:N7	1:B:65:A:N7	0.64	2.46	7	9
1:A:6:A:O2'	1:A:7:U:C5'	0.64	2.45	9	3
1:B:44:G:H8	1:B:44:G:O5'	0.64	1.74	14	2
1:A:21:A:N3	1:B:81:A:C8	0.64	2.65	17	1
1:B:61:G:O2'	1:B:62:G:C5'	0.64	2.46	4	18
1:A:21:A:C6	1:A:22:A:C5	0.64	2.86	9	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:69:U:HO2'	1:B:70:G:H5'	0.64	1.50	5	2
1:B:49:A:N3	1:B:51:G:C8	0.63	2.66	18	10
1:A:21:A:N6	1:A:22:A:N1	0.63	2.46	10	3
1:B:49:A:HO2'	1:B:50:U:H2'	0.63	1.51	11	1
1:A:20:G:O2'	1:A:22:A:N7	0.63	2.30	16	1
1:A:30:U:O2'	1:A:31:C:H5'	0.63	1.93	15	6
1:A:6:A:C2	1:A:38:A:C6	0.63	2.87	17	1
1:B:47:A:O2'	1:B:48:U:H5'	0.63	1.93	17	6
1:B:84:C:O2'	1:B:85:C:C5'	0.63	2.46	11	18
1:B:49:A:C5	1:B:51:G:C5	0.63	2.86	7	10
1:B:60:G:C5	1:B:70:G:N2	0.63	2.67	11	10
1:B:64:A:C2'	1:B:65:A:O4'	0.62	2.47	6	1
1:A:8:G:C6	1:A:9:G:N7	0.62	2.66	9	4
1:A:4:A:O2'	1:A:5:U:C5'	0.62	2.47	10	14
1:B:50:U:O2'	1:B:51:G:O5'	0.62	2.18	11	15
1:A:37:A:H1'	1:A:38:A:N7	0.62	2.09	10	1
1:B:60:G:O2'	1:B:61:G:C5'	0.62	2.45	3	3
1:A:21:A:C8	1:A:21:A:O5'	0.62	2.53	16	1
1:A:36:U:C4	1:A:37:A:C6	0.61	2.88	14	2
1:A:21:A:C8	1:A:21:A:OP2	0.61	2.53	16	1
1:B:77:C:O2'	1:B:78:C:OP1	0.61	2.18	19	2
1:B:50:U:H1'	1:B:51:G:OP2	0.61	1.94	14	1
1:B:49:A:C8	1:B:51:G:C6	0.61	2.88	12	4
1:B:48:U:O2'	1:B:49:A:H5"	0.61	1.94	4	2
1:A:24:C:O2'	1:B:52:G:O2'	0.61	2.17	20	1
1:A:21:A:O5'	1:A:21:A:C8	0.61	2.52	17	18
1:B:49:A:O2'	1:B:50:U:O5'	0.61	2.19	10	7
1:A:6:A:C4	1:A:8:G:C5	0.61	2.89	20	4
1:B:50:U:C1'	1:B:51:G:OP1	0.61	2.48	5	5
1:B:74:C:C4	1:B:75:U:C4	0.61	2.89	19	1
1:A:9:G:O2'	1:B:67:C:O2'	0.61	2.18	11	1
1:A:8:G:N3	1:B:66:A:C2	0.61	2.69	12	1
1:B:48:U:H4'	1:B:49:A:OP1	0.61	1.95	17	6
1:A:22:A:N6	1:B:51:G:O2'	0.61	2.28	20	3
1:B:50:U:OP1	1:B:50:U:C6	0.61	2.53	3	2
1:A:7:U:O4	1:A:39:G:C2	0.60	2.53	5	3
1:B:64:A:O5'	1:B:64:A:C8	0.60	2.53	8	18
1:A:30:U:C4	1:A:31:C:C4	0.60	2.90	11	3
1:B:69:U:C4	1:B:70:G:C5	0.60	2.90	7	6
1:B:79:U:O4	1:B:80:A:N6	0.60	2.35	6	4
1:A:32:U:O2'	1:A:33:U:C5'	0.60	2.50	12	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:U:O2'	1:A:30:U:C5'	0.60	2.50	15	9
1:A:18:G:HO2'	1:A:19:G:H5'	0.60	1.55	9	1
1:B:62:G:O6	1:B:63:G:N1	0.60	2.34	11	3
1:A:38:A:O5'	1:A:38:A:H8	0.60	1.80	12	1
1:B:51:G:C5	1:B:52:G:C8	0.60	2.90	5	6
1:A:8:G:H1'	1:B:65:A:N1	0.59	2.11	12	4
1:A:40:U:H6	1:A:40:U:O5'	0.59	1.80	11	16
1:A:7:U:OP2	1:A:7:U:N1	0.59	2.35	17	1
1:B:62:G:C8	1:B:63:G:N7	0.59	2.70	5	6
1:A:5:U:C5	1:A:37:A:C6	0.59	2.91	17	1
1:A:7:U:C1'	1:A:8:G:OP1	0.59	2.51	7	1
1:B:44:G:O5'	1:B:44:G:C8	0.59	2.54	20	3
1:B:50:U:OP1	1:B:50:U:N1	0.59	2.36	19	2
1:A:6:A:O2'	1:A:7:U:O5'	0.59	2.20	14	4
1:B:79:U:C4	1:B:80:A:C6	0.59	2.91	18	4
1:A:7:U:O2'	1:A:8:G:O5'	0.58	2.21	7	11
1:A:7:U:C5	1:A:7:U:OP1	0.58	2.56	12	1
1:A:8:G:O2'	1:A:9:G:OP1	0.58	2.21	3	3
1:B:48:U:C4	1:B:80:A:C5	0.58	2.91	4	1
1:B:65:A:C2'	1:B:66:A:OP1	0.58	2.50	11	1
1:A:6:A:N1	1:B:64:A:N1	0.58	2.52	12	1
1:A:25:U:O2'	1:A:26:U:C5'	0.58	2.48	14	9
1:A:15:C:O2'	1:A:16:C:H5'	0.58	1.98	8	4
1:B:65:A:O2'	1:B:66:A:OP1	0.58	2.20	11	3
1:B:49:A:HO2'	1:B:50:U:H3'	0.58	1.59	17	2
1:B:49:A:HO2'	1:B:50:U:P	0.58	2.20	15	3
1:A:9:G:OP1	1:A:9:G:C4'	0.58	2.51	3	4
1:A:7:U:O2	1:A:7:U:C2'	0.58	2.52	14	1
1:B:49:A:O2'	1:B:50:U:C3'	0.58	2.51	1	2
1:B:50:U:O2'	1:B:51:G:OP1	0.58	2.20	5	2
1:B:55:G:O6	1:B:56:A:N6	0.58	2.36	16	1
1:B:50:U:O4	1:B:82:G:N2	0.58	2.37	3	3
1:A:20:G:C2'	1:A:21:A:OP1	0.58	2.52	16	1
1:B:58:C:C5	1:B:59:C:C4	0.57	2.92	1	6
1:B:62:G:C6	1:B:63:G:C2	0.57	2.92	11	3
1:B:79:U:O2'	1:B:80:A:OP1	0.57	2.20	17	3
1:A:9:G:C4'	1:A:9:G:OP1	0.57	2.51	7	1
1:A:8:G:O6	1:A:9:G:C6	0.57	2.57	20	7
1:A:6:A:O2'	1:A:7:U:H3'	0.57	1.98	7	1
1:A:6:A:O2'	1:A:7:U:OP2	0.57	2.22	6	8
1:A:6:A:C4'	1:A:7:U:OP1	0.57	2.53	11	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:64:A:H4'	1:B:65:A:OP1	0.57	1.98	6	1
1:A:7:U:OP1	1:A:7:U:N1	0.57	2.36	15	1
1:B:49:A:C1'	1:B:50:U:OP1	0.57	2.52	18	3
1:B:49:A:C1'	1:B:50:U:O5'	0.57	2.52	14	3
1:B:50:U:O2	1:B:50:U:O2'	0.57	2.22	10	3
1:A:21:A:O5'	1:A:21:A:H8	0.57	1.83	16	1
1:A:22:A:OP2	1:A:22:A:C8	0.57	2.54	16	1
1:A:6:A:P	1:A:6:A:O4'	0.57	2.61	18	1
1:B:69:U:H2'	1:B:70:G:O4'	0.57	2.00	15	18
1:B:70:G:O2'	1:B:71:G:C8	0.57	2.56	1	2
1:A:21:A:C6	1:A:22:A:C6	0.57	2.92	10	8
1:A:37:A:O2'	1:A:38:A:OP2	0.57	2.22	10	1
1:A:19:G:O6	1:A:20:G:N1	0.57	2.38	9	13
1:A:21:A:C5	1:A:22:A:C5	0.57	2.92	14	15
1:A:7:U:O2'	1:A:8:G:OP1	0.57	2.23	9	4
1:B:79:U:C4'	1:B:79:U:OP1	0.57	2.52	14	2
1:A:36:U:C2'	1:A:37:A:OP1	0.57	2.52	5	1
1:A:15:C:H2'	1:A:16:C:O4'	0.57	2.00	8	1
1:A:8:G:C2'	1:A:9:G:O4'	0.57	2.52	12	1
1:B:51:G:O2'	1:B:52:G:OP1	0.57	2.21	18	1
1:A:36:U:O2'	1:A:37:A:P	0.57	2.63	19	2
1:A:7:U:OP2	1:A:7:U:C6	0.57	2.57	17	1
1:A:37:A:C2	1:A:38:A:N6	0.57	2.72	10	2
1:A:30:U:O4	1:A:31:C:N4	0.57	2.38	11	1
1:B:79:U:OP1	1:B:79:U:H4'	0.57	1.99	14	1
1:A:36:U:H4'	1:A:36:U:OP1	0.57	2.00	5	3
1:A:6:A:C1'	1:A:7:U:OP1	0.57	2.53	13	3
1:A:36:U:O2'	1:A:37:A:C5'	0.57	2.51	12	1
1:A:8:G:N7	1:A:9:G:N7	0.56	2.52	20	2
1:B:50:U:H6	1:B:51:G:N7	0.56	1.97	10	2
1:A:5:U:O2'	1:A:6:A:O5'	0.56	2.21	14	1
1:A:21:A:C5	1:A:22:A:N7	0.56	2.73	9	8
1:A:24:C:O2'	1:A:25:U:C5'	0.56	2.47	17	6
1:A:19:G:C6	1:A:20:G:C6	0.56	2.93	9	5
1:B:52:G:OP1	1:B:52:G:C4'	0.56	2.53	18	3
1:A:36:U:O2'	1:A:37:A:OP1	0.56	2.23	19	2
1:B:49:A:C4'	1:B:50:U:OP1	0.56	2.52	18	3
1:A:22:A:C5	1:A:23:A:C6	0.56	2.93	16	3
1:A:38:A:O4'	1:B:64:A:C1'	0.56	2.54	10	3
1:B:44:G:H2'	1:B:45:G:O4'	0.56	2.00	20	2
1:A:7:U:C2'	1:A:8:G:O5'	0.56	2.54	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:A:O5'	1:A:23:A:C8	0.56	2.59	9	6
1:A:34:C:O2'	1:A:35:C:OP1	0.56	2.23	11	2
1:B:49:A:N7	1:B:51:G:C6	0.56	2.74	12	3
1:A:8:G:C2'	1:A:9:G:OP1	0.56	2.53	3	3
1:A:6:A:OP2	1:A:6:A:C4'	0.56	2.53	18	2
1:B:77:C:C2'	1:B:78:C:O5'	0.56	2.53	14	1
1:B:81:A:C2'	1:B:82:G:OP1	0.56	2.53	19	1
1:A:21:A:C1'	1:B:81:A:O4'	0.55	2.53	17	5
1:B:50:U:OP1	1:B:50:U:C2'	0.55	2.53	3	2
1:B:83:U:O2'	1:B:84:C:H5'	0.55	2.00	19	8
1:B:78:C:OP1	1:B:78:C:C4'	0.55	2.54	5	1
1:A:6:A:C8	1:A:8:G:O6	0.55	2.59	12	4
1:B:48:U:O2'	1:B:49:A:C5'	0.55	2.54	4	1
1:A:6:A:C8	1:A:8:G:C6	0.55	2.94	6	3
1:B:51:G:C2'	1:B:52:G:O5'	0.55	2.54	14	4
1:A:35:C:OP1	1:A:35:C:C4'	0.55	2.54	11	1
1:B:58:C:C5	1:B:59:C:C5	0.55	2.94	1	5
1:A:7:U:HO2'	1:A:8:G:P	0.55	2.24	3	6
1:B:49:A:O2'	1:B:50:U:OP2	0.55	2.21	16	6
1:B:50:U:C2'	1:B:50:U:O2	0.55	2.54	20	1
1:A:26:U:O2'	1:A:27:G:O4'	0.55	2.25	6	16
1:B:49:A:C8	1:B:51:G:O6	0.55	2.60	12	5
1:B:68:U:O2'	1:B:69:U:C5'	0.55	2.55	12	2
1:A:10:A:OP1	1:B:68:U:C5'	0.55	2.55	13	2
1:B:48:U:C2'	1:B:49:A:OP1	0.55	2.55	19	1
1:A:6:A:H61	1:B:64:A:H61	0.54	1.44	18	13
1:B:46:G:O2'	1:B:47:A:C5'	0.54	2.49	19	5
1:A:6:A:C5	1:A:8:G:N7	0.54	2.76	5	6
1:B:77:C:O2'	1:B:78:C:O5'	0.54	2.25	19	2
1:A:23:A:C2	1:B:52:G:O4'	0.54	2.60	20	1
1:A:26:U:H2'	1:A:27:G:O4'	0.54	2.02	19	20
1:A:34:C:C2'	1:A:35:C:OP1	0.54	2.55	11	1
1:A:17:G:C5	1:A:27:G:N2	0.54	2.76	6	13
1:A:22:A:N1	1:B:51:G:H1'	0.54	2.18	2	7
1:A:22:A:C5	1:A:23:A:N6	0.53	2.77	16	1
1:A:21:A:C8	1:A:22:A:C8	0.53	2.96	15	3
1:A:6:A:C8	1:A:8:G:C5	0.53	2.95	6	1
1:A:36:U:C4'	1:A:36:U:OP1	0.53	2.57	16	1
1:A:6:A:C6	1:A:8:G:C4	0.53	2.95	5	7
1:A:6:A:H61	1:B:64:A:N6	0.53	2.02	18	9
1:A:36:U:C4	1:A:37:A:N6	0.53	2.77	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:U:O4'	1:A:7:U:O2	0.53	2.22	20	3
1:A:36:U:HO2'	1:A:37:A:P	0.53	2.27	19	1
1:A:19:G:H2'	1:A:20:G:O4'	0.53	2.03	1	6
1:B:66:A:OP1	1:B:66:A:O4'	0.53	2.26	11	1
1:A:39:G:OP1	1:A:39:G:C4'	0.53	2.57	8	1
1:A:21:A:C2	1:B:80:A:O4'	0.53	2.61	10	1
1:B:84:C:HO2'	1:B:85:C:H5'	0.53	1.59	3	2
1:B:48:U:O2'	1:B:49:A:OP1	0.53	2.23	4	6
1:B:64:A:O2'	1:B:65:A:OP1	0.53	2.26	6	2
1:B:65:A:C6	1:B:66:A:C2	0.53	2.96	11	2
1:A:5:U:O2'	1:A:6:A:C5'	0.53	2.56	14	1
1:A:6:A:N6	1:B:64:A:H61	0.53	2.02	18	10
1:A:38:A:C8	1:B:64:A:N3	0.53	2.77	10	1
1:A:5:U:C2'	1:A:6:A:OP1	0.53	2.57	20	2
1:B:69:U:O2'	1:B:70:G:O4'	0.53	2.27	20	5
1:A:7:U:H6	1:A:8:G:N7	0.53	1.99	14	1
1:B:82:G:OP1	1:B:82:G:C4'	0.53	2.57	19	1
1:A:21:A:H61	1:B:49:A:H61	0.52	1.46	6	6
1:A:5:U:HO2'	1:A:6:A:P	0.52	2.27	9	3
1:B:49:A:O2'	1:B:50:U:N1	0.52	2.33	20	3
1:B:70:G:H2'	1:B:71:G:N7	0.52	2.18	1	6
1:B:62:G:C6	1:B:63:G:N1	0.52	2.77	11	1
1:B:49:A:C2	1:B:81:A:N1	0.52	2.77	13	1
1:A:21:A:OP2	1:A:21:A:N7	0.52	2.42	16	1
1:B:81:A:N6	1:B:82:G:C6	0.52	2.77	19	1
1:A:22:A:N6	1:A:23:A:N1	0.52	2.57	20	1
1:B:62:G:C5	1:B:63:G:C4	0.52	2.97	20	4
1:A:38:A:O4'	1:B:64:A:H1'	0.52	2.04	10	3
1:A:19:G:N7	1:A:20:G:C6	0.52	2.77	13	8
1:A:38:A:C2'	1:A:39:G:OP1	0.52	2.57	8	1
1:A:8:G:N3	1:B:66:A:H2	0.52	2.02	12	1
1:A:6:A:N1	1:A:8:G:C8	0.52	2.77	14	1
1:A:21:A:N6	1:B:49:A:H61	0.52	2.03	6	5
1:B:49:A:N1	1:B:51:G:C8	0.52	2.78	14	2
1:B:49:A:C2'	1:B:50:U:C6	0.52	2.93	20	3
1:B:50:U:O2	1:B:50:U:O4'	0.52	2.28	11	14
1:B:66:A:O5'	1:B:66:A:H8	0.52	1.87	13	7
1:A:6:A:N1	1:B:64:A:C6	0.52	2.78	12	1
1:A:17:G:O2'	1:A:18:G:C5'	0.52	2.52	2	4
1:A:6:A:C5	1:A:8:G:C8	0.52	2.98	3	2
1:A:21:A:N6	1:A:22:A:N6	0.52	2.58	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:50:U:O2	1:B:50:U:C2'	0.52	2.57	14	2
1:A:17:G:HO2'	1:A:18:G:H5'	0.52	1.65	6	4
1:B:50:U:HO2'	1:B:51:G:P	0.52	2.21	5	1
1:B:44:G:O5'	1:B:44:G:H8	0.52	1.88	20	2
1:A:15:C:C5	1:A:16:C:C5	0.51	2.98	19	7
1:B:79:U:O2'	1:B:80:A:H5'	0.51	2.04	10	1
1:B:48:U:O2'	1:B:49:A:O5'	0.51	2.27	16	4
1:A:37:A:OP1	1:A:37:A:C4'	0.51	2.59	5	1
1:B:79:U:C4	1:B:80:A:N6	0.51	2.78	12	4
1:B:50:U:C2'	1:B:51:G:O5'	0.51	2.58	4	1
1:A:13:A:O2'	1:A:14:A:H5'	0.51	2.05	11	1
1:B:62:G:C6	1:B:63:G:C6	0.51	2.98	19	2
1:B:50:U:C4'	1:B:51:G:O5'	0.51	2.59	14	1
1:A:5:U:C2'	1:A:6:A:OP2	0.51	2.58	15	2
1:A:1:G:H2'	1:A:2:G:O4'	0.51	2.04	6	2
1:A:6:A:C2'	1:A:8:G:N7	0.51	2.74	12	2
1:B:51:G:H2'	1:B:52:G:O5'	0.51	2.05	14	4
1:A:6:A:HO2'	1:A:7:U:P	0.51	2.29	4	2
1:B:49:A:N3	1:B:50:U:C5	0.51	2.79	13	2
1:A:8:G:C4	1:A:9:G:C8	0.51	2.98	9	6
1:A:6:A:O2'	1:A:7:U:OP1	0.51	2.28	17	1
1:A:7:U:O4	1:A:38:A:N1	0.51	2.44	6	1
1:A:19:G:N7	1:A:20:G:N7	0.50	2.59	9	8
1:B:64:A:O2'	1:B:65:A:O5'	0.50	2.29	6	1
1:A:17:G:O6	1:A:27:G:C2	0.50	2.65	11	1
1:A:8:G:C6	1:A:9:G:C6	0.50	2.99	6	4
1:A:36:U:O4	1:A:37:A:N6	0.50	2.44	7	1
1:B:69:U:O4	1:B:70:G:C6	0.50	2.64	7	1
1:B:73:U:O2'	1:B:74:C:C5'	0.50	2.56	18	4
1:A:19:G:C5	1:A:20:G:C6	0.50	3.00	9	5
1:B:64:A:C6	1:B:65:A:C5	0.50	3.00	7	16
1:A:7:U:O4	1:A:38:A:N6	0.50	2.45	5	1
1:A:19:G:O6	1:A:20:G:C6	0.50	2.65	9	3
1:B:79:U:O4	1:B:80:A:C6	0.50	2.64	8	1
1:A:6:A:O2'	1:A:8:G:N7	0.50	2.44	17	1
1:A:6:A:C2	1:A:38:A:N1	0.50	2.80	17	1
1:A:19:G:C6	1:A:20:G:N1	0.50	2.80	9	5
1:B:74:C:C2'	1:B:75:U:O4'	0.50	2.60	4	1
1:B:78:C:OP1	1:B:78:C:O4'	0.50	2.29	5	1
1:A:6:A:O4'	1:A:7:U:OP1	0.49	2.30	5	3
1:A:7:U:OP1	1:A:7:U:H5	0.49	1.88	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:G:OP1	1:A:39:G:O4'	0.49	2.29	8	1
1:A:5:U:C4'	1:A:6:A:OP1	0.49	2.60	14	1
1:A:7:U:O2	1:A:7:U:O4'	0.49	2.29	7	8
1:B:65:A:C5	1:B:66:A:C6	0.49	2.99	9	6
1:A:7:U:OP2	1:A:7:U:C2	0.49	2.66	17	1
1:B:79:U:H4'	1:B:80:A:OP1	0.49	2.07	17	1
1:B:64:A:C8	1:B:65:A:N7	0.49	2.80	7	3
1:A:35:C:C2'	1:A:36:U:O5'	0.49	2.60	3	2
1:A:6:A:O2'	1:A:7:U:N1	0.49	2.42	14	1
1:B:81:A:O5'	1:B:81:A:C8	0.49	2.66	19	1
1:A:37:A:OP1	1:A:37:A:O4'	0.49	2.31	5	1
1:B:48:U:C2'	1:B:49:A:OP2	0.49	2.60	14	2
1:B:50:U:O4'	1:B:51:G:OP1	0.49	2.30	11	1
1:A:10:A:OP1	1:B:68:U:H5"	0.49	2.07	13	1
1:B:49:A:N7	1:B:80:A:N1	0.49	2.60	6	1
1:A:21:A:C5	1:A:22:A:C8	0.49	3.00	15	3
1:B:81:A:C2'	1:B:82:G:O5'	0.49	2.60	4	2
1:B:49:A:O2'	1:B:50:U:C5'	0.49	2.50	8	1
1:A:26:U:C2'	1:A:27:G:O4'	0.49	2.61	19	17
1:A:37:A:O4'	1:B:64:A:C2	0.49	2.66	6	1
1:B:49:A:C4	1:B:51:G:C5	0.49	3.01	7	2
1:A:34:C:C4	1:A:35:C:C5	0.49	3.00	11	1
1:B:65:A:O2'	1:B:66:A:P	0.49	2.70	11	1
1:A:19:G:C8	1:A:20:G:C8	0.48	3.01	7	7
1:B:65:A:C2	1:B:66:A:C4	0.48	3.01	19	8
1:A:35:C:OP1	1:A:35:C:O4'	0.48	2.31	11	1
1:B:44:G:C8	1:B:44:G:O5'	0.48	2.66	7	2
1:B:50:U:H4'	1:B:51:G:O5'	0.48	2.08	14	1
1:A:22:A:C2	1:A:23:A:N3	0.48	2.81	9	11
1:B:49:A:OP2	1:B:49:A:H8	0.48	1.92	14	1
1:A:7:U:OP1	1:A:7:U:H2'	0.48	2.08	17	2
1:A:20:G:H2'	1:A:21:A:OP1	0.48	2.08	16	1
1:A:38:A:O4'	1:B:64:A:O4'	0.48	2.32	16	2
1:B:50:U:C2'	1:B:51:G:OP1	0.48	2.61	5	2
1:B:58:C:C4	1:B:59:C:N4	0.48	2.81	9	3
1:B:49:A:H2'	1:B:50:U:C5	0.48	2.44	20	3
1:A:21:A:H61	1:B:49:A:N6	0.48	2.07	1	5
1:B:77:C:C2'	1:B:78:C:OP1	0.48	2.61	5	1
1:A:6:A:C2	1:A:8:G:O4'	0.48	2.66	20	2
1:A:30:U:C4	1:A:31:C:N4	0.48	2.82	11	1
1:B:70:G:H2'	1:B:71:G:C8	0.48	2.44	1	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:71:G:O2'	1:B:72:U:H5'	0.48	2.09	4	1
1:A:8:G:C6	1:A:9:G:C8	0.48	3.00	9	1
1:A:14:A:C5	1:A:15:C:N4	0.48	2.82	10	2
1:A:8:G:C5	1:A:9:G:C5	0.48	3.02	20	1
1:A:4:A:HO2'	1:A:5:U:H5'	0.48	1.69	10	4
1:A:6:A:N7	1:A:8:G:C6	0.48	2.82	19	5
1:B:77:C:HO2'	1:B:78:C:P	0.48	2.32	14	1
1:A:21:A:OP1	1:A:21:A:C3'	0.48	2.52	16	1
1:B:49:A:C2	1:B:51:G:O4'	0.47	2.67	4	2
1:A:14:A:N6	1:A:15:C:N4	0.47	2.61	10	1
1:A:5:U:O2'	1:A:6:A:OP2	0.47	2.31	16	3
1:A:35:C:N4	1:A:36:U:O4	0.47	2.48	12	1
1:A:6:A:C2'	1:A:7:U:C6	0.47	2.97	14	1
1:A:24:C:HO2'	1:A:25:U:H5'	0.47	1.65	12	2
1:B:65:A:C2	1:B:66:A:N3	0.47	2.82	7	11
1:A:8:G:H3'	1:A:8:G:OP2	0.47	2.10	2	1
1:B:77:C:N3	1:B:78:C:C5	0.47	2.83	14	1
1:B:50:U:HO2'	1:B:51:G:H5'	0.47	1.70	5	1
1:A:21:A:C2	1:B:81:A:N7	0.47	2.82	17	1
1:B:64:A:N7	1:B:65:A:C5	0.47	2.83	7	2
1:B:49:A:C6	1:B:51:G:N7	0.47	2.83	14	2
1:A:22:A:C2	1:A:23:A:C4	0.47	3.03	5	15
1:B:80:A:H1'	1:B:81:A:N7	0.47	2.25	12	2
1:B:49:A:C6	1:B:51:G:C4	0.47	3.03	18	1
1:B:69:U:C2'	1:B:70:G:O4'	0.46	2.63	15	4
1:A:41:C:O2'	1:A:42:C:O4'	0.46	2.28	8	1
1:A:38:A:O5'	1:A:38:A:C8	0.46	2.66	12	1
1:A:7:U:H4'	1:A:8:G:O5'	0.46	2.09	14	1
1:B:79:U:C2'	1:B:80:A:O5'	0.46	2.63	13	1
1:A:21:A:OP1	1:A:22:A:C8	0.46	2.68	16	1
1:A:22:A:N6	1:A:23:A:C6	0.46	2.83	20	1
1:B:50:U:H3'	1:B:50:U:OP2	0.46	2.10	17	2
1:B:51:G:O6	1:B:52:G:C6	0.46	2.69	4	1
1:B:51:G:C4	1:B:52:G:C8	0.46	3.04	18	4
1:B:53:A:O2'	1:B:54:A:C5'	0.46	2.64	8	2
1:B:78:C:HO2'	1:B:79:U:P	0.46	2.33	19	1
1:B:56:A:H2'	1:B:57:A:C8	0.46	2.45	4	2
1:B:81:A:O5'	1:B:81:A:H8	0.46	1.93	19	1
1:B:51:G:N1	1:B:52:G:N7	0.46	2.63	20	1
1:B:78:C:O2'	1:B:79:U:OP1	0.46	2.27	7	3
1:B:64:A:C6	1:B:65:A:C4	0.46	3.03	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:79:U:OP1	1:B:79:U:O4'	0.46	2.33	7	1
1:A:12:G:O6	1:A:13:A:N6	0.46	2.48	11	1
1:A:6:A:C2	1:B:64:A:N6	0.46	2.84	12	1
1:B:77:C:H2'	1:B:78:C:O5'	0.46	2.11	14	1
1:A:7:U:OP1	1:A:7:U:C1'	0.46	2.64	15	1
1:A:36:U:C2'	1:A:37:A:O5'	0.46	2.62	19	1
1:A:35:C:HO2'	1:A:36:U:P	0.46	2.34	7	1
1:A:35:C:O2'	1:A:36:U:OP1	0.46	2.34	7	1
1:A:8:G:C8	1:A:9:G:C8	0.46	3.03	20	2
1:B:50:U:C1'	1:B:51:G:P	0.46	3.04	11	2
1:B:49:A:C2'	1:B:50:U:O5'	0.46	2.64	14	1
1:B:62:G:O6	1:B:63:G:C6	0.45	2.70	12	4
1:A:6:A:N1	1:A:38:A:C6	0.45	2.84	17	1
1:A:6:A:C2	1:A:7:U:C5	0.45	3.04	6	1
1:A:7:U:OP1	1:A:7:U:C6	0.45	2.69	15	1
1:A:7:U:O2	1:A:7:U:O2'	0.45	2.32	14	1
1:A:35:C:H2'	1:A:36:U:O4'	0.45	2.12	14	1
1:B:49:A:OP2	1:B:49:A:C8	0.45	2.69	14	1
1:A:7:U:HO2'	1:A:8:G:H5'	0.45	1.69	16	1
1:B:51:G:C2	1:B:52:G:C8	0.45	3.04	20	1
1:A:10:A:O2'	1:A:11:A:C5'	0.45	2.64	9	2
1:B:82:G:OP1	1:B:82:G:O4'	0.45	2.35	19	1
1:A:7:U:O2'	1:A:8:G:H8	0.45	1.92	7	1
1:B:69:U:C4	1:B:70:G:N7	0.45	2.85	7	1
1:A:2:G:O2'	1:A:3:G:C5'	0.45	2.65	17	2
1:A:15:C:C4	1:A:16:C:N3	0.45	2.84	8	1
1:A:36:U:O2'	1:A:37:A:O5'	0.45	2.25	17	1
1:B:53:A:N6	1:B:77:C:N4	0.45	2.64	18	1
1:A:38:A:C8	1:B:64:A:C5	0.45	3.05	6	1
1:B:64:A:O2'	1:B:65:A:O4'	0.45	2.35	6	1
1:A:38:A:N7	1:B:64:A:C2	0.45	2.85	10	1
1:B:70:G:C2'	1:B:71:G:C8	0.45	3.00	1	1
1:B:51:G:H3'	1:B:51:G:OP2	0.45	2.12	16	1
1:A:34:C:N4	1:A:35:C:N4	0.44	2.64	11	1
1:B:57:A:C6	1:B:58:C:C4	0.44	3.06	13	1
1:A:30:U:O2'	1:A:31:C:C5'	0.44	2.65	15	1
1:A:20:G:H21	1:A:23:A:H62	0.44	1.56	4	3
1:A:21:A:C6	1:A:22:A:C2	0.44	3.05	10	1
1:B:50:U:C4	1:B:52:G:O6	0.44	2.70	10	1
1:B:51:G:C2'	1:B:52:G:OP1	0.44	2.64	18	1
1:A:27:G:H2'	1:A:28:G:C8	0.44	2.47	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:48:U:HO2'	1:B:49:A:P	0.44	2.34	19	1
1:A:19:G:C6	1:A:20:G:C2	0.44	3.04	13	2
1:B:49:A:C1'	1:B:50:U:P	0.44	3.05	10	2
1:A:6:A:H2'	1:A:7:U:C5	0.44	2.46	14	1
1:A:1:G:C8	1:A:1:G:O5'	0.44	2.68	8	1
1:B:74:C:N4	1:B:75:U:O4	0.44	2.50	19	1
1:B:49:A:O2'	1:B:51:G:C8	0.44	2.65	13	1
1:A:35:C:O2'	1:A:36:U:P	0.44	2.76	7	1
1:A:27:G:H2'	1:A:28:G:N7	0.44	2.27	8	1
1:B:73:U:O4	1:B:74:C:N4	0.44	2.51	8	1
1:B:60:G:O6	1:B:70:G:C2	0.44	2.70	10	3
1:A:9:G:OP1	1:A:9:G:O4'	0.44	2.35	7	3
1:B:50:U:OP1	1:B:50:U:C1'	0.44	2.66	19	2
1:B:49:A:C8	1:B:80:A:N1	0.44	2.86	6	1
1:B:45:G:O2'	1:B:46:G:C5'	0.44	2.62	14	1
1:B:61:G:HO2'	1:B:62:G:H5'	0.44	1.69	17	1
1:A:4:A:H2'	1:A:5:U:O4'	0.44	2.13	14	1
1:B:58:C:N4	1:B:59:C:C4	0.43	2.86	1	2
1:A:7:U:OP1	1:A:7:U:C2'	0.43	2.66	15	1
1:A:6:A:C1'	1:A:8:G:N7	0.43	2.81	17	1
1:A:21:A:O4'	1:B:81:A:O4'	0.43	2.34	18	1
1:B:49:A:C2	1:B:51:G:N9	0.43	2.86	18	1
1:B:76:U:O2'	1:B:77:C:H5'	0.43	2.13	2	1
1:B:48:U:C4'	1:B:49:A:OP1	0.43	2.65	17	5
1:A:31:C:C4	1:A:32:U:O4	0.43	2.71	4	1
1:A:36:U:O4	1:A:37:A:C6	0.43	2.71	7	1
1:A:1:G:O5'	1:A:1:G:H8	0.43	1.96	8	1
1:A:21:A:C6	1:A:22:A:N1	0.43	2.87	10	1
1:A:29:U:HO2'	1:A:30:U:C5'	0.43	2.26	15	1
1:A:28:G:O2'	1:A:29:U:H5'	0.43	2.13	20	2
1:A:10:A:O2'	1:A:11:A:H5'	0.43	2.13	16	2
1:A:38:A:HO2'	1:A:39:G:P	0.43	2.36	15	1
1:B:72:U:HO2'	1:B:73:U:H5'	0.43	1.72	19	1
1:B:58:C:HO2'	1:B:59:C:H5'	0.43	1.72	2	1
1:A:26:U:HO2'	1:A:27:G:C4'	0.43	2.27	18	1
1:B:49:A:C2'	1:B:51:G:N7	0.43	2.81	2	2
1:B:66:A:OP1	1:B:66:A:C4'	0.43	2.67	11	1
1:A:8:G:C1'	1:B:65:A:H61	0.43	2.27	12	1
1:B:81:A:O2'	1:B:82:G:OP1	0.43	2.37	19	1
1:B:84:C:O2'	1:B:85:C:O4'	0.43	2.35	2	1
1:B:65:A:C6	1:B:66:A:C5	0.43	3.06	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:U:C5'	1:A:6:A:OP2	0.43	2.61	13	1
1:B:66:A:C2'	1:B:67:C:O4'	0.43	2.59	2	1
1:A:26:U:O2'	1:A:27:G:C4'	0.43	2.67	4	2
1:B:50:U:C4'	1:B:51:G:OP1	0.43	2.67	16	2
1:A:6:A:C4	1:A:7:U:C5	0.43	3.06	20	1
1:A:8:G:O4'	1:B:64:A:N6	0.43	2.51	12	1
1:A:37:A:H8	1:A:37:A:O5'	0.43	1.96	12	1
1:A:6:A:C6	1:A:8:G:C8	0.43	3.07	14	1
1:A:6:A:OP2	1:A:6:A:H4'	0.43	2.12	18	1
1:B:49:A:N9	1:B:51:G:N7	0.42	2.67	6	1
1:B:64:A:C8	1:B:65:A:C8	0.42	3.06	7	1
1:A:36:U:OP1	1:A:36:U:C4'	0.42	2.66	2	1
1:B:51:G:C2'	1:B:52:G:O4'	0.42	2.60	10	1
1:A:41:C:H2'	1:A:42:C:C6	0.42	2.50	8	4
1:B:69:U:C4	1:B:70:G:C6	0.42	3.08	10	2
1:A:6:A:H1'	1:A:7:U:O5'	0.42	2.15	11	1
1:A:39:G:H8	1:A:39:G:O5'	0.42	1.98	13	1
1:B:83:U:O5'	1:B:83:U:C6	0.42	2.65	19	2
1:B:80:A:C4'	1:B:81:A:OP1	0.42	2.64	15	1
1:A:21:A:C2	1:B:81:A:C8	0.42	3.08	17	1
1:B:49:A:H4'	1:B:50:U:OP2	0.42	2.13	3	1
1:A:5:U:O3'	1:A:6:A:H4'	0.42	2.15	13	1
1:A:20:G:C2'	1:A:22:A:N7	0.42	2.83	16	1
1:B:48:U:H2'	1:B:80:A:N1	0.42	2.30	17	1
1:A:6:A:O4'	1:A:6:A:OP2	0.42	2.37	18	1
1:A:7:U:C5'	1:A:7:U:C6	0.42	3.03	12	1
1:B:79:U:O2'	1:B:80:A:O5'	0.42	2.38	17	1
1:B:64:A:C4'	1:B:65:A:OP1	0.42	2.65	6	1
1:B:79:U:H4'	1:B:79:U:OP1	0.42	2.15	13	1
1:B:78:C:C2'	1:B:79:U:O5'	0.42	2.68	20	1
1:B:76:U:O2'	1:B:77:C:C5'	0.41	2.68	2	1
1:A:6:A:C6	1:A:8:G:N9	0.41	2.87	3	1
1:B:48:U:C4	1:B:80:A:N7	0.41	2.88	4	1
1:B:62:G:C5	1:B:63:G:C6	0.41	3.08	11	1
1:B:64:A:C6	1:B:65:A:C2	0.41	3.08	14	1
1:A:8:G:C2'	1:A:9:G:O5'	0.41	2.66	17	1
1:A:38:A:C1'	1:B:64:A:C8	0.41	3.03	6	1
1:A:40:U:C4	1:A:41:C:N4	0.41	2.88	10	1
1:A:38:A:C2'	1:A:39:G:O5'	0.41	2.69	15	1
1:A:21:A:O2'	1:A:22:A:OP1	0.41	2.31	12	1
1:A:22:A:C6	1:A:23:A:N6	0.41	2.88	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:69:U:N3	1:B:70:G:C5	0.41	2.88	7	1
1:A:21:A:C6	1:B:49:A:N1	0.41	2.88	13	1
1:A:26:U:C4	1:A:27:G:C5	0.41	3.09	9	1
1:B:85:C:H6	1:B:85:C:O5'	0.41	1.99	19	1
1:A:6:A:OP2	1:A:6:A:O4'	0.41	2.39	9	1
1:A:21:A:C4	1:A:22:A:C8	0.41	3.09	9	1
1:A:22:A:N1	1:A:23:A:C6	0.41	2.89	15	1
1:A:15:C:N4	1:A:16:C:H42	0.41	2.11	20	1
1:A:24:C:O5'	1:A:24:C:H6	0.41	1.98	6	1
1:B:49:A:C5	1:B:51:G:C8	0.41	3.08	6	1
1:A:6:A:C2	1:A:8:G:N9	0.41	2.89	13	1
1:A:31:C:H2'	1:A:32:U:C6	0.41	2.50	15	1
1:B:58:C:C4	1:B:59:C:N3	0.41	2.88	1	1
1:B:69:U:O4	1:B:70:G:O6	0.41	2.39	7	1
1:A:5:U:O3'	1:A:6:A:C4'	0.41	2.68	13	1
1:A:32:U:H2'	1:A:33:U:C6	0.41	2.51	13	1
1:A:6:A:C4'	1:A:7:U:OP2	0.41	2.69	17	1
1:A:1:G:HO2'	1:A:2:G:H5'	0.41	1.74	18	1
1:A:7:U:H2'	1:A:8:G:O5'	0.41	2.15	20	1
1:A:8:G:N7	1:A:9:G:C8	0.40	2.89	1	1
1:B:49:A:N7	1:B:51:G:C5	0.40	2.89	6	1
1:A:22:A:C4'	1:A:22:A:OP1	0.40	2.69	19	1
1:B:65:A:N1	1:B:66:A:C6	0.40	2.88	19	1
1:B:57:A:O5'	1:B:57:A:H8	0.40	1.99	4	1
1:A:7:U:C4	1:A:39:G:N2	0.40	2.89	10	1
1:B:65:A:C5	1:B:66:A:C5	0.40	3.09	11	1
1:A:34:C:O2'	1:A:35:C:H5'	0.40	2.16	13	1
1:B:67:C:O2'	1:B:68:U:C5'	0.40	2.55	13	1
1:B:84:C:H2'	1:B:85:C:C6	0.40	2.51	19	1
1:A:35:C:H2'	1:A:36:U:O5'	0.40	2.17	3	1
1:A:36:U:OP1	1:A:36:U:O4'	0.40	2.39	16	1
1:B:49:A:H2'	1:B:51:G:N7	0.40	2.31	2	1
1:A:6:A:C6	1:A:8:G:C5	0.40	3.09	5	1
1:A:6:A:C2	1:A:7:U:C6	0.40	3.09	6	1
1:A:14:A:C5	1:A:15:C:C4	0.40	3.10	10	1
1:B:49:A:P	1:B:49:A:O4'	0.40	2.78	19	1
1:A:8:G:O2'	1:A:9:G:O5'	0.40	2.35	12	1
1:B:68:U:O2'	1:B:69:U:O4'	0.40	2.35	12	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	42/43 (98%)	11±1 (25±3%)	2±1 (4±3%)	0.33±0.02
1	B	42/43 (98%)	11±1 (26±3%)	2±1 (5±2%)	0.36±0.02
All	All	1680/1720 (98%)	429 (26%)	71 (4%)	0.34

The overall RNA backbone suiteness is 0.34.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	9	G	20
1	A	23	A	20
1	B	52	G	20
1	B	66	A	20
1	A	7	U	19
1	A	8	G	19
1	A	20	G	19
1	A	36	U	19
1	B	51	G	19
1	B	63	G	19
1	A	6	A	18
1	B	49	A	18
1	B	50	U	18
1	A	22	A	17
1	A	38	A	17
1	B	64	A	17
1	B	65	A	17
1	B	79	U	17
1	A	21	A	15
1	B	81	A	13
1	B	82	G	12

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Mol	Chain	Res	Type	Models (Total)
1	B	78	C	10
1	A	39	G	10
1	B	80	A	9
1	A	37	A	9
1	A	35	C	8
1	B	77	C	5
1	A	34	C	4
1	B	53	A	1

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	50	U	10
1	A	21	A	7
1	A	6	A	7
1	B	48	U	6
1	B	49	A	6
1	B	65	A	5
1	B	64	A	5
1	B	81	A	4
1	A	7	U	4
1	A	22	A	3
1	A	5	U	3
1	A	35	C	2
1	A	38	A	2
1	B	79	U	2
1	A	39	G	1
1	A	23	A	1
1	B	78	C	1
1	B	77	C	1
1	B	82	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)

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