



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 12:19 AM BST

PDB ID : 2L1F
Title : Structure of a conserved retroviral RNA packaging element by NMR spectroscopy and cryo-electron tomography
Authors : Summers, M.F.; Irobalieva, R.N.; Tolbert, B.; Smalls-Manty, A.; Iyalla, K.; Loeliger, K.; D'Souza, V.; Khant, H.; Schmid, M.; Garcia, E.; Telesnitsky, A.; Chiu, W.; Miyazaki, Y.
Deposited on : 2010-07-28

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

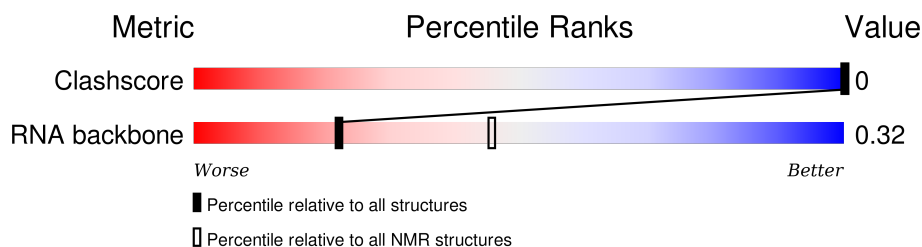
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

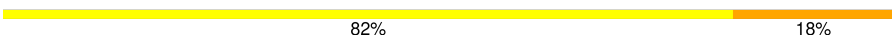
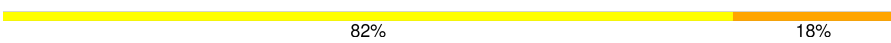
The overall completeness of chemical shifts assignment is 8%.

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
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	A	65	 82% 18%
2	B	66	 82% 18%

2 Ensemble composition and analysis ⓘ

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4246 atoms, of which 1427 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called RNA (65-MER).

Mol	Chain	Residues	Atoms						Trace
1	A	65	Total	C	H	N	O	P	0
			2106	622	708	262	449	65	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	328	A	U	ENGINEERED MUTATION	GB AF033811.1
A	333	U	A	ENGINEERED MUTATION	GB AF033811.1

- Molecule 2 is a RNA chain called RNA (66-MER).

Mol	Chain	Residues	Atoms						Trace
2	B	66	Total	C	H	N	O	P	0
			2140	632	719	267	456	66	

There are 2 discrepancies between the modelled and reference sequences:

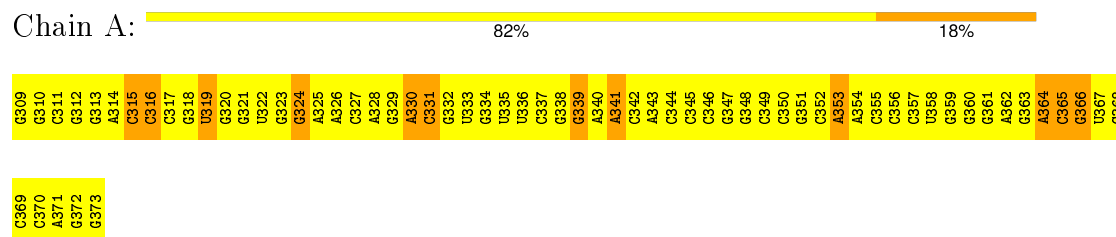
Chain	Residue	Modelled	Actual	Comment	Reference
B	728	A	U	ENGINEERED MUTATION	GB AF033811.1
B	733	U	A	ENGINEERED MUTATION	GB AF033811.1

4 Residue-property plots

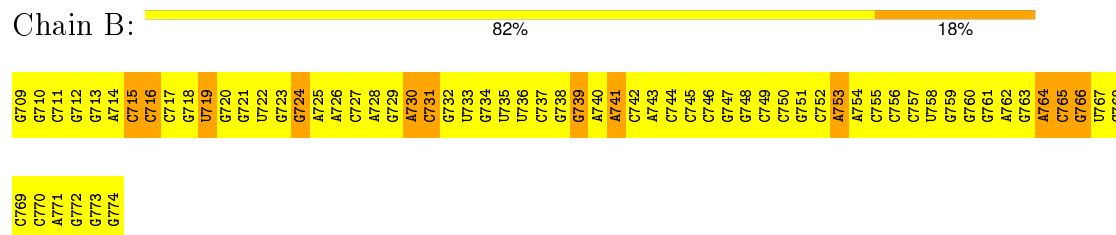
4.1 Average score per residue in the NMR ensemble

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: RNA (65-MER)



- Molecule 2: RNA (66-MER)

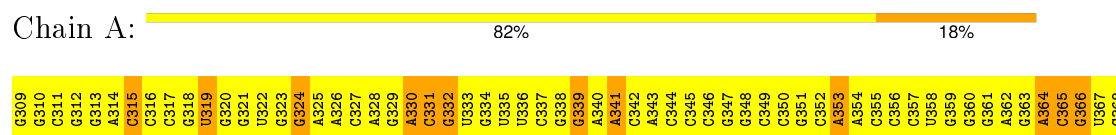


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: RNA (65-MER)



C369
C370
A371
G372
G373

- Molecule 2: RNA (66-MER)

Chain B:



G709 G710 G711 G712 G713 G714 G715 G716 G717 G718 G719 G720 G721 G722 G723 G724 G725 A726 A727 A728 G729 A730 A731 G732 G733 G734 U735 U736 G737 G738 G739 A740 A741 G742 A743 C744 C745 C746 G747 G748 C749 C750 G751 G752 A753 A754 C755 C756 C757 U758 G759 G760 G761 A762 G763 A764 C765 G766 U767 C768

C769
C770
A771
G772
G773
G774

4.2.2 Score per residue for model 2

- Molecule 1: RNA (65-MER)

Chain A:



G309 G310 G311 G312 G313 A314 G315 G316 C317 G318 U319 G320 G321 U322 G323 G324 A325 A326 C327 A328 G329 A330 A331 G332 U333 G334 U335 U336 G337 G338 G339 A340 A341 C342 A343 C344 C345 C346 G347 G348 C349 C350 G351 C352 A353 A354 C355 C356 C357 U358 G359 G360 G361 A362 G363 A364 C365 G366 U367 C368

C369
C370
A371
G372
G373

- Molecule 2: RNA (66-MER)

Chain B:



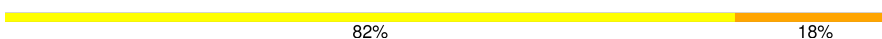
G709 G710 G711 G712 G713 G714 G715 G716 G717 G718 U719 G720 G721 U722 G723 G724 A725 A726 A727 A728 G729 A730 A731 G732 G733 G734 U735 U736 G737 G738 G739 A740 A741 G742 A743 C744 C745 C746 G747 G748 C749 C750 G751 G752 A753 A754 C755 C756 C757 U758 G759 G760 G761 A762 G763 A764 C765 G766 U767 C768

C769
C770
A771
G772
G773
G774

4.2.3 Score per residue for model 3

- Molecule 1: RNA (65-MER)

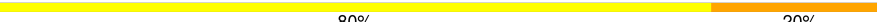
Chain A:



G309 G310 G311 G312 G313 A314 G315 G316 C317 G318 U319 G320 G321 U322 G323 G324 A325 A326 C327 A328 G329 A330 A331 G332 U333 G334 U335 U336 G337 G338 G339 A340 A341 C342 A343 C344 C345 C346 G347 G348 C349 C350 G351 C352 A353 A354 C355 C356 C357 U358 G359 G360 G361 A362 G363 A364 C365 G366 U367 C368

C369
C370
A371
G372
G373

- Molecule 2: RNA (66-MER)


Chain B:  80% 20%

G709	G710	G711	G712	G713	A714	C715	C716	C717	G718	U719	G720	G721	U722	G723	G724	A725	A726	C727	A728	G729	A730	C731	G732	U733	G734	U735	U736	C737	G738	G739	A740	A741	C742	A743	C744	C745	C746	G747	G748	C749	C750	G751	C752	A753	A754	C755	C756	C757	U758	G759	G760	A761	A762	G763	A764	C765	G766	U767	C768
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C769	C770	A771	G772	G773	G774
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4.2.4 Score per residue for model 4


- Molecule 1: RNA (65-MER)

Chain A:  80% 20%

G309	G310	C311	G312	G313	A314	C315	C316	C317	G318	U319	G320	G321	U322	G323	G324	A325	A326	C327	A328	G329	A330	C331	G332	U333	G334	U335	U336	C337	G338	G339	A340	A341	C342	A343	C344	C345	C346	G347	G348	C349	C350	G351	C352	A353	A354	C355	C356	C357	U358	G359	G360	G361	A362	G363	A364	C365	G366	U367	C368
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C369	C370	A371	G372	G373
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- Molecule 2: RNA (66-MER)


Chain B:  80% 20%

G709	G710	C711	G712	G713	A714	C715	C716	C717	G718	U719	G720	G721	U722	G723	G724	A725	A726	C727	A728	G729	A730	C731	G732	U733	G734	U735	U736	C737	G738	G739	A740	A741	C742	A743	C744	C745	C746	G747	G748	C749	C750	G751	C752	A753	A754	C755	C756	C757	U758	G759	G760	A761	A762	G763	A764	C765	G766	U767	C768
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C769	C770	A771	G772	G773	G774
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4.2.5 Score per residue for model 5

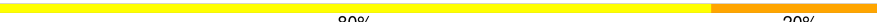
- Molecule 1: RNA (65-MER)

Chain A:  80% 20%

G309	G310	C311	G312	G313	A314	C315	C316	C317	G318	U319	G320	G321	U322	G323	G324	A325	A326	C327	A328	G329	A330	C331	G332	U333	G334	U335	U336	C337	G338	G339	A340	A341	C342	A343	C344	C345	C346	G347	G348	C349	C350	G351	C352	A353	A354	C355	C356	C357	U358	G359	G360	G361	A362	G363	A364	C365	G366	U367	C368
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C369	C370	A371	G372	G373
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- Molecule 2: RNA (66-MER)

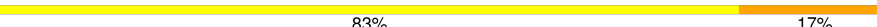
Chain B:  80% 20%

G709	G710	C711	G712	G713	A714	C715	C716	C717	G718	U719	G720	G721	U722	G723	G724	A725	A726	C727	A728	G729	A730	C731	G732	U733	G734	U735	U736	C737	G738	G739	A740	A741	C742	A743	C744	C745	C746	G747	G748	C749	C750	G751	C752	A753	A754	C755	C756	C757	U758	G759	G760	A761	A762	G763	A764	C765	G766	U767	C768
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C769
C770
A771
G772
G773
G774

4.2.6 Score per residue for model 6


- Molecule 1: RNA (65-MER)

Chain A:  83% 17%

G309 G310 G311 G312 G313 G314 G315 G316 G317 G318 G319 G320 G321 G322 G323 G324 G325 A326 G327 A328 G329 A330 A331 G332 G333 G334 G335 G336 G337 G338 G339 A340 A341 A343 G344 G345 G346 G347 G348 G349 G350 G351 G352 A353 A354 G355 G356 G357 G358 G359 G360 G361 A362 G363 A364 G365 G366 G367 G368

C369
C370
A371
G372
G373

- Molecule 2: RNA (66-MER)


Chain B:  82% 18%

G709 G710 G711 G712 G713 A714 G715 G716 G717 G718 G719 G720 G721 G722 G723 G724 A725 A726 G727 A728 G729 A730 A731 G732 G733 G734 G735 G736 G737 G738 G739 A740 A741 A743 G744 G745 G746 G747 G748 G749 G750 G751 G752 A753 A754 G755 G756 G757 G758 G759 G760 G761 A762 G763 A764 G765 G766 G767 G768

C769
C770
A771
G772
G773
G774

4.2.7 Score per residue for model 7


- Molecule 1: RNA (65-MER)

Chain A:  78% 22%

G309 G310 G311 G312 G313 G314 G315 G316 G317 G318 G319 G320 G321 G322 G323 G324 A325 A326 G327 A328 G329 A330 A331 G332 G333 G334 G335 G336 G337 G338 G339 A340 A341 A343 G344 G345 G346 G347 G348 G349 G350 G351 G352 A353 A354 G355 G356 G357 G358 G359 G360 G361 A362 G363 A364 G365 G366 G367 G368

C369
C370
A371
G372
G373

- Molecule 2: RNA (66-MER)

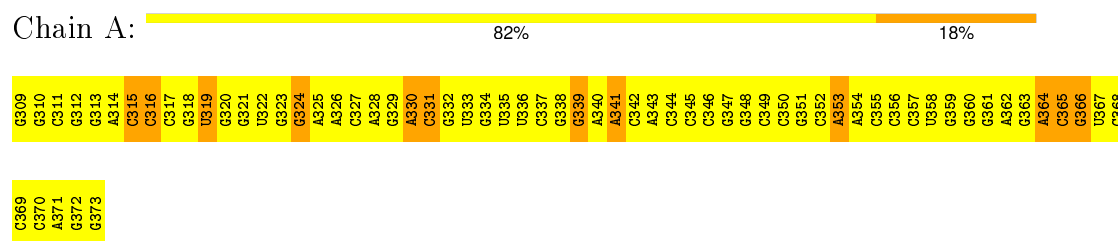
Chain B:  82% 18%

G709 G710 G711 G712 G713 A714 G715 G716 G717 G718 G719 G720 G721 G722 G723 G724 A725 A726 G727 A728 G729 A730 A731 G732 G733 G734 G735 G736 G737 G738 G739 A740 A741 A743 G744 G745 G746 G747 G748 G749 G750 G751 G752 A753 A754 G755 G756 G757 G758 G759 G760 G761 A762 G763 A764 G765 G766 G767 G768

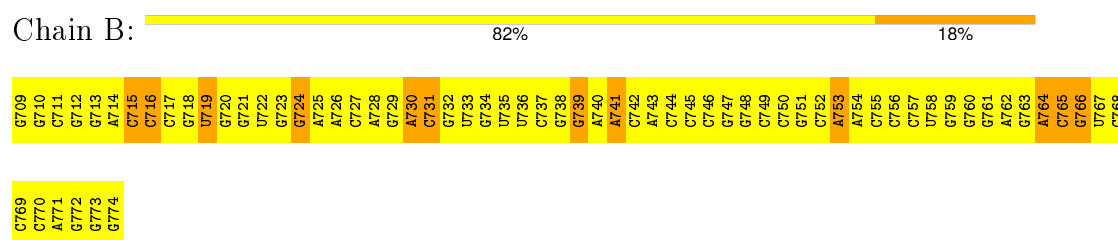
C769
C770
A771
G772
G773
G774

4.2.8 Score per residue for model 8

- Molecule 1: RNA (65-MER)

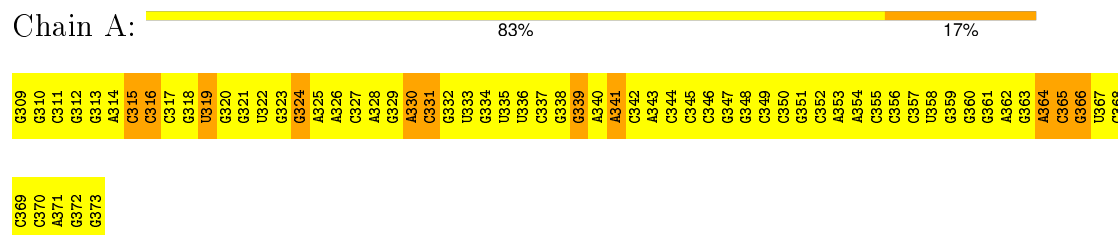


- Molecule 2: RNA (66-MER)

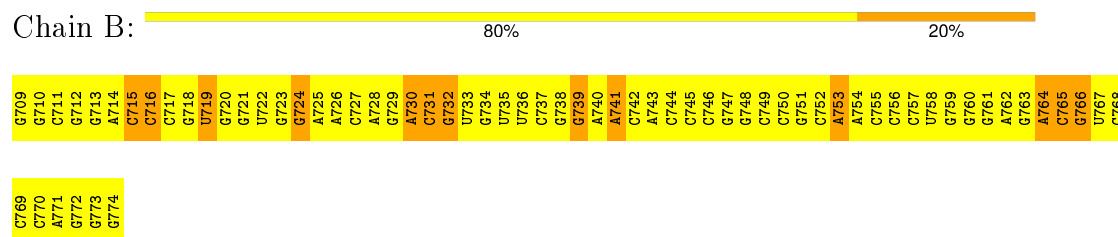


4.2.9 Score per residue for model 9

- Molecule 1: RNA (65-MER)

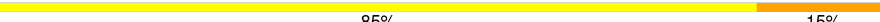


- Molecule 2: RNA (66-MER)



4.2.10 Score per residue for model 10


- Molecule 1: RNA (65-MER)

Chain A:  85% 15%

G309	G310	G311	G312	G313	A314	C315	C316	C317	G318	U319	G320	G321	U322	G323	G324	A325	A326	C327	A328	G329	A330	C331	G332	U333	G334	U335	U336	C337	G338	G339	A340	A341	C342	A343	C344	C345	C346	G347	G348	C349	C350	G351	C352	A353	A354	C355	C356	C357	U358	G359	G360	G361	A362	G363	A364	C365	G366	U367	C368
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G369	C370	A371	G372	G373
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- Molecule 2: RNA (66-MER)


Chain B:  80% 20%

G709	G710	G711	G712	G713	A714	C715	C716	C717	G718	U719	G720	G721	U722	G723	G724	A725	A726	C727	A728	G729	A730	C731	G732	U733	G734	U735	U736	C737	G738	G739	A740	A741	C742	A743	C744	C745	C746	G747	G748	C749	C750	G751	C752	A753	A754	C755	C756	C757	U758	G759	G760	G761	A762	G763	A764	C765	G766	U767	C768
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G769	C770	A771	G772	G773	G774
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4.2.11 Score per residue for model 11

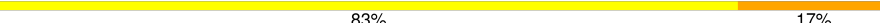
- Molecule 1: RNA (65-MER)

Chain A:  80% 20%

G309	G310	C311	G312	G313	A314	C315	C316	C317	G318	U319	G320	G321	U322	G323	G324	A325	A326	C327	A328	G329	A330	C331	G332	U333	G334	U335	U336	C337	G338	G339	A340	A341	C342	A343	C344	C345	C346	G347	G348	C349	C350	G351	C352	A353	A354	C355	C356	C357	U358	G359	G360	G361	A362	G363	A364	C365	G366	U367	C368
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G369	C370	A371	G372	G373
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- Molecule 2: RNA (66-MER)

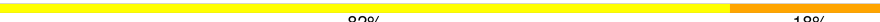
Chain B:  83% 17%

G709	G710	G711	G712	G713	A714	C715	C716	C717	G718	U719	G720	G721	U722	G723	G724	A725	A726	C727	A728	G729	A730	C731	G732	U733	G734	U735	U736	C737	G738	G739	A740	A741	C742	A743	C744	C745	C746	G747	G748	C749	C750	G751	C752	A753	A754	C755	C756	C757	U758	G759	G760	G761	A762	G763	A764	C765	G766	U767	C768
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G769	C770	A771	G772	G773	G774
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4.2.12 Score per residue for model 12


- Molecule 1: RNA (65-MER)

Chain A:  82% 18%

G309	G310	C311	G312	G313	A314	C315	C316	C317	G318	U319	G320	G321	U322	G323	G324	A325	A326	C327	A328	G329	A330	C331	G332	U333	G334	U335	U336	C337	G338	G339	A340	A341	C342	A343	C344	C345	C346	G347	G348	C349	C350	G351	C352	A353	A354	C355	C356	C357	U358	G359	G360	G361	A362	G363	A364	C365	G366	U367	C368
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C369
C370
A371
G372
G373

- Molecule 2: RNA (66-MER)


Chain B:  80% 20%

G709 G710 G711 G712 G713 G714 A715 C716 C717 G718 G719 U720 G721 U722 G723 G724 A725 A726 A727 A728 G729 A730 C731 C732 U733 G734 U735 U736 C737 C738 G739 A740 A741 C742 A743 C744 C745 C746 G747 G748 C749 C750 G751 C752 A753 A754 C755 C756 C757 U758 G759 G760 G761 A762 G763 A764 C765 G766 U767 C768

C769
C770
A771
G772
G773
G774

4.2.13 Score per residue for model 13


- Molecule 1: RNA (65-MER)

Chain A:  80% 20%

G309 G310 G311 G312 G313 G314 A315 C316 C317 G318 U319 G320 G321 U322 G323 G324 A325 A326 C327 A328 G329 A330 C331 G332 U333 G334 U335 U336 C337 G338 G339 A340 A341 C342 A343 C344 C345 C346 G347 G348 C349 C350 G351 C352 A353 A354 C355 C356 C357 U358 G359 G360 G361 A362 G363 A364 C365 G366 U367 C368

C369
C370
A371
G372
G373

- Molecule 2: RNA (66-MER)

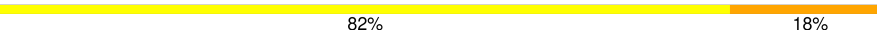
Chain B:  83% 17%

G709 G710 G711 G712 G713 G714 A715 C716 C717 G718 U719 G720 G721 U722 G723 G724 A725 A726 A727 A728 G729 A730 C731 C732 U733 G734 U735 U736 C737 C738 G739 A740 A741 C742 A743 C744 C745 C746 G747 G748 C749 C750 G751 C752 A753 A754 C755 C756 C757 U758 G759 G760 G761 A762 G763 A764 C765 G766 U767 C768

C769
C770
A771
G772
G773
G774

4.2.14 Score per residue for model 14


- Molecule 1: RNA (65-MER)

Chain A:  82% 18%

G309 G310 G311 G312 G313 G314 A315 C316 C317 G318 U319 G320 G321 U322 G323 G324 A325 A326 C327 A328 G329 A330 C331 G332 U333 G334 U335 U336 C337 G338 G339 A340 A341 C342 A343 C344 C345 C346 G347 G348 C349 C350 G351 C352 A353 A354 C355 C356 C357 U358 G359 G360 G361 A362 G363 A364 C365 G366 U367 C368

C369
C370
A371
G372
G373

- Molecule 2: RNA (66-MER)


Chain B:  83% 17%

G709	G710	G711	G712	G713	A714	C715	C716	C717	G718	U719	G720	G721	U722	G723	G724	A725	A726	C727	A728	G729	A730	C731	G732	U733	G734	U735	U736	C737	G738	G739	A740	A741	C742	A743	C744	C745	C746	G747	G748	C749	C750	G751	C752	A753	A754	C755	C756	C757	U758	G759	G760	G761	A762	G763	A764	C765	G766	U767	C768
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

C769	C770	A771	G772	G773	G774
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4.2.15 Score per residue for model 15


- Molecule 1: RNA (65-MER)

Chain A:  83% 17%

G309	G310	C311	G312	G313	A314	C315	C316	C317	G318	U319	G320	G321	U322	G323	G324	A325	A326	C327	A328	G329	A330	C331	G332	U333	G334	U335	U336	C337	G338	G339	A340	A341	C342	A343	C344	C345	C346	G347	G348	C349	C350	G351	C352	A353	A354	C355	C356	C357	U358	G359	G360	G361	A362	G363	A364	C365	G366	U367	C368
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

C369	C370	A371	G372	G373
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- Molecule 2: RNA (66-MER)


Chain B:  83% 17%

G709	G710	G711	G712	G713	A714	C715	C716	C717	G718	U719	G720	G721	U722	G723	G724	A725	A726	C727	A728	G729	A730	C731	G732	U733	G734	U735	U736	C737	G738	G739	A740	A741	C742	A743	C744	C745	C746	G747	G748	C749	C750	G751	C752	A753	A754	C755	C756	C757	U758	G759	G760	G761	A762	G763	A764	C765	G766	U767	C768
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

C769	C770	A771	G772	G773	G774
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4.2.16 Score per residue for model 16


- Molecule 1: RNA (65-MER)

Chain A:  82% 18%

G309	G310	C311	G312	G313	A314	C315	C316	C317	G318	U319	G320	G321	U322	G323	G324	A325	A326	C327	A328	G329	A330	C331	G332	U333	G334	U335	U336	C337	G338	G339	A340	A341	C342	A343	C344	C345	C346	G347	G348	C349	C350	G351	C352	A353	A354	C355	C356	C357	U358	G359	G360	G361	A362	G363	A364	C365	G366	U367	C368
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

C369	C370	A371	G372	G373
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- Molecule 2: RNA (66-MER)

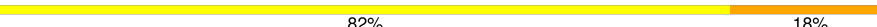
Chain B:  83% 17%

G709	G710	G711	G712	G713	A714	C715	C716	C717	G718	U719	G720	G721	U722	G723	G724	A725	A726	C727	A728	G729	A730	C731	G732	U733	G734	U735	U736	C737	G738	G739	A740	A741	C742	A743	C744	C745	C746	G747	G748	C749	C750	G751	C752	A753	A754	C755	C756	C757	U758	G759	G760	G761	A762	G763	A764	C765	G766	U767	C768
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

G769
C770
A771
G772
G773
G774

4.2.17 Score per residue for model 17


- Molecule 1: RNA (65-MER)

Chain A:  82% 18%

G309 G310 G311 G312 G313 G314 G315 G316 G317 G318 G319 G320 G321 G322 G323 G324 G325 A326 G327 A328 G329 A330 G331 G332 G333 G334 G335 G336 G337 G338 G339 G340 A341 A342 A343 G344 G345 G346 G347 G348 G349 G350 G351 G352 A353 A354 G355 G356 G357 G358 G359 G360 G361 G362 G363 A364 G365 G366 G367 G368

C369
C370
A371
G372
G373

- Molecule 2: RNA (66-MER)


Chain B:  82% 18%

G709 G710 G711 G712 G713 A714 G715 G716 G717 G718 G719 G720 G721 G722 G723 G724 A725 A726 G727 A728 G729 A730 G731 G732 G733 G734 G735 G736 G737 G738 G739 A740 A741 G742 G743 G744 G745 G746 G747 G748 G749 G750 G751 G752 A753 A754 G755 G756 G757 G758 G759 G760 G761 A762 G763 G764 G765 G766 G767 G768

G769
C770
A771
G772
G773
G774

4.2.18 Score per residue for model 18


- Molecule 1: RNA (65-MER)

Chain A:  83% 17%

G309 G310 G311 G312 G313 G314 G315 G316 G317 G318 G319 G320 G321 G322 G323 G324 A325 A326 G327 A328 G329 A330 G331 G332 G333 G334 G335 G336 G337 G338 G339 A340 A341 A342 A343 G344 G345 G346 G347 G348 G349 G350 G351 G352 A353 A354 G355 G356 G357 G358 G359 G360 G361 A362 G363 G364 A365 G366 G367 G368

C369
C370
A371
G372
G373

- Molecule 2: RNA (66-MER)

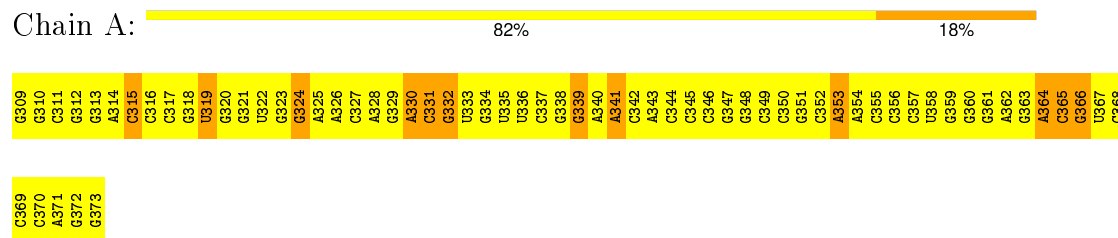
Chain B:  80% 20%

G709 G710 G711 G712 G713 A714 G715 G716 G717 G718 G719 G720 G721 G722 G723 G724 A725 A726 G727 A728 G729 A730 G731 G732 G733 G734 G735 G736 G737 G738 G739 A740 A741 G742 G743 G744 G745 G746 G747 G748 G749 G750 G751 G752 A753 A754 G755 G756 G757 G758 G759 G760 G761 A762 G763 G764 G765 G766 G767 G768

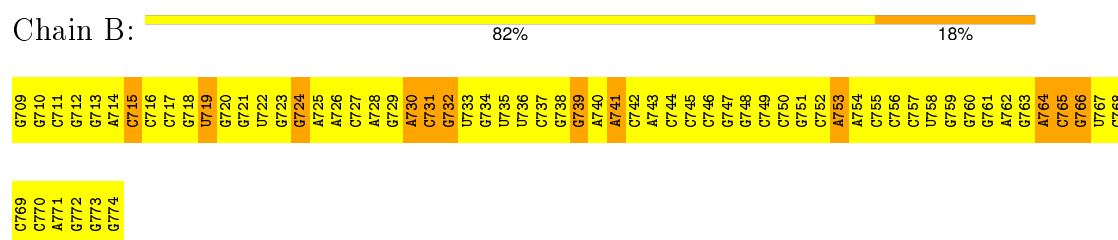
G769
C770
A771
G772
G773
G774

4.2.19 Score per residue for model 19

- Molecule 1: RNA (65-MER)

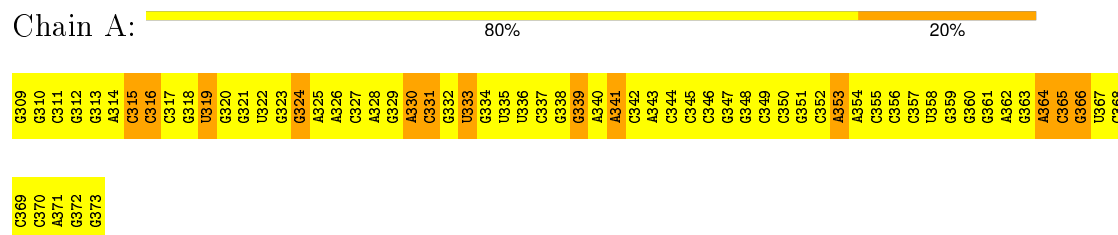


- Molecule 2: RNA (66-MER)

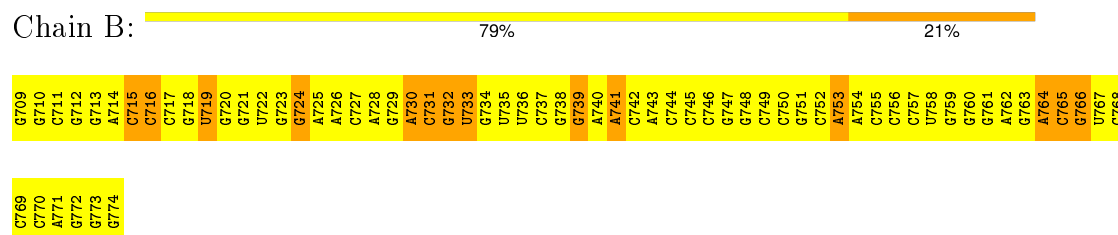


4.2.20 Score per residue for model 20

- Molecule 1: RNA (65-MER)



- Molecule 2: RNA (66-MER)



5 Refinement protocol and experimental data overview

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

Of the 340 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
CYANA	structure solution	2.1
CYANA	refinement	2.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 17083
Number of chemical shift lists	1
Total number of shifts	208
Number of shifts mapped to atoms	208
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	8%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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	1.55±0.00	0±0/1564 (0.0±0.0%)	3.37±0.01	262±2/2439 (10.7±0.1%)
2	B	1.55±0.00	0±0/1590 (0.0±0.0%)	3.39±0.01	268±2/2480 (10.8±0.1%)
All	All	1.55	0/63080 (0.0%)	3.38	10603/98380 (10.8%)

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	339	G	O4'-C4'-C3'	-14.23	89.77	104.00	16	20
2	B	739	G	O4'-C4'-C3'	-14.06	89.94	104.00	9	20
1	A	340	A	O4'-C4'-C3'	-13.95	90.06	104.00	5	20
1	A	328	A	O4'-C4'-C3'	-13.68	90.32	104.00	9	20
2	B	728	A	O4'-C4'-C3'	-13.52	90.48	104.00	19	20
2	B	762	A	O4'-C4'-C3'	-13.36	90.64	104.00	15	20
1	A	362	A	O4'-C4'-C3'	-13.32	90.68	104.00	16	20
2	B	734	G	O4'-C4'-C3'	-13.29	90.71	104.00	9	20
2	B	719	U	O4'-C4'-C3'	-13.22	90.78	104.00	7	20
1	A	319	U	O4'-C4'-C3'	-13.18	90.82	104.00	9	20
1	A	334	G	O4'-C4'-C3'	-13.11	90.89	104.00	8	20
2	B	764	A	O4'-C4'-C3'	-12.96	91.04	104.00	7	20
2	B	741	A	O4'-C4'-C3'	-12.92	91.08	104.00	7	20
2	B	740	A	O4'-C4'-C3'	-12.83	91.17	104.00	7	20
1	A	341	A	O4'-C4'-C3'	-12.82	91.18	104.00	7	20
1	A	314	A	O4'-C4'-C3'	-12.78	91.22	104.00	10	20
1	A	364	A	O4'-C4'-C3'	-12.78	91.22	104.00	11	20
2	B	714	A	O4'-C4'-C3'	-12.77	91.23	104.00	13	20
2	B	720	G	O4'-C4'-C3'	-12.62	91.38	104.00	3	20
1	A	323	G	O4'-C4'-C3'	-12.60	91.40	104.00	5	20
2	B	730	A	O4'-C4'-C3'	-12.49	91.51	104.00	17	14
1	A	330	A	O4'-C4'-C3'	-12.47	91.53	104.00	16	12
2	B	758	U	O4'-C4'-C3'	-12.14	91.86	104.00	16	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	358	U	O4'-C4'-C3'	-12.13	91.87	104.00	9	20
2	B	709	G	O4'-C4'-C3'	-12.07	91.93	104.00	11	20
2	B	774	G	O4'-C4'-C3'	-12.05	91.95	104.00	6	20
1	A	348	G	C5-C6-N1	12.03	117.52	111.50	7	20
2	B	712	G	C5-C6-N1	12.03	117.52	111.50	10	20
2	B	723	G	C5-C6-N1	12.01	117.50	111.50	1	20
1	A	320	G	C5-C6-N1	12.00	117.50	111.50	8	20
2	B	718	G	C5-C6-N1	12.00	117.50	111.50	9	20
2	B	739	G	C5-C6-N1	12.00	117.50	111.50	1	20
2	B	773	G	C5-C6-N1	12.00	117.50	111.50	12	20
1	A	359	G	C5-C6-N1	11.99	117.50	111.50	1	20
1	A	363	G	C5-C6-N1	11.97	117.49	111.50	9	20
2	B	724	G	C5-C6-N1	11.97	117.49	111.50	19	20
1	A	373	G	C5-C6-N1	11.97	117.49	111.50	2	20
1	A	372	G	C5-C6-N1	11.97	117.48	111.50	15	20
1	A	366	G	C5-C6-N1	11.97	117.48	111.50	14	20
1	A	323	G	C5-C6-N1	11.96	117.48	111.50	1	20
1	A	339	G	C5-C6-N1	11.96	117.48	111.50	13	20
2	B	713	G	C5-C6-N1	11.96	117.48	111.50	6	20
2	B	729	G	C5-C6-N1	11.96	117.48	111.50	13	20
2	B	710	G	C5-C6-N1	11.95	117.48	111.50	1	20
1	A	309	G	C5-C6-N1	11.95	117.47	111.50	14	20
2	B	721	G	C5-C6-N1	11.95	117.47	111.50	1	20
2	B	723	G	O4'-C4'-C3'	-11.95	92.05	104.00	16	20
1	A	334	G	C5-C6-N1	11.95	117.47	111.50	19	20
1	A	347	G	C5-C6-N1	11.94	117.47	111.50	6	20
1	A	360	G	C5-C6-N1	11.95	117.47	111.50	19	20
2	B	732	G	C5-C6-N1	11.94	117.47	111.50	12	20
2	B	766	G	C5-C6-N1	11.94	117.47	111.50	14	20
1	A	313	G	C5-C6-N1	11.94	117.47	111.50	5	20
1	A	332	G	C5-C6-N1	11.94	117.47	111.50	6	20
2	B	738	G	C5-C6-N1	11.93	117.47	111.50	8	20
2	B	774	G	C5-C6-N1	11.93	117.47	111.50	6	20
1	A	312	G	C5-C6-N1	11.93	117.46	111.50	16	20
2	B	747	G	C5-C6-N1	11.93	117.47	111.50	19	20
1	A	361	G	C5-C6-N1	11.93	117.46	111.50	1	20
2	B	748	G	C5-C6-N1	11.93	117.46	111.50	4	20
2	B	760	G	C5-C6-N1	11.93	117.46	111.50	10	20
1	A	310	G	C5-C6-N1	11.92	117.46	111.50	16	20
2	B	761	G	C5-C6-N1	11.92	117.46	111.50	12	20
1	A	318	G	C5-C6-N1	11.92	117.46	111.50	14	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	329	G	C5-C6-N1	11.92	117.46	111.50	18	20
2	B	759	G	C5-C6-N1	11.91	117.45	111.50	14	20
2	B	772	G	C5-C6-N1	11.91	117.45	111.50	14	20
2	B	709	G	C5-C6-N1	11.90	117.45	111.50	2	20
2	B	751	G	C5-C6-N1	11.90	117.45	111.50	17	20
1	A	338	G	C5-C6-N1	11.90	117.45	111.50	7	20
1	A	321	G	C5-C6-N1	11.89	117.45	111.50	12	20
1	A	324	G	C5-C6-N1	11.89	117.45	111.50	15	20
2	B	720	G	C5-C6-N1	11.89	117.44	111.50	10	20
2	B	734	G	C5-C6-N1	11.89	117.44	111.50	17	20
2	B	763	G	C5-C6-N1	11.88	117.44	111.50	3	20
1	A	351	G	C5-C6-N1	11.88	117.44	111.50	5	20
1	A	344	C	O4'-C4'-C3'	-11.73	92.27	104.00	14	20
2	B	744	C	O4'-C4'-C3'	-11.71	92.29	104.00	15	20
1	A	370	C	O4'-C4'-C3'	-11.28	92.72	104.00	20	20
1	A	363	G	O4'-C4'-C3'	-11.26	92.74	104.00	2	20
2	B	770	C	O4'-C4'-C3'	-11.25	92.75	104.00	1	20
2	B	718	G	C6-N1-C2	-11.19	118.39	125.10	4	20
2	B	766	G	C6-N1-C2	-11.18	118.39	125.10	14	20
1	A	339	G	C6-N1-C2	-11.17	118.40	125.10	13	20
1	A	359	G	C6-N1-C2	-11.17	118.40	125.10	14	20
2	B	723	G	C6-N1-C2	-11.17	118.40	125.10	1	20
2	B	739	G	C6-N1-C2	-11.17	118.40	125.10	1	20
2	B	724	G	C6-N1-C2	-11.17	118.40	125.10	19	20
1	A	351	G	C6-N1-C2	-11.16	118.40	125.10	5	20
1	A	361	G	C6-N1-C2	-11.15	118.41	125.10	1	20
2	B	712	G	C6-N1-C2	-11.15	118.41	125.10	10	20
1	A	309	G	C6-N1-C2	-11.15	118.41	125.10	4	20
1	A	324	G	C6-N1-C2	-11.15	118.41	125.10	20	20
2	B	772	G	C6-N1-C2	-11.15	118.41	125.10	2	20
2	B	751	G	C6-N1-C2	-11.15	118.41	125.10	1	20
1	A	373	G	C6-N1-C2	-11.14	118.42	125.10	11	20
2	B	721	G	C6-N1-C2	-11.14	118.42	125.10	6	20
2	B	759	G	C6-N1-C2	-11.14	118.42	125.10	17	20
2	B	710	G	C6-N1-C2	-11.14	118.42	125.10	3	20
1	A	312	G	C6-N1-C2	-11.13	118.42	125.10	4	20
1	A	329	G	C6-N1-C2	-11.13	118.42	125.10	10	20
1	A	348	G	C6-N1-C2	-11.13	118.42	125.10	19	20
1	A	372	G	C6-N1-C2	-11.13	118.42	125.10	4	20
1	A	363	G	C6-N1-C2	-11.13	118.42	125.10	9	20
1	A	332	G	C6-N1-C2	-11.13	118.42	125.10	15	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	318	G	C6-N1-C2	-11.12	118.43	125.10	3	20
1	A	366	G	C6-N1-C2	-11.12	118.43	125.10	14	20
2	B	761	G	C6-N1-C2	-11.12	118.43	125.10	19	20
2	B	763	G	O4'-C4'-C3'	-11.12	92.88	104.00	18	20
1	A	310	G	C6-N1-C2	-11.11	118.43	125.10	1	20
1	A	320	G	C6-N1-C2	-11.11	118.43	125.10	1	20
2	B	732	G	C6-N1-C2	-11.11	118.43	125.10	19	20
2	B	713	G	C6-N1-C2	-11.11	118.43	125.10	4	20
1	A	334	G	C6-N1-C2	-11.11	118.44	125.10	19	20
2	B	773	G	C6-N1-C2	-11.11	118.44	125.10	12	20
1	A	360	G	C6-N1-C2	-11.10	118.44	125.10	8	20
1	A	347	G	C6-N1-C2	-11.10	118.44	125.10	8	20
2	B	760	G	C6-N1-C2	-11.10	118.44	125.10	19	20
2	B	732	G	O4'-C4'-C3'	-11.09	92.91	104.00	18	20
2	B	738	G	C6-N1-C2	-11.09	118.44	125.10	1	20
1	A	313	G	C6-N1-C2	-11.09	118.45	125.10	20	20
2	B	720	G	C6-N1-C2	-11.08	118.45	125.10	10	20
1	A	338	G	C6-N1-C2	-11.08	118.45	125.10	13	20
1	A	321	G	C6-N1-C2	-11.08	118.45	125.10	9	20
2	B	748	G	C6-N1-C2	-11.08	118.45	125.10	1	20
1	A	323	G	C6-N1-C2	-11.07	118.46	125.10	20	20
2	B	774	G	C6-N1-C2	-11.07	118.46	125.10	20	20
2	B	729	G	C6-N1-C2	-11.06	118.46	125.10	11	20
2	B	763	G	C6-N1-C2	-11.06	118.46	125.10	10	20
2	B	734	G	C6-N1-C2	-11.06	118.46	125.10	1	20
2	B	747	G	C6-N1-C2	-11.06	118.46	125.10	4	20
2	B	709	G	C6-N1-C2	-11.04	118.47	125.10	11	20
1	A	333	U	O4'-C4'-C3'	-11.03	92.97	104.00	18	20
1	A	342	C	O4'-C4'-C3'	-10.78	93.22	104.00	11	20
1	A	360	G	O4'-C4'-C3'	-10.70	93.30	104.00	8	20
1	A	329	G	O4'-C4'-C3'	-10.68	93.32	104.00	16	20
2	B	733	U	O4'-C4'-C3'	-10.67	93.33	104.00	4	20
1	A	337	C	O4'-C4'-C3'	-10.65	93.34	104.00	19	20
2	B	760	G	O4'-C4'-C3'	-10.62	93.38	104.00	6	20
2	B	737	C	O4'-C4'-C3'	-10.61	93.39	104.00	19	20
2	B	729	G	O4'-C4'-C3'	-10.59	93.41	104.00	15	20
2	B	735	U	O4'-C4'-C3'	-10.53	93.47	104.00	20	20
2	B	765	C	O4'-C4'-C3'	-10.50	93.50	104.00	14	10
1	A	311	C	O4'-C4'-C3'	-10.43	93.57	104.00	14	20
1	A	335	U	O4'-C4'-C3'	-10.43	93.57	104.00	10	20
1	A	320	G	O4'-C4'-C3'	-10.41	93.59	104.00	15	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	355	C	O4'-C4'-C3'	-10.40	93.60	104.00	16	20
1	A	332	G	O4'-C4'-C3'	-10.37	93.63	104.00	7	20
1	A	353	A	O4'-C4'-C3'	-10.37	93.63	104.00	16	20
2	B	711	C	O4'-C4'-C3'	-10.36	93.64	104.00	1	20
2	B	753	A	O4'-C4'-C3'	-10.34	93.66	104.00	11	20
2	B	755	C	O4'-C4'-C3'	-10.33	93.67	104.00	4	20
1	A	359	G	O4'-C4'-C3'	-10.30	93.70	104.00	10	20
2	B	759	G	O4'-C4'-C3'	-10.27	93.73	104.00	10	20
1	A	372	G	O4'-C4'-C3'	-10.24	93.76	104.00	7	20
2	B	751	G	O4'-C4'-C3'	-10.21	93.79	104.00	15	20
2	B	772	G	O4'-C4'-C3'	-10.21	93.79	104.00	3	20
1	A	352	C	O4'-C4'-C3'	-10.20	93.81	104.00	15	20
2	B	752	C	O4'-C4'-C3'	-10.19	93.81	104.00	13	20
2	B	767	U	O4'-C4'-C3'	-10.19	93.81	104.00	7	20
1	A	351	G	O4'-C4'-C3'	-10.18	93.82	104.00	14	20
1	A	367	U	O4'-C4'-C3'	-10.15	93.84	104.00	3	20
2	B	773	G	O4'-C4'-C3'	-10.15	93.85	104.00	7	20
1	A	373	G	O4'-C4'-C3'	-10.10	93.90	104.00	3	20
2	B	750	C	O4'-C4'-C3'	-10.10	93.90	104.00	5	20
2	B	768	C	O4'-C4'-C3'	-9.94	94.06	104.00	13	20
1	A	312	G	O4'-C4'-C3'	-9.94	94.06	104.00	14	20
2	B	717	C	O4'-C4'-C3'	-9.93	94.07	104.00	19	20
1	A	369	C	O4'-C4'-C3'	-9.91	94.09	104.00	20	20
1	A	357	C	O4'-C4'-C3'	-9.90	94.09	104.00	3	20
2	B	712	G	O4'-C4'-C3'	-9.90	94.10	104.00	7	20
1	A	368	C	O4'-C4'-C3'	-9.90	94.10	104.00	3	20
1	A	350	C	O4'-C4'-C3'	-9.89	94.11	104.00	8	20
2	B	727	C	O4'-C4'-C3'	-9.85	94.15	104.00	4	20
2	B	742	C	O4'-C4'-C3'	-9.85	94.15	104.00	7	20
2	B	757	C	O4'-C4'-C3'	-9.85	94.15	104.00	20	20
2	B	769	C	O4'-C4'-C3'	-9.84	94.16	104.00	3	20
1	A	315	C	C1'-O4'-C4'	9.81	117.75	109.90	11	20
1	A	317	C	O4'-C4'-C3'	-9.79	94.21	104.00	19	20
2	B	715	C	C1'-O4'-C4'	9.78	117.72	109.90	8	20
1	A	327	C	O4'-C4'-C3'	-9.73	94.27	104.00	3	20
2	B	736	U	O4'-C4'-C3'	-9.70	94.30	104.00	9	20
2	B	743	A	C1'-O4'-C4'	9.69	117.65	109.90	3	20
1	A	336	U	O4'-C4'-C3'	-9.68	94.32	104.00	8	20
1	A	365	C	O4'-C4'-C3'	-9.57	94.43	104.00	12	13
1	A	343	A	C1'-O4'-C4'	9.57	117.55	109.90	1	20
1	A	316	C	C1'-O4'-C4'	9.52	117.52	109.90	19	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	765	C	C1'-O4'-C4'	9.52	117.52	109.90	10	20
1	A	318	G	O4'-C4'-C3'	-9.51	94.49	104.00	3	20
1	A	361	G	C1'-O4'-C4'	9.49	117.50	109.90	1	20
2	B	761	G	C1'-O4'-C4'	9.49	117.49	109.90	13	20
1	A	322	U	C1'-O4'-C4'	9.48	117.48	109.90	15	20
2	B	716	C	C1'-O4'-C4'	9.46	117.47	109.90	15	20
1	A	327	C	C1'-O4'-C4'	9.43	117.45	109.90	1	20
2	B	722	U	C1'-O4'-C4'	9.43	117.44	109.90	6	20
2	B	745	C	C1'-O4'-C4'	9.42	117.44	109.90	17	20
1	A	345	C	O4'-C4'-C3'	-9.42	94.58	104.00	11	20
1	A	366	G	C1'-O4'-C4'	9.40	117.42	109.90	11	20
1	A	345	C	C1'-O4'-C4'	9.39	117.41	109.90	6	20
2	B	727	C	C1'-O4'-C4'	9.37	117.39	109.90	11	20
2	B	766	G	C1'-O4'-C4'	9.34	117.38	109.90	1	20
1	A	313	G	C1'-O4'-C4'	9.29	117.33	109.90	13	20
1	A	326	A	C1'-O4'-C4'	9.28	117.33	109.90	10	20
2	B	749	C	C1'-O4'-C4'	9.28	117.32	109.90	5	20
2	B	713	G	C1'-O4'-C4'	9.28	117.32	109.90	13	20
1	A	349	C	C1'-O4'-C4'	9.27	117.32	109.90	2	20
1	A	331	C	C1'-O4'-C4'	9.27	117.32	109.90	20	20
2	B	756	C	C1'-O4'-C4'	9.26	117.31	109.90	6	20
2	B	717	C	C1'-O4'-C4'	9.26	117.31	109.90	4	20
2	B	726	A	C1'-O4'-C4'	9.25	117.30	109.90	6	20
2	B	741	A	C1'-O4'-C4'	9.25	117.30	109.90	15	19
1	A	317	C	C1'-O4'-C4'	9.25	117.30	109.90	10	20
1	A	347	G	C1'-O4'-C4'	9.25	117.30	109.90	5	20
1	A	356	C	C1'-O4'-C4'	9.25	117.30	109.90	12	20
2	B	729	G	C1'-O4'-C4'	9.24	117.30	109.90	8	20
1	A	341	A	C1'-O4'-C4'	9.24	117.29	109.90	3	18
1	A	365	C	C1'-O4'-C4'	9.23	117.29	109.90	14	20
2	B	731	C	C1'-O4'-C4'	9.23	117.28	109.90	1	20
2	B	722	U	O4'-C4'-C3'	-9.22	94.78	104.00	7	20
1	A	342	C	C1'-O4'-C4'	9.21	117.27	109.90	9	20
1	A	318	G	C1'-O4'-C4'	9.20	117.26	109.90	6	20
2	B	742	C	C1'-O4'-C4'	9.20	117.26	109.90	2	20
2	B	754	A	C1'-O4'-C4'	9.20	117.26	109.90	1	20
1	A	354	A	C1'-O4'-C4'	9.18	117.25	109.90	10	20
2	B	747	G	C1'-O4'-C4'	9.18	117.24	109.90	7	20
1	A	329	G	C1'-O4'-C4'	9.17	117.23	109.90	1	20
2	B	733	U	C1'-O4'-C4'	9.15	117.22	109.90	10	20
1	A	333	U	C1'-O4'-C4'	9.14	117.21	109.90	17	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	322	U	O4'-C4'-C3'	-9.09	94.91	104.00	3	20
1	A	346	C	C1'-O4'-C4'	9.09	117.17	109.90	11	20
2	B	769	C	C1'-O4'-C4'	9.08	117.17	109.90	6	20
2	B	713	G	O4'-C4'-C3'	-9.07	94.93	104.00	15	20
1	A	373	G	C1'-O4'-C4'	9.07	117.15	109.90	8	20
2	B	718	G	C1'-O4'-C4'	9.04	117.13	109.90	6	20
2	B	773	G	C1'-O4'-C4'	9.03	117.12	109.90	10	20
1	A	309	G	O4'-C4'-C3'	-9.02	94.98	104.00	2	20
2	B	753	A	C1'-O4'-C4'	9.02	117.11	109.90	13	20
1	A	337	C	C1'-O4'-C4'	9.01	117.11	109.90	7	20
1	A	313	G	O4'-C4'-C3'	-9.01	95.00	104.00	14	20
2	B	737	C	C1'-O4'-C4'	8.99	117.09	109.90	7	20
1	A	353	A	C1'-O4'-C4'	8.99	117.09	109.90	3	20
1	A	331	C	O4'-C4'-C3'	-8.98	95.02	104.00	4	19
1	A	369	C	C1'-O4'-C4'	8.96	117.07	109.90	9	20
1	A	357	C	C1'-O4'-C4'	8.94	117.05	109.90	18	20
2	B	757	C	C1'-O4'-C4'	8.92	117.03	109.90	18	20
1	A	351	G	C1'-O4'-C4'	8.91	117.03	109.90	8	20
2	B	751	G	C1'-O4'-C4'	8.88	117.01	109.90	8	20
2	B	750	C	C1'-O4'-C4'	8.87	117.00	109.90	17	20
1	A	332	G	N1-C2-N3	8.87	129.22	123.90	15	20
1	A	318	G	N1-C2-N3	8.86	129.21	123.90	3	20
1	A	371	A	O4'-C4'-C3'	-8.86	95.14	104.00	4	20
1	A	311	C	C1'-O4'-C4'	8.85	116.98	109.90	9	20
2	B	751	G	N1-C2-N3	8.85	129.21	123.90	1	20
1	A	359	G	N1-C2-N3	8.84	129.21	123.90	14	20
1	A	350	C	C1'-O4'-C4'	8.84	116.97	109.90	5	20
2	B	714	A	C1'-O4'-C4'	8.84	116.97	109.90	16	20
1	A	363	G	N1-C2-N3	8.83	129.20	123.90	12	20
2	B	739	G	N1-C2-N3	8.83	129.20	123.90	18	20
2	B	759	G	N1-C2-N3	8.83	129.20	123.90	15	20
1	A	334	G	N1-C2-N3	8.83	129.20	123.90	1	20
1	A	347	G	N1-C2-N3	8.83	129.20	123.90	8	20
1	A	361	G	N1-C2-N3	8.83	129.20	123.90	13	20
2	B	731	C	O4'-C4'-C3'	-8.83	95.17	104.00	3	19
1	A	360	G	N1-C2-N3	8.82	129.19	123.90	8	20
2	B	760	G	N1-C2-N3	8.82	129.19	123.90	13	20
1	A	348	G	N1-C2-N3	8.81	129.19	123.90	19	20
2	B	771	A	O4'-C4'-C3'	-8.81	95.19	104.00	8	20
1	A	321	G	C1'-O4'-C4'	8.81	116.95	109.90	1	20
1	A	348	G	C1'-O4'-C4'	8.81	116.95	109.90	13	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	734	G	N1-C2-N3	8.81	129.19	123.90	12	20
1	A	351	G	N1-C2-N3	8.81	129.19	123.90	5	20
1	A	329	G	N1-C2-N3	8.81	129.18	123.90	14	20
1	A	338	G	O4'-C4'-C3'	-8.81	95.19	104.00	7	20
1	A	372	G	N1-C2-N3	8.80	129.18	123.90	6	20
2	B	711	C	C1'-O4'-C4'	8.80	116.94	109.90	11	20
2	B	718	G	N1-C2-N3	8.80	129.18	123.90	4	20
2	B	720	G	N1-C2-N3	8.80	129.18	123.90	17	20
2	B	745	C	O4'-C4'-C3'	-8.80	95.20	104.00	7	20
2	B	724	G	N1-C2-N3	8.79	129.18	123.90	15	20
2	B	772	G	N1-C2-N3	8.79	129.18	123.90	2	20
1	A	320	G	N1-C2-N3	8.79	129.18	123.90	1	20
1	A	312	G	N1-C2-N3	8.79	129.17	123.90	8	20
1	A	313	G	N1-C2-N3	8.78	129.17	123.90	5	20
1	A	339	G	N1-C2-N3	8.78	129.17	123.90	2	20
2	B	721	G	C1'-O4'-C4'	8.78	116.92	109.90	12	20
2	B	732	G	N1-C2-N3	8.78	129.17	123.90	19	20
2	B	747	G	N1-C2-N3	8.78	129.17	123.90	20	20
1	A	366	G	N1-C2-N3	8.78	129.17	123.90	14	20
2	B	709	G	N1-C2-N3	8.78	129.17	123.90	8	20
2	B	721	G	N1-C2-N3	8.78	129.17	123.90	6	20
1	A	309	G	N1-C2-N3	8.78	129.17	123.90	4	20
1	A	338	G	N1-C2-N3	8.78	129.17	123.90	13	20
1	A	373	G	N1-C2-N3	8.78	129.16	123.90	1	20
1	A	324	G	N1-C2-N3	8.77	129.16	123.90	20	20
2	B	723	G	N1-C2-N3	8.77	129.16	123.90	1	20
2	B	721	G	O4'-C4'-C3'	-8.77	95.23	104.00	7	20
2	B	748	G	N1-C2-N3	8.77	129.16	123.90	18	20
2	B	738	G	N1-C2-N3	8.77	129.16	123.90	19	20
2	B	766	G	N1-C2-N3	8.77	129.16	123.90	14	20
1	A	321	G	N1-C2-N3	8.77	129.16	123.90	9	20
2	B	773	G	N1-C2-N3	8.77	129.16	123.90	16	20
1	A	310	G	N1-C2-N3	8.76	129.16	123.90	9	20
2	B	710	G	N1-C2-N3	8.76	129.16	123.90	12	20
2	B	712	G	N1-C2-N3	8.76	129.16	123.90	10	20
2	B	736	U	C1'-O4'-C4'	8.76	116.91	109.90	4	20
2	B	748	G	C1'-O4'-C4'	8.76	116.91	109.90	13	20
2	B	761	G	N1-C2-N3	8.76	129.16	123.90	18	20
2	B	763	G	N1-C2-N3	8.76	129.16	123.90	1	20
1	A	371	A	C1'-O4'-C4'	8.76	116.91	109.90	1	20
2	B	713	G	N1-C2-N3	8.75	129.15	123.90	13	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	323	G	N1-C2-N3	8.75	129.15	123.90	11	20
2	B	738	G	C1'-O4'-C4'	8.75	116.90	109.90	4	20
2	B	729	G	N1-C2-N3	8.75	129.15	123.90	20	20
2	B	774	G	N1-C2-N3	8.75	129.15	123.90	19	20
1	A	321	G	O4'-C4'-C3'	-8.74	95.26	104.00	4	20
2	B	771	A	C1'-O4'-C4'	8.73	116.89	109.90	13	20
1	A	348	G	O4'-C4'-C3'	-8.73	95.27	104.00	11	20
1	A	314	A	C1'-O4'-C4'	8.72	116.88	109.90	6	20
2	B	709	G	C1'-O4'-C4'	8.72	116.87	109.90	19	20
1	A	356	C	O4'-C4'-C3'	-8.71	95.29	104.00	13	20
1	A	338	G	C1'-O4'-C4'	8.70	116.86	109.90	2	20
2	B	748	G	O4'-C4'-C3'	-8.70	95.30	104.00	20	20
1	A	320	G	C1'-O4'-C4'	8.70	116.86	109.90	3	20
1	A	336	U	C1'-O4'-C4'	8.70	116.86	109.90	14	20
1	A	309	G	C1'-O4'-C4'	8.69	116.85	109.90	13	20
1	A	360	G	C1'-O4'-C4'	8.68	116.85	109.90	14	20
1	A	354	A	O4'-C4'-C3'	-8.68	95.32	104.00	1	20
2	B	720	G	C1'-O4'-C4'	8.68	116.84	109.90	1	20
2	B	760	G	C1'-O4'-C4'	8.66	116.83	109.90	3	20
2	B	756	C	O4'-C4'-C3'	-8.66	95.34	104.00	20	20
2	B	755	C	C1'-O4'-C4'	8.63	116.81	109.90	14	20
1	A	335	U	C1'-O4'-C4'	8.62	116.80	109.90	19	20
1	A	332	G	C1'-O4'-C4'	8.62	116.79	109.90	6	20
2	B	746	C	C1'-O4'-C4'	8.62	116.79	109.90	11	20
2	B	754	A	O4'-C4'-C3'	-8.61	95.39	104.00	10	20
2	B	735	U	C1'-O4'-C4'	8.60	116.78	109.90	19	20
2	B	738	G	O4'-C4'-C3'	-8.60	95.40	104.00	7	20
1	A	355	C	C1'-O4'-C4'	8.59	116.77	109.90	1	20
2	B	732	G	C1'-O4'-C4'	8.59	116.77	109.90	5	20
1	A	372	G	C1'-O4'-C4'	8.56	116.75	109.90	10	20
2	B	718	G	O4'-C4'-C3'	-8.54	95.46	104.00	1	20
2	B	767	U	C1'-O4'-C4'	8.54	116.73	109.90	8	20
1	A	352	C	C1'-O4'-C4'	8.54	116.73	109.90	19	20
1	A	367	U	C1'-O4'-C4'	8.54	116.73	109.90	9	20
1	A	368	C	C1'-O4'-C4'	8.54	116.73	109.90	11	20
2	B	768	C	C1'-O4'-C4'	8.53	116.72	109.90	16	20
2	B	752	C	C1'-O4'-C4'	8.53	116.72	109.90	19	20
1	A	363	G	C1'-O4'-C4'	8.52	116.72	109.90	1	20
2	B	772	G	C1'-O4'-C4'	8.50	116.70	109.90	2	20
1	A	312	G	C1'-O4'-C4'	8.49	116.69	109.90	19	20
1	A	359	G	C1'-O4'-C4'	8.47	116.67	109.90	20	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	712	G	C1'-O4'-C4'	8.46	116.67	109.90	15	20
2	B	763	G	C1'-O4'-C4'	8.45	116.66	109.90	19	20
2	B	710	G	C1'-O4'-C4'	8.43	116.65	109.90	1	20
1	A	325	A	C1'-O4'-C4'	8.42	116.63	109.90	19	20
1	A	310	G	C1'-O4'-C4'	8.41	116.63	109.90	10	20
2	B	759	G	C1'-O4'-C4'	8.41	116.63	109.90	8	20
1	A	325	A	O4'-C4'-C3'	-8.33	95.67	104.00	14	20
2	B	725	A	C1'-O4'-C4'	8.30	116.54	109.90	17	20
2	B	725	A	O4'-C4'-C3'	-8.25	95.75	104.00	18	20
2	B	715	C	O4'-C4'-C3'	-8.23	95.77	104.00	12	17
1	A	315	C	O4'-C4'-C3'	-8.19	95.81	104.00	13	15
1	A	361	G	O4'-C4'-C3'	-8.16	95.84	104.00	9	20
2	B	716	C	O4'-C4'-C3'	-8.14	95.86	104.00	3	8
1	A	344	C	C1'-O4'-C4'	8.14	116.41	109.90	11	20
2	B	766	G	O4'-C4'-C3'	-8.12	95.88	104.00	19	16
2	B	761	G	O4'-C4'-C3'	-8.12	95.88	104.00	18	20
1	A	343	A	O4'-C4'-C3'	-8.04	95.96	104.00	13	20
1	A	323	G	C1'-O4'-C4'	8.03	116.33	109.90	12	20
1	A	366	G	O4'-C4'-C3'	-8.03	95.97	104.00	19	17
2	B	723	G	C1'-O4'-C4'	8.02	116.32	109.90	18	20
2	B	770	C	C1'-O4'-C4'	8.02	116.31	109.90	6	20
1	A	370	C	C1'-O4'-C4'	8.01	116.31	109.90	6	20
2	B	744	C	C1'-O4'-C4'	7.99	116.29	109.90	20	20
1	A	316	C	O4'-C4'-C3'	-7.91	96.09	104.00	17	8
2	B	743	A	O4'-C4'-C3'	-7.90	96.10	104.00	11	20
2	B	734	G	C1'-O4'-C4'	7.87	116.20	109.90	4	18
2	B	746	C	O4'-C4'-C3'	-7.76	96.24	104.00	13	20
1	A	364	A	C1'-O4'-C4'	7.73	116.09	109.90	6	7
1	A	339	G	C1'-O4'-C4'	7.73	116.08	109.90	1	11
1	A	346	C	O4'-C4'-C3'	-7.71	96.29	104.00	7	20
2	B	764	A	C1'-O4'-C4'	7.67	116.04	109.90	9	5
2	B	739	G	C1'-O4'-C4'	7.67	116.04	109.90	14	15
1	A	334	G	C1'-O4'-C4'	7.60	115.98	109.90	2	20
1	A	324	G	C1'-O4'-C4'	7.45	115.86	109.90	7	20
1	A	358	U	C1'-O4'-C4'	7.44	115.85	109.90	13	20
1	A	319	U	C1'-O4'-C4'	7.42	115.84	109.90	6	1
2	B	758	U	C1'-O4'-C4'	7.39	115.81	109.90	7	20
2	B	747	G	O4'-C4'-C3'	-7.37	96.63	104.00	7	20
1	A	349	C	O4'-C4'-C3'	-7.37	96.64	104.00	2	20
2	B	774	G	C1'-O4'-C4'	7.32	115.76	109.90	11	20
2	B	749	C	O4'-C4'-C3'	-7.28	96.72	104.00	20	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	347	G	O4'-C4'-C3'	-7.24	96.76	104.00	14	20
2	B	740	A	C1'-O4'-C4'	7.21	115.67	109.90	11	19
1	A	340	A	C1'-O4'-C4'	7.16	115.63	109.90	16	17
2	B	724	G	C1'-O4'-C4'	7.14	115.61	109.90	18	20
1	A	330	A	C1'-O4'-C4'	6.97	115.48	109.90	11	9
2	B	730	A	C1'-O4'-C4'	6.95	115.46	109.90	9	9
1	A	328	A	C5'-C4'-O4'	-6.52	101.27	109.10	9	20
2	B	762	A	C1'-O4'-C4'	6.51	115.11	109.90	12	20
1	A	324	G	O4'-C4'-C3'	-6.42	97.58	104.00	19	20
1	A	310	G	O4'-C4'-C3'	-6.38	97.62	104.00	7	20
2	B	728	A	C5'-C4'-O4'	-6.36	101.47	109.10	19	20
1	A	362	A	C1'-O4'-C4'	6.33	114.97	109.90	15	20
2	B	710	G	O4'-C4'-C3'	-6.26	97.74	104.00	14	20
2	B	724	G	O4'-C4'-C3'	-6.18	97.82	104.00	14	20
2	B	714	A	C5'-C4'-O4'	-6.03	101.86	109.10	13	7
1	A	314	A	C5'-C4'-O4'	-5.91	102.00	109.10	10	14
1	A	326	A	O4'-C4'-C3'	-5.88	98.12	104.00	19	20
2	B	726	A	O4'-C4'-C3'	-5.84	98.16	104.00	19	20
1	A	336	U	C2-N3-C4	-5.83	123.50	127.00	2	20
1	A	358	U	C2-N3-C4	-5.80	123.52	127.00	11	20
1	A	322	U	C2-N3-C4	-5.79	123.53	127.00	10	20
2	B	735	U	C2-N3-C4	-5.79	123.53	127.00	8	20
2	B	736	U	C2-N3-C4	-5.79	123.53	127.00	4	20
2	B	733	U	C2-N3-C4	-5.79	123.53	127.00	11	20
1	A	335	U	C2-N3-C4	-5.79	123.53	127.00	18	20
2	B	722	U	C2-N3-C4	-5.78	123.53	127.00	3	20
1	A	319	U	C2-N3-C4	-5.77	123.54	127.00	6	20
1	A	333	U	C2-N3-C4	-5.77	123.54	127.00	12	20
2	B	719	U	C2-N3-C4	-5.77	123.54	127.00	11	20
1	A	367	U	C2-N3-C4	-5.76	123.55	127.00	5	20
2	B	713	G	C5'-C4'-O4'	-5.76	102.19	109.10	19	4
2	B	767	U	C2-N3-C4	-5.76	123.54	127.00	13	20
2	B	758	U	C2-N3-C4	-5.75	123.55	127.00	11	20
1	A	313	G	C5'-C4'-O4'	-5.74	102.21	109.10	15	7
1	A	323	G	C5'-C4'-O4'	-5.73	102.22	109.10	11	6
2	B	721	G	C5'-C4'-O4'	-5.64	102.33	109.10	10	17
1	A	321	G	C5'-C4'-O4'	-5.59	102.39	109.10	20	17
1	A	318	G	N1-C2-N2	-5.57	111.18	116.20	11	20
1	A	361	G	N1-C2-N2	-5.56	111.20	116.20	1	20
2	B	718	G	N1-C2-N2	-5.55	111.20	116.20	4	20
2	B	729	G	N1-C2-N2	-5.55	111.20	116.20	8	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	761	G	N1-C2-N2	-5.55	111.20	116.20	19	20
1	A	360	G	C5-C6-O6	-5.55	125.27	128.60	2	20
2	B	710	G	N1-C2-N2	-5.55	111.20	116.20	3	20
2	B	759	G	N1-C2-N2	-5.55	111.20	116.20	17	20
1	A	372	G	N1-C2-N2	-5.55	111.21	116.20	4	20
2	B	721	G	N1-C2-N2	-5.55	111.21	116.20	13	20
1	A	366	G	N1-C2-N2	-5.54	111.21	116.20	14	20
1	A	339	G	N1-C2-N2	-5.54	111.21	116.20	19	20
2	B	720	G	N1-C2-N2	-5.54	111.21	116.20	17	20
1	A	313	G	N1-C2-N2	-5.54	111.22	116.20	19	20
1	A	332	G	N1-C2-N2	-5.54	111.22	116.20	15	20
1	A	338	G	N1-C2-N2	-5.54	111.22	116.20	1	20
1	A	312	G	N1-C2-N2	-5.54	111.22	116.20	20	20
2	B	763	G	N1-C2-N2	-5.54	111.22	116.20	8	20
1	A	342	C	C5'-C4'-O4'	-5.53	102.46	109.10	11	1
1	A	363	G	N1-C2-N2	-5.53	111.22	116.20	3	20
1	A	334	G	N1-C2-N2	-5.53	111.23	116.20	17	20
1	A	373	G	N1-C2-N2	-5.53	111.23	116.20	10	20
1	A	310	G	N1-C2-N2	-5.52	111.23	116.20	15	20
1	A	324	G	C5-C6-O6	-5.52	125.29	128.60	4	20
2	B	712	G	N1-C2-N2	-5.52	111.23	116.20	10	20
2	B	760	G	N1-C2-N2	-5.52	111.23	116.20	18	20
1	A	324	G	N1-C2-N2	-5.52	111.23	116.20	20	20
1	A	351	G	N1-C2-N2	-5.52	111.23	116.20	11	20
1	A	359	G	N1-C2-N2	-5.52	111.23	116.20	10	20
2	B	723	G	C5-C6-O6	-5.52	125.29	128.60	19	20
1	A	321	G	N1-C2-N2	-5.52	111.24	116.20	10	20
2	B	709	G	N1-C2-N2	-5.51	111.24	116.20	11	20
2	B	713	G	N1-C2-N2	-5.51	111.24	116.20	5	20
2	B	723	G	N1-C2-N2	-5.51	111.24	116.20	10	20
2	B	724	G	N1-C2-N2	-5.51	111.24	116.20	4	20
2	B	766	G	N1-C2-N2	-5.51	111.24	116.20	9	20
1	A	320	G	N1-C2-N2	-5.51	111.24	116.20	15	20
1	A	348	G	C5-C6-O6	-5.51	125.29	128.60	5	20
2	B	751	G	N1-C2-N2	-5.51	111.24	116.20	16	20
1	A	309	G	N1-C2-N2	-5.51	111.24	116.20	4	20
1	A	329	G	N1-C2-N2	-5.51	111.24	116.20	13	20
1	A	347	G	N1-C2-N2	-5.51	111.24	116.20	8	20
1	A	348	G	N1-C2-N2	-5.51	111.24	116.20	11	20
2	B	748	G	N1-C2-N2	-5.51	111.24	116.20	14	20
2	B	732	G	N1-C2-N2	-5.51	111.24	116.20	2	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	773	G	N1-C2-N2	-5.51	111.25	116.20	19	20
1	A	372	G	C5-C6-O6	-5.50	125.30	128.60	15	20
2	B	772	G	C5-C6-O6	-5.50	125.30	128.60	12	20
2	B	739	G	N1-C2-N2	-5.50	111.25	116.20	16	20
2	B	712	G	C5-C6-O6	-5.50	125.30	128.60	17	20
2	B	772	G	N1-C2-N2	-5.50	111.25	116.20	2	20
2	B	748	G	C5-C6-O6	-5.50	125.30	128.60	10	20
1	A	339	G	C5-C6-O6	-5.50	125.30	128.60	4	20
1	A	347	G	C5-C6-O6	-5.50	125.30	128.60	1	20
2	B	734	G	N1-C2-N2	-5.50	111.25	116.20	12	20
2	B	738	G	N1-C2-N2	-5.50	111.25	116.20	20	20
2	B	738	G	C5-C6-O6	-5.50	125.30	128.60	8	20
1	A	323	G	N1-C2-N2	-5.49	111.26	116.20	7	20
2	B	729	G	C5-C6-O6	-5.49	125.30	128.60	13	20
1	A	334	G	C5-C6-O6	-5.49	125.31	128.60	20	20
1	A	366	G	C5-C6-O6	-5.49	125.31	128.60	14	20
2	B	747	G	N1-C2-N2	-5.49	111.26	116.20	9	20
2	B	774	G	N1-C2-N2	-5.48	111.27	116.20	1	20
1	A	363	G	C5-C6-O6	-5.48	125.31	128.60	18	20
1	A	313	G	C5-C6-O6	-5.48	125.31	128.60	6	20
1	A	329	G	C5-C6-O6	-5.48	125.31	128.60	3	20
1	A	360	G	N1-C2-N2	-5.48	111.27	116.20	13	20
1	A	361	G	C5-C6-O6	-5.48	125.31	128.60	10	20
2	B	734	G	C5-C6-O6	-5.48	125.31	128.60	17	20
2	B	747	G	C5-C6-O6	-5.48	125.31	128.60	2	20
2	B	773	G	C5-C6-O6	-5.48	125.31	128.60	1	20
1	A	351	G	C5-C6-O6	-5.48	125.31	128.60	8	20
2	B	774	G	C5-C6-O6	-5.47	125.32	128.60	6	20
2	B	761	G	C5-C6-O6	-5.47	125.32	128.60	17	20
2	B	720	G	C5-C6-O6	-5.46	125.32	128.60	18	20
2	B	766	G	C5-C6-O6	-5.46	125.32	128.60	11	20
1	A	338	G	C5-C6-O6	-5.46	125.32	128.60	3	20
1	A	359	G	C5-C6-O6	-5.46	125.33	128.60	5	20
1	A	310	G	C5-C6-O6	-5.46	125.33	128.60	15	20
1	A	320	G	C5-C6-O6	-5.46	125.33	128.60	18	20
1	A	318	G	C5-C6-O6	-5.45	125.33	128.60	6	20
1	A	373	G	C5-C6-O6	-5.45	125.33	128.60	18	20
2	B	709	G	C5-C6-O6	-5.45	125.33	128.60	16	20
2	B	732	G	C5-C6-O6	-5.45	125.33	128.60	2	20
1	A	309	G	C5-C6-O6	-5.45	125.33	128.60	19	20
2	B	721	G	C5-C6-O6	-5.45	125.33	128.60	1	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	323	G	C5-C6-O6	-5.45	125.33	128.60	16	20
2	B	724	G	C5-C6-O6	-5.45	125.33	128.60	2	20
2	B	760	G	C5-C6-O6	-5.45	125.33	128.60	8	20
2	B	718	G	C5-C6-O6	-5.44	125.34	128.60	14	20
2	B	710	G	C5-C6-O6	-5.44	125.34	128.60	4	20
2	B	739	G	C5-C6-O6	-5.44	125.34	128.60	18	20
1	A	312	G	C5-C6-O6	-5.43	125.34	128.60	1	20
2	B	763	G	C5-C6-O6	-5.43	125.34	128.60	6	20
2	B	759	G	C5-C6-O6	-5.43	125.34	128.60	13	20
2	B	713	G	C5-C6-O6	-5.42	125.35	128.60	17	20
2	B	751	G	C5-C6-O6	-5.42	125.35	128.60	2	20
1	A	321	G	C5-C6-O6	-5.42	125.35	128.60	18	20
2	B	765	C	C5'-C4'-O4'	-5.42	102.60	109.10	14	3
1	A	332	G	C5-C6-O6	-5.39	125.36	128.60	6	20
2	B	719	U	N3-C4-C5	5.32	117.79	114.60	11	20
1	A	322	U	N3-C4-C5	5.32	117.79	114.60	17	20
1	A	358	U	N3-C4-C5	5.31	117.78	114.60	1	20
1	A	367	U	N3-C4-C5	5.30	117.78	114.60	5	20
1	A	339	G	C5'-C4'-O4'	-5.30	102.74	109.10	11	1
2	B	758	U	N3-C4-C5	5.30	117.78	114.60	11	20
1	A	336	U	N3-C4-C5	5.29	117.78	114.60	1	20
2	B	733	U	N3-C4-C5	5.29	117.78	114.60	7	20
2	B	722	U	N3-C4-C5	5.29	117.77	114.60	8	20
2	B	728	A	C1'-O4'-C4'	5.29	114.13	109.90	18	2
1	A	319	U	N3-C4-C5	5.28	117.77	114.60	6	20
1	A	335	U	N3-C4-C5	5.28	117.77	114.60	11	20
2	B	735	U	N3-C4-C5	5.26	117.76	114.60	19	20
2	B	736	U	N3-C4-C5	5.25	117.75	114.60	10	20
2	B	767	U	N3-C4-C5	5.25	117.75	114.60	13	20
1	A	328	A	C1'-O4'-C4'	5.24	114.09	109.90	12	1
1	A	333	U	N3-C4-C5	5.23	117.74	114.60	4	20
2	B	739	G	C5'-C4'-O4'	-5.18	102.88	109.10	5	2
2	B	723	G	C5'-C4'-O4'	-5.12	102.96	109.10	7	3
1	A	365	C	C5'-C4'-O4'	-5.04	103.05	109.10	11	1
2	B	748	G	C2-N3-C4	-5.00	109.40	111.90	2	1

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
All	All	56380	28540	28580	-

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 -.

There are no clashes.

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	64/65 (98%)	12±1 (19±1%)	0±0 (0±0%)	0.32±0.01
2	B	65/66 (98%)	12±1 (19±2%)	0±0 (0±0%)	0.32±0.01
All	All	2580/2620 (98%)	484 (19%)	0 (0%)	0.32

The overall RNA backbone suiteness is 0.32.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	331	C	20
2	B	719	U	20
2	B	741	A	20
2	B	764	A	20
2	B	739	G	20
1	A	330	A	20

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Mol	Chain	Res	Type	Models (Total)
1	A	366	G	20
2	B	730	A	20
1	A	324	G	20
2	B	766	G	20
2	B	724	G	20
1	A	319	U	20
1	A	365	C	20
1	A	364	A	20
1	A	339	G	20
2	B	731	C	20
1	A	341	A	20
2	B	765	C	19
2	B	715	C	19
1	A	315	C	19
2	B	753	A	18
1	A	353	A	16
2	B	716	C	15
1	A	316	C	13
2	B	732	G	7
1	A	332	G	6
1	A	333	U	5
2	B	733	U	2
2	B	710	G	2
1	A	340	A	2
2	B	740	A	1

There are no RNA pucker outliers to report.

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

The completeness of assignment taking into account all chemical shift lists is 8% for the well-defined parts and 8% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 17083

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	208
Number of shifts mapped to atoms	208
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

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

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 8%, i.e. 203 atoms were assigned a chemical shift out of a possible 2510. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	203/2510 (8%)	203/1462 (14%)	0/868 (0%)	0/180 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 203 atoms were assigned a chemical shift out of a possible 2510. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	203/2510 (8%)	203/1462 (14%)	0/868 (0%)	0/180 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
2	B	734	G	H4'	2.79	5.12 – 3.72	-11.6
2	B	768	C	H4'	2.76	5.08 – 3.58	-10.5
2	B	733	U	H1'	3.87	6.46 – 4.76	-10.3

7.1.5 Random Coil Index (RCI) plots [i](#)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.