



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 07:37 pm GMT

PDB ID : 1R2P
Title : Solution structure of domain 5 from the ai5(gamma) group II intron
Authors : Sigel, R.K.O.; Sashital, D.G.; Abramovitz, D.L.; Palmer III, A.G.; Butcher, S.E.; Pyle, A.M.
Deposited on : 2003-09-29

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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

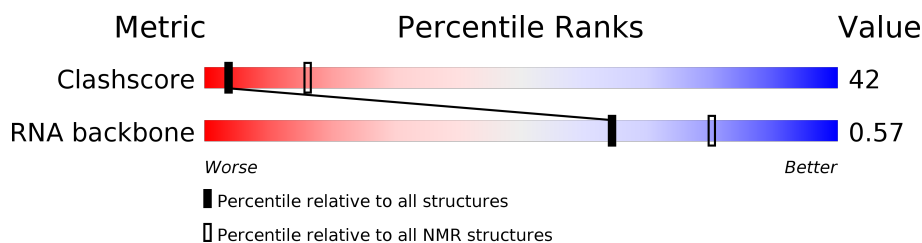
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR


The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
RNA backbone	3398	623

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	34	 <div style="display: flex; justify-content: space-between; width: 100%;"> . 76% 21% </div>

2 Ensemble composition and analysis ⓘ

This entry contains 10 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 1094 atoms, of which 368 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 34-MER.

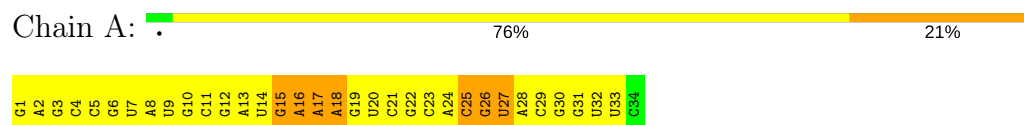
Mol	Chain	Residues	Atoms						Trace
1	A	34	Total	C	H	N	O	P	0
			1094	325	368	133	235	33	

4 Residue-property plots [i](#)

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: 34-MER

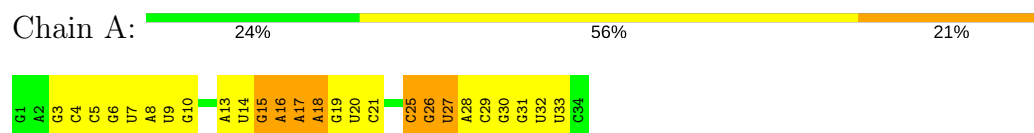


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

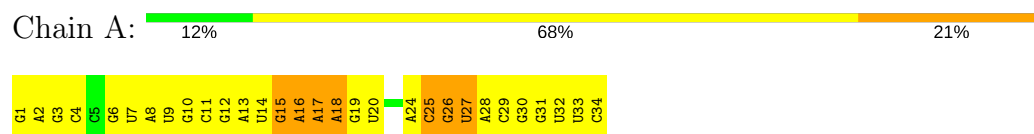
4.2.1 Score per residue for model 1

- Molecule 1: 34-MER



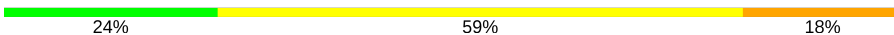
4.2.2 Score per residue for model 2

- Molecule 1: 34-MER



4.2.3 Score per residue for model 3

- Molecule 1: 34-MER

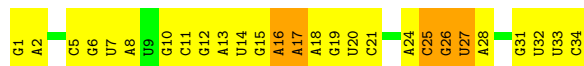
Chain A:  24% 59% 18%



4.2.4 Score per residue for model 4

- Molecule 1: 34-MER

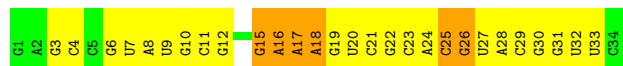
Chain A:  21% 65% 15%



4.2.5 Score per residue for model 5

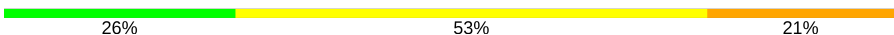
- Molecule 1: 34-MER

Chain A:  18% 65% 18%



4.2.6 Score per residue for model 6

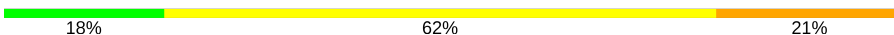
- Molecule 1: 34-MER

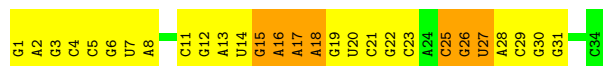
Chain A:  26% 53% 21%



4.2.7 Score per residue for model 7

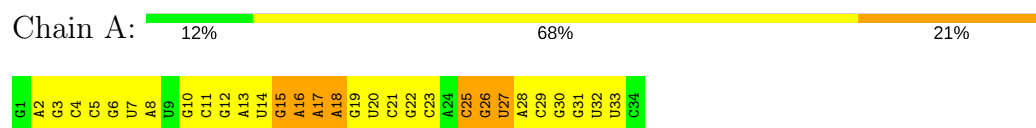
- Molecule 1: 34-MER

Chain A:  18% 62% 21%



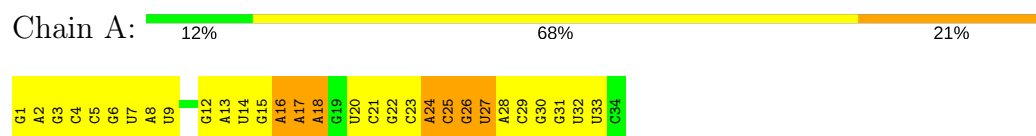
4.2.8 Score per residue for model 8

- Molecule 1: 34-MER



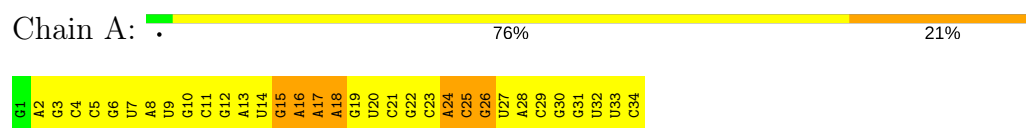
4.2.9 Score per residue for model 9

- Molecule 1: 34-MER



4.2.10 Score per residue for model 10

- Molecule 1: 34-MER



5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE MOLECULAR DYNAMICS CARTESIAN SPACE SIMULATED ANNEALING AND MOLECULAR DYNAMICS RESIDUAL DIPOLAR COUPLINGS*.

Of the 100 calculated structures, 10 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	1.1
CNS	refinement	1.1

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 5962
Number of chemical shift lists	1
Total number of shifts	410
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	410
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
All	All	0	1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	15	G	Sidechain	1

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	726	368	369	46±13
All	All	7260	3680	3690	462

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 42.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:C:HO2'	1:A:27:U:H5	0.89	0.95	4	2
1:A:26:G:N3	1:A:26:G:H3'	0.86	1.86	2	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:U:O2'	1:A:28:A:H5'	0.80	1.77	8	10
1:A:18:A:H8	1:A:18:A:O5'	0.75	1.65	3	3
1:A:17:A:H2'	1:A:18:A:C8	0.74	2.17	3	10
1:A:7:U:O2'	1:A:8:A:H5'	0.73	1.83	7	9
1:A:26:G:H2'	1:A:27:U:C6	0.72	2.20	5	1
1:A:18:A:O5'	1:A:18:A:H8	0.71	1.68	9	7
1:A:27:U:H2'	1:A:28:A:O4'	0.70	1.85	5	2
1:A:29:C:O2'	1:A:30:G:H5'	0.70	1.87	3	5
1:A:27:U:O5'	1:A:27:U:H6	0.69	1.70	5	1
1:A:16:A:C3'	1:A:17:A:H5''	0.69	2.17	8	2
1:A:16:A:C2'	1:A:17:A:H5''	0.69	2.17	9	2
1:A:17:A:C6	1:A:18:A:C2	0.69	2.80	9	7
1:A:25:C:O2'	1:A:27:U:H5	0.68	1.71	4	1
1:A:16:A:H2'	1:A:17:A:C8	0.68	2.24	1	10
1:A:33:U:O5'	1:A:33:U:H6	0.67	1.72	9	4
1:A:26:G:C8	1:A:28:A:N7	0.66	2.64	8	2
1:A:20:U:O2'	1:A:21:C:H5'	0.66	1.91	10	8
1:A:6:G:O2'	1:A:7:U:H5'	0.65	1.91	4	4
1:A:31:G:H8	1:A:31:G:O5'	0.64	1.74	1	3
1:A:13:A:H8	1:A:13:A:O5'	0.64	1.74	4	3
1:A:24:A:H2'	1:A:25:C:O4'	0.63	1.93	4	4
1:A:5:C:H2'	1:A:6:G:C8	0.63	2.29	7	3
1:A:7:U:O5'	1:A:7:U:H6	0.63	1.77	7	5
1:A:17:A:N7	1:A:18:A:C6	0.63	2.67	9	4
1:A:3:G:O2'	1:A:4:C:H5'	0.63	1.94	2	4
1:A:8:A:N6	1:A:26:G:C8	0.62	2.68	5	1
1:A:6:G:O5'	1:A:6:G:H8	0.62	1.78	10	4
1:A:15:G:N2	1:A:17:A:H3'	0.61	2.10	8	2
1:A:12:G:H8	1:A:12:G:O5'	0.61	1.78	4	1
1:A:25:C:O2'	1:A:27:U:C5	0.61	2.51	4	1
1:A:6:G:H8	1:A:6:G:O5'	0.61	1.78	7	2
1:A:1:G:H2'	1:A:2:A:C8	0.60	2.32	9	3
1:A:25:C:H6	1:A:25:C:O5'	0.59	1.78	7	2
1:A:26:G:N3	1:A:26:G:C3'	0.59	2.62	2	2
1:A:28:A:C2	1:A:29:C:C2	0.59	2.90	8	1
1:A:32:U:H2'	1:A:33:U:C6	0.59	2.32	9	9
1:A:5:C:O5'	1:A:5:C:H6	0.59	1.80	7	4
1:A:26:G:O2'	1:A:27:U:C6	0.59	2.55	9	6
1:A:30:G:O2'	1:A:31:G:H5'	0.58	1.97	3	4
1:A:25:C:H3'	1:A:26:G:O4'	0.58	1.99	9	4
1:A:31:G:O5'	1:A:31:G:H8	0.58	1.80	10	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:G:O2'	1:A:13:A:H5'	0.58	1.99	10	4
1:A:26:G:N7	1:A:28:A:N6	0.58	2.52	9	2
1:A:31:G:H2'	1:A:32:U:O4'	0.58	1.98	10	4
1:A:21:C:O2'	1:A:22:G:H5'	0.58	1.99	9	3
1:A:29:C:H6	1:A:29:C:O5'	0.58	1.82	9	2
1:A:10:G:O2'	1:A:11:C:H5'	0.58	1.99	8	1
1:A:8:A:N6	1:A:27:U:C4	0.57	2.71	1	2
1:A:10:G:H8	1:A:10:G:O5'	0.57	1.83	1	2
1:A:4:C:H2'	1:A:5:C:C6	0.56	2.35	1	5
1:A:17:A:C5	1:A:18:A:C6	0.56	2.92	3	1
1:A:5:C:C2	1:A:31:G:N2	0.56	2.75	9	1
1:A:26:G:H1'	1:A:27:U:C5	0.55	2.36	6	3
1:A:2:A:H2'	1:A:3:G:C8	0.55	2.36	9	2
1:A:17:A:H2'	1:A:18:A:O4'	0.55	2.01	8	2
1:A:29:C:O5'	1:A:29:C:H6	0.55	1.83	7	2
1:A:25:C:C3'	1:A:26:G:O4'	0.55	2.55	10	1
1:A:14:U:C4	1:A:15:G:C6	0.55	2.95	9	6
1:A:2:A:H8	1:A:2:A:O5'	0.55	1.85	9	2
1:A:2:A:O5'	1:A:2:A:C8	0.54	2.60	9	3
1:A:17:A:C5	1:A:18:A:C2	0.54	2.96	8	6
1:A:13:A:C5	1:A:14:U:C4	0.54	2.96	9	3
1:A:18:A:C8	1:A:18:A:O5'	0.54	2.57	9	4
1:A:5:C:O2'	1:A:6:G:H5'	0.54	2.03	4	5
1:A:27:U:C2'	1:A:28:A:H5'	0.54	2.33	10	7
1:A:18:A:O5'	1:A:18:A:C8	0.53	2.61	10	4
1:A:26:G:O2'	1:A:27:U:H3'	0.53	2.02	4	1
1:A:17:A:H2'	1:A:18:A:N9	0.53	2.18	7	3
1:A:30:G:H2'	1:A:31:G:C8	0.53	2.38	9	3
1:A:11:C:H2'	1:A:12:G:C8	0.53	2.38	4	4
1:A:27:U:C4	1:A:28:A:C5	0.53	2.97	5	1
1:A:4:C:H6	1:A:4:C:O5'	0.53	1.87	9	2
1:A:12:G:O5'	1:A:12:G:H8	0.53	1.86	5	1
1:A:14:U:C5	1:A:15:G:C5	0.53	2.97	4	2
1:A:7:U:O5'	1:A:7:U:C6	0.52	2.61	7	2
1:A:31:G:C8	1:A:31:G:O5'	0.52	2.61	9	1
1:A:18:A:H2'	1:A:19:G:O4'	0.52	2.05	4	4
1:A:31:G:O2'	1:A:32:U:H5'	0.52	2.04	10	4
1:A:6:G:H2'	1:A:7:U:O4'	0.52	2.04	10	1
1:A:30:G:O5'	1:A:30:G:H8	0.52	1.87	9	3
1:A:17:A:C8	1:A:18:A:C6	0.52	2.97	10	3
1:A:26:G:C5	1:A:28:A:N6	0.52	2.77	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:G:O2'	1:A:2:A:H5'	0.52	2.04	3	2
1:A:26:G:C2'	1:A:27:U:C6	0.52	2.93	5	1
1:A:7:U:C6	1:A:7:U:O5'	0.51	2.61	8	1
1:A:9:U:C4	1:A:25:C:C4	0.51	2.97	2	1
1:A:26:G:H2'	1:A:27:U:C5	0.51	2.40	5	1
1:A:6:G:C2	1:A:30:G:C2	0.51	2.98	7	1
1:A:28:A:H2'	1:A:29:C:C6	0.51	2.41	9	3
1:A:6:G:C4	1:A:30:G:N2	0.51	2.79	9	1
1:A:15:G:H1'	1:A:18:A:N6	0.51	2.21	8	2
1:A:26:G:H3'	1:A:26:G:N3	0.51	2.21	1	2
1:A:26:G:O2'	1:A:27:U:O5'	0.51	2.29	6	5
1:A:11:C:O5'	1:A:11:C:H6	0.51	1.88	5	1
1:A:5:C:O5'	1:A:5:C:C6	0.50	2.65	9	2
1:A:26:G:H4'	1:A:27:U:OP1	0.50	2.06	1	2
1:A:27:U:H2'	1:A:28:A:C5'	0.50	2.37	5	1
1:A:4:C:C6	1:A:4:C:O5'	0.50	2.65	9	1
1:A:26:G:O2'	1:A:27:U:P	0.50	2.70	6	4
1:A:33:U:H2'	1:A:34:C:C6	0.50	2.42	2	3
1:A:16:A:C6	1:A:17:A:C2	0.50	2.99	9	1
1:A:28:A:C8	1:A:28:A:O5'	0.50	2.65	6	3
1:A:15:G:H1'	1:A:18:A:H61	0.49	1.66	8	2
1:A:27:U:C2	1:A:28:A:C8	0.49	3.00	5	1
1:A:7:U:C5	1:A:25:C:C5	0.49	3.00	8	1
1:A:6:G:H2'	1:A:7:U:C6	0.49	2.43	8	1
1:A:14:U:C4	1:A:15:G:C5	0.49	3.01	3	7
1:A:29:C:H2'	1:A:30:G:C8	0.48	2.43	9	2
1:A:27:U:C4	1:A:28:A:N7	0.48	2.81	5	1
1:A:9:U:O2'	1:A:10:G:H5'	0.48	2.08	10	1
1:A:26:G:H4'	1:A:27:U:O5'	0.48	2.09	4	1
1:A:12:G:C8	1:A:12:G:O5'	0.48	2.65	4	1
1:A:19:G:H2'	1:A:20:U:O4'	0.48	2.08	6	5
1:A:13:A:H2'	1:A:14:U:O4'	0.48	2.08	10	3
1:A:6:G:O5'	1:A:6:G:C8	0.48	2.64	7	3
1:A:16:A:H2'	1:A:17:A:O4'	0.48	2.09	7	1
1:A:22:G:O2'	1:A:23:C:H5'	0.48	2.08	9	6
1:A:17:A:C6	1:A:18:A:N1	0.48	2.82	3	1
1:A:17:A:C8	1:A:17:A:C5'	0.48	2.96	8	1
1:A:15:G:C3'	1:A:16:A:C5'	0.47	2.92	9	4
1:A:15:G:N2	1:A:17:A:H5'	0.47	2.24	8	1
1:A:8:A:H2'	1:A:9:U:O4'	0.47	2.09	9	1
1:A:16:A:C2	1:A:17:A:C2	0.47	3.01	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:A:C8	1:A:18:A:C5	0.47	3.02	9	1
1:A:17:A:C5'	1:A:17:A:C8	0.47	2.98	9	1
1:A:8:A:H61	1:A:27:U:H3	0.47	1.53	5	1
1:A:28:A:O5'	1:A:28:A:C8	0.46	2.68	7	3
1:A:15:G:H2'	1:A:16:A:C5'	0.46	2.40	6	5
1:A:7:U:O4	1:A:26:G:N7	0.46	2.49	7	1
1:A:16:A:O2'	1:A:17:A:O4'	0.46	2.29	3	4
1:A:5:C:C2	1:A:31:G:C2	0.46	3.04	9	1
1:A:3:G:C2	1:A:4:C:C2	0.46	3.03	10	1
1:A:10:G:O5'	1:A:10:G:H8	0.46	1.94	2	1
1:A:34:C:H6	1:A:34:C:O5'	0.46	1.93	10	2
1:A:3:G:H8	1:A:3:G:O5'	0.46	1.93	9	2
1:A:29:C:C6	1:A:29:C:O5'	0.46	2.69	7	1
1:A:3:G:H2'	1:A:4:C:O4'	0.45	2.11	7	1
1:A:6:G:C8	1:A:6:G:O5'	0.45	2.66	10	1
1:A:13:A:O2'	1:A:14:U:H5'	0.45	2.10	8	1
1:A:16:A:H2'	1:A:17:A:N7	0.45	2.26	8	1
1:A:33:U:C6	1:A:33:U:O5'	0.45	2.64	10	1
1:A:26:G:N7	1:A:28:A:N7	0.45	2.64	8	1
1:A:13:A:C6	1:A:14:U:N3	0.45	2.84	2	1
1:A:18:A:C2	1:A:19:G:C4	0.45	3.04	3	1
1:A:14:U:O4	1:A:15:G:C6	0.45	2.69	9	6
1:A:16:A:C2'	1:A:17:A:O4'	0.45	2.64	7	1
1:A:17:A:N7	1:A:18:A:N6	0.45	2.65	3	1
1:A:28:A:O5'	1:A:28:A:H8	0.45	1.95	10	3
1:A:8:A:O2'	1:A:9:U:H5'	0.45	2.12	10	1
1:A:10:G:O5'	1:A:10:G:C8	0.45	2.67	1	1
1:A:26:G:N3	1:A:26:G:O5'	0.45	2.50	5	2
1:A:29:C:O5'	1:A:29:C:C6	0.45	2.69	9	2
1:A:17:A:C2'	1:A:18:A:C8	0.44	2.97	3	1
1:A:15:G:H2'	1:A:16:A:H5''	0.44	1.89	9	1
1:A:25:C:H3'	1:A:26:G:C5'	0.44	2.42	10	1
1:A:27:U:C2'	1:A:28:A:C5'	0.44	2.96	5	1
1:A:30:G:O5'	1:A:30:G:C8	0.44	2.71	9	1
1:A:21:C:H2'	1:A:22:G:O4'	0.44	2.12	8	1
1:A:20:U:C2'	1:A:21:C:H5'	0.44	2.43	10	1
1:A:31:G:O5'	1:A:31:G:C8	0.44	2.68	10	2
1:A:19:G:O2'	1:A:20:U:H5'	0.43	2.13	8	1
1:A:13:A:H2'	1:A:14:U:C6	0.43	2.48	9	2
1:A:16:A:O2'	1:A:17:A:H5''	0.43	2.13	8	2
1:A:5:C:H2'	1:A:6:G:O4'	0.43	2.14	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:G:C2'	1:A:16:A:H5''	0.43	2.43	9	1
1:A:2:A:C8	1:A:2:A:O5'	0.43	2.72	4	1
1:A:33:U:O5'	1:A:33:U:C6	0.43	2.63	9	1
1:A:26:G:H2'	1:A:27:U:O5'	0.43	2.13	8	1
1:A:10:G:H2'	1:A:11:C:C6	0.42	2.49	4	1
1:A:9:U:C2'	1:A:10:G:H5'	0.42	2.44	5	1
1:A:16:A:C3'	1:A:17:A:C5'	0.42	2.95	8	1
1:A:15:G:H2'	1:A:16:A:H5'	0.42	1.91	3	1
1:A:18:A:N7	1:A:19:G:C5	0.42	2.87	8	1
1:A:7:U:H2'	1:A:8:A:C8	0.42	2.50	5	1
1:A:26:G:H4'	1:A:26:G:OP1	0.42	2.13	10	1
1:A:3:G:C8	1:A:3:G:O5'	0.41	2.72	9	1
1:A:27:U:HO2'	1:A:28:A:H5'	0.41	1.70	9	1
1:A:26:G:H5''	1:A:26:G:N3	0.41	2.30	10	1
1:A:30:G:H8	1:A:30:G:O5'	0.41	1.98	1	1
1:A:18:A:C8	1:A:19:G:N7	0.41	2.88	8	1
1:A:25:C:O5'	1:A:25:C:H6	0.41	1.99	5	1
1:A:26:G:N3	1:A:26:G:C5'	0.41	2.83	5	1
1:A:10:G:C8	1:A:10:G:O5'	0.41	2.74	2	1
1:A:24:A:C2'	1:A:25:C:O4'	0.41	2.67	4	1
1:A:18:A:H2'	1:A:19:G:C8	0.41	2.51	7	1
1:A:9:U:O4	1:A:25:C:C2	0.41	2.74	1	1
1:A:11:C:H6	1:A:11:C:O5'	0.41	1.98	4	1
1:A:11:C:O2'	1:A:12:G:H5'	0.41	2.16	7	2
1:A:17:A:C5'	1:A:17:A:H8	0.41	2.29	9	1
1:A:2:A:O2'	1:A:3:G:H5'	0.41	2.16	8	1
1:A:15:G:H22	1:A:17:A:H3'	0.40	1.76	7	1
1:A:19:G:N1	1:A:20:U:C2	0.40	2.89	3	1
1:A:19:G:C2'	1:A:20:U:H5'	0.40	2.47	1	1
1:A:4:C:O5'	1:A:4:C:H6	0.40	1.99	5	1
1:A:6:G:C2	1:A:7:U:C2	0.40	3.09	10	1
1:A:16:A:C2'	1:A:17:A:C8	0.40	3.03	8	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	33/34 (97%)	7±1 (21±3%)	0±0 (0±0%)	0.57±0.04
All	All	330/340 (97%)	68 (21%)	0 (0%)	0.57

The overall RNA backbone suiteness is 0.57.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	17	A	10
1	A	16	A	10
1	A	26	G	10
1	A	25	C	10
1	A	18	A	9
1	A	27	U	8
1	A	15	G	6
1	A	24	A	5

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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5962

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	410
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	410
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Chain not found in structure. All 410 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	15	U	H2'	4.209	0.005	1
UNMAPPED	21	U	H5	5.134	0.005	1
UNMAPPED	22	C	H5''	4.071	0.005	1
UNMAPPED	27	G	H2'	4.703	0.005	1
UNMAPPED	31	G	H5''	4.097	0.005	1
UNMAPPED	6	C	H2'	4.6	0.005	1
UNMAPPED	35	C	H5	5.685	0.005	1
UNMAPPED	29	A	H61	7.849	0.005	1
UNMAPPED	28	U	H3'	4.607	0.005	1
UNMAPPED	8	U	H3	13.55	0.005	1
UNMAPPED	13	G	H5''	4.134	0.005	1
UNMAPPED	30	C	C6	140.4	0.05	1
UNMAPPED	26	C	H5	5.408	0.005	1
UNMAPPED	8	U	H5	5.103	0.005	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	30	C	H5''	4.049	0.005	1
UNMAPPED	13	G	H3'	4.105	0.005	1
UNMAPPED	17	A	H5''	3.966	0.005	1
UNMAPPED	13	G	H22	5.75	0.005	1
UNMAPPED	24	C	H41	8.152	0.005	1
UNMAPPED	8	U	C6	141.5	0.05	1
UNMAPPED	15	U	C5	104.2	0.05	1
UNMAPPED	16	G	H8	7.634	0.005	1
UNMAPPED	25	A	H1'	5.839	0.005	1
UNMAPPED	6	C	N3	196.1	0.05	1
UNMAPPED	9	A	C3'	73.17	0.05	1
UNMAPPED	25	A	C4'	84.87	0.05	1
UNMAPPED	22	C	H3'	4.51	0.005	1
UNMAPPED	23	G	H3'	4.424	0.005	1
UNMAPPED	23	G	H1	12.75	0.005	1
UNMAPPED	12	C	C6	140.9	0.05	1
UNMAPPED	29	A	H2'	4.564	0.005	1
UNMAPPED	22	C	H6	7.823	0.005	1
UNMAPPED	9	A	C1'	92.71	0.05	1
UNMAPPED	3	A	H5'	4.509	0.005	1
UNMAPPED	36	C	H1'	5.704	0.005	1
UNMAPPED	1	G	H2'	4.928	0.005	1
UNMAPPED	5	C	H42	7.039	0.005	1
UNMAPPED	3	A	C4'	82.39	0.05	1
UNMAPPED	29	A	C4'	82.23	0.05	1
UNMAPPED	2	G	H21	7.933	0.005	1
UNMAPPED	2	G	H1'	5.896	0.005	1
UNMAPPED	23	G	N1	147.1	0.05	1
UNMAPPED	20	G	H8	7.772	0.005	1
UNMAPPED	1	G	H3'	4.542	0.005	1
UNMAPPED	32	G	H2'	4.638	0.005	1
UNMAPPED	4	G	H8	7.038	0.005	1
UNMAPPED	34	U	C6	143.2	0.05	1
UNMAPPED	7	G	H1	12.81	0.005	1
UNMAPPED	3	A	H2	7.362	0.005	1
UNMAPPED	20	G	C8	137.7	0.05	1
UNMAPPED	3	A	H8	7.858	0.005	1
UNMAPPED	14	A	N1	221.7	0.05	1
UNMAPPED	3	A	H3'	4.66	0.005	1
UNMAPPED	4	G	H5''	4.012	0.005	1
UNMAPPED	33	U	C6	140.5	0.05	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	2	G	N1	146.5	0.05	1
UNMAPPED	3	A	C2'	76.12	0.05	1
UNMAPPED	28	U	H6	7.847	0.005	1
UNMAPPED	22	C	C6	141.2	0.05	1
UNMAPPED	27	G	C2'	75.08	0.05	1
UNMAPPED	25	A	H2'	4.183	0.005	1
UNMAPPED	7	G	H2'	4.477	0.005	1
UNMAPPED	15	U	C1'	93.12	0.05	1
UNMAPPED	4	G	H1'	5.655	0.005	1
UNMAPPED	24	C	H3'	4.393	0.005	1
UNMAPPED	9	A	C2'	75.83	0.05	1
UNMAPPED	14	A	H8	7.674	0.005	1
UNMAPPED	6	C	H3'	4.411	0.005	1
UNMAPPED	14	A	H2	7.755	0.005	1
UNMAPPED	1	G	C8	139.1	0.05	1
UNMAPPED	4	G	H3'	4.206	0.005	1
UNMAPPED	35	C	H42	7.058	0.005	1
UNMAPPED	32	G	C8	135.9	0.05	1
UNMAPPED	10	U	C6	141.3	0.05	1
UNMAPPED	34	U	H3'	4.538	0.005	1
UNMAPPED	5	C	H5	5.263	0.005	1
UNMAPPED	3	A	C5'	65.8	0.05	1
UNMAPPED	2	G	H4'	4.55	0.005	1
UNMAPPED	24	C	C5	97.12	0.05	1
UNMAPPED	23	G	H22	5.855	0.005	1
UNMAPPED	25	A	C8	139.6	0.05	1
UNMAPPED	34	U	H2'	4.501	0.005	1
UNMAPPED	8	U	H1'	5.533	0.005	1
UNMAPPED	33	U	H3	12.22	0.005	1
UNMAPPED	21	U	C5	102.4	0.05	1
UNMAPPED	1	G	C1'	89.41	0.05	1
UNMAPPED	9	A	H1'	6.01	0.005	1
UNMAPPED	17	A	N3	215.8	0.05	1
UNMAPPED	25	A	C5'	66.52	0.05	1
UNMAPPED	9	A	H2'	4.509	0.005	1
UNMAPPED	33	U	H3'	4.54	0.005	1
UNMAPPED	15	U	H5'	4.47	0.005	1
UNMAPPED	27	G	C5'	67.71	0.05	1
UNMAPPED	2	G	H22	5.827	0.005	1
UNMAPPED	8	U	H2'	4.545	0.005	1
UNMAPPED	16	G	N1	145.6	0.05	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	12	C	H3'	4.472	0.005	1
UNMAPPED	29	A	C1'	92.67	0.05	1
UNMAPPED	13	G	H1	12.0	0.005	1
UNMAPPED	35	C	H2'	4.206	0.005	1
UNMAPPED	34	U	N3	162.8	0.05	1
UNMAPPED	5	C	N3	197.4	0.05	1
UNMAPPED	4	G	H1	11.72	0.005	1
UNMAPPED	19	A	C4'	82.69	0.05	1
UNMAPPED	32	G	H22	6.181	0.005	1
UNMAPPED	19	A	H8	8.192	0.005	1
UNMAPPED	25	A	H8	7.929	0.005	1
UNMAPPED	17	A	H2'	4.678	0.005	1
UNMAPPED	5	C	H3'	4.45	0.005	1
UNMAPPED	16	G	H1'	5.632	0.005	1
UNMAPPED	15	U	C2'	75.72	0.05	1
UNMAPPED	11	G	H3'	4.454	0.005	1
UNMAPPED	9	A	N1	223.0	0.05	1
UNMAPPED	18	A	N1	226.4	0.05	1
UNMAPPED	36	C	C5	97.51	0.05	1
UNMAPPED	14	A	C8	139.1	0.05	1
UNMAPPED	20	G	H1'	4.04	0.005	1
UNMAPPED	36	C	C6	140.9	0.05	1
UNMAPPED	30	C	H1'	5.406	0.005	1
UNMAPPED	14	A	C2	153.9	0.05	1
UNMAPPED	27	G	C1'	86.12	0.05	1
UNMAPPED	21	U	H3	14.35	0.005	1
UNMAPPED	13	G	H1'	5.665	0.005	1
UNMAPPED	33	U	C5	103.8	0.05	1
UNMAPPED	22	C	C5	97.54	0.05	1
UNMAPPED	14	A	H61	8.047	0.005	1
UNMAPPED	33	U	N3	158.5	0.05	1
UNMAPPED	23	G	H5''	4.066	0.005	1
UNMAPPED	35	C	C6	142.0	0.05	1
UNMAPPED	32	G	H3'	4.374	0.005	1
UNMAPPED	26	C	C6	141.8	0.05	1
UNMAPPED	17	A	H3'	4.461	0.005	1
UNMAPPED	36	C	H6	7.671	0.005	1
UNMAPPED	29	A	H4'	4.547	0.005	1
UNMAPPED	5	C	C5	97.12	0.05	1
UNMAPPED	3	A	H4'	4.526	0.005	1
UNMAPPED	32	G	H8	7.209	0.005	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	15	U	C6	139.1	0.05	1
UNMAPPED	6	C	H41	8.37	0.005	1
UNMAPPED	22	C	H42	6.908	0.005	1
UNMAPPED	8	U	N3	159.7	0.05	1
UNMAPPED	1	G	C2'	77.45	0.05	1
UNMAPPED	20	G	H5''	3.805	0.005	1
UNMAPPED	29	A	N1	222.3	0.05	1
UNMAPPED	12	C	H2'	4.561	0.005	1
UNMAPPED	26	C	H5'	4.236	0.005	1
UNMAPPED	29	A	C8	140.1	0.05	1
UNMAPPED	11	G	H1'	5.71	0.005	1
UNMAPPED	10	U	H6	7.519	0.005	1
UNMAPPED	30	C	H6	7.467	0.005	1
UNMAPPED	19	A	H1'	5.994	0.005	1
UNMAPPED	23	G	H4'	4.534	0.005	1
UNMAPPED	9	A	C8	139.8	0.05	1
UNMAPPED	14	A	H5'	4.444	0.005	1
UNMAPPED	15	U	C5'	64.02	0.05	1
UNMAPPED	28	U	H1'	5.659	0.005	1
UNMAPPED	1	G	H8	8.186	0.005	1
UNMAPPED	35	C	H41	8.497	0.005	1
UNMAPPED	20	G	H3'	4.457	0.005	1
UNMAPPED	32	G	H5''	4.07	0.005	1
UNMAPPED	24	C	H1'	5.397	0.005	1
UNMAPPED	3	A	C2	153.0	0.05	1
UNMAPPED	24	C	H4'	4.537	0.005	1
UNMAPPED	12	C	H42	6.669	0.005	1
UNMAPPED	33	U	H2'	4.172	0.005	1
UNMAPPED	5	C	H6	7.664	0.005	1
UNMAPPED	3	A	C8	137.8	0.05	1
UNMAPPED	26	C	H4'	4.371	0.005	1
UNMAPPED	23	G	H2'	4.462	0.005	1
UNMAPPED	22	C	H2'	4.456	0.005	1
UNMAPPED	35	C	H4'	4.447	0.005	1
UNMAPPED	34	U	H6	8.088	0.005	1
UNMAPPED	31	G	H21	8.04	0.005	1
UNMAPPED	32	G	H1'	5.723	0.005	1
UNMAPPED	15	U	H5''	4.047	0.005	1
UNMAPPED	24	C	N3	196.1	0.05	1
UNMAPPED	33	U	H6	7.743	0.005	1
UNMAPPED	30	C	H42	6.83	0.005	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	21	U	N3	162.4	0.05	1
UNMAPPED	3	A	H1'	6.033	0.005	1
UNMAPPED	27	G	H4'	4.555	0.005	1
UNMAPPED	31	G	H5'	4.409	0.005	1
UNMAPPED	29	A	H1'	6.022	0.005	1
UNMAPPED	19	A	C2'	76.43	0.05	1
UNMAPPED	21	U	H1'	5.477	0.005	1
UNMAPPED	14	A	H2'	4.493	0.005	1
UNMAPPED	3	A	N3	213.2	0.05	1
UNMAPPED	10	U	H2'	4.247	0.005	1
UNMAPPED	26	C	H2'	4.113	0.005	1
UNMAPPED	9	A	C5'	65.61	0.05	1
UNMAPPED	25	A	N1	225.1	0.05	1
UNMAPPED	24	C	H2'	4.352	0.005	1
UNMAPPED	3	A	H62	6.604	0.005	1
UNMAPPED	27	G	H3'	4.68	0.005	1
UNMAPPED	11	G	H1	12.52	0.005	1
UNMAPPED	14	A	H1'	5.918	0.005	1
UNMAPPED	7	G	H3'	4.503	0.005	1
UNMAPPED	25	A	H3'	4.533	0.005	1
UNMAPPED	13	G	N1	145.9	0.05	1
UNMAPPED	33	U	H1'	5.536	0.005	1
UNMAPPED	36	C	N3	197.8	0.05	1
UNMAPPED	15	U	H3	11.35	0.005	1
UNMAPPED	16	G	C8	137.1	0.05	1
UNMAPPED	14	A	N3	212.9	0.05	1
UNMAPPED	15	U	H5	5.3	0.005	1
UNMAPPED	3	A	H2'	4.628	0.005	1
UNMAPPED	29	A	C2'	75.65	0.05	1
UNMAPPED	19	A	H2'	4.618	0.005	1
UNMAPPED	31	G	H1'	5.695	0.005	1
UNMAPPED	14	A	H62	6.648	0.005	1
UNMAPPED	18	A	H5''	3.938	0.005	1
UNMAPPED	35	C	C5	97.83	0.05	1
UNMAPPED	35	C	H6	7.894	0.005	1
UNMAPPED	26	C	C5	97.41	0.05	1
UNMAPPED	20	G	H2'	4.369	0.005	1
UNMAPPED	28	U	N3	161.7	0.05	1
UNMAPPED	33	U	H5	5.427	0.005	1
UNMAPPED	32	G	H1	13.43	0.005	1
UNMAPPED	30	C	H5'	4.432	0.005	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	22	C	H41	8.306	0.005	1
UNMAPPED	32	G	H5'	4.492	0.005	1
UNMAPPED	26	C	H6	7.434	0.005	1
UNMAPPED	34	U	H4'	4.412	0.005	1
UNMAPPED	10	U	H5	5.386	0.005	1
UNMAPPED	30	C	H5	5.181	0.005	1
UNMAPPED	13	G	H21	7.591	0.005	1
UNMAPPED	22	C	H4'	4.411	0.005	1
UNMAPPED	6	C	H1'	5.509	0.005	1
UNMAPPED	9	A	H8	8.046	0.005	1
UNMAPPED	24	C	H42	6.874	0.005	1
UNMAPPED	16	G	H1	10.7	0.005	1
UNMAPPED	2	G	C8	137.0	0.05	1
UNMAPPED	24	C	H5''	4.069	0.005	1
UNMAPPED	8	U	C5	102.8	0.05	1
UNMAPPED	19	A	N1	226.2	0.05	1
UNMAPPED	27	G	C3'	75.02	0.05	1
UNMAPPED	11	G	N1	147.5	0.05	1
UNMAPPED	30	C	N3	196.7	0.05	1
UNMAPPED	9	A	H4'	4.524	0.005	1
UNMAPPED	25	A	C2	154.0	0.05	1
UNMAPPED	29	A	H8	8.25	0.005	1
UNMAPPED	19	A	C5'	65.75	0.05	1
UNMAPPED	30	C	H4'	4.405	0.005	1
UNMAPPED	20	G	H4'	4.283	0.005	1
UNMAPPED	4	G	H4'	4.474	0.005	1
UNMAPPED	12	C	C5	97.19	0.05	1
UNMAPPED	23	G	H8	7.508	0.005	1
UNMAPPED	22	C	H5	5.588	0.005	1
UNMAPPED	17	A	N1	224.7	0.05	1
UNMAPPED	1	G	H4'	4.536	0.005	1
UNMAPPED	7	G	H5''	4.087	0.005	1
UNMAPPED	29	A	H5''	4.207	0.005	1
UNMAPPED	5	C	H41	8.431	0.005	1
UNMAPPED	18	A	H2'	4.393	0.005	1
UNMAPPED	2	G	H5''	4.231	0.005	1
UNMAPPED	13	G	H5'	4.408	0.005	1
UNMAPPED	17	A	H5'	4.177	0.005	1
UNMAPPED	19	A	C8	141.1	0.05	1
UNMAPPED	31	G	C8	136.1	0.05	1
UNMAPPED	7	G	H8	7.536	0.005	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	19	A	H2	8.159	0.005	1
UNMAPPED	25	A	H2	7.161	0.005	1
UNMAPPED	8	U	H3'	4.576	0.005	1
UNMAPPED	4	G	N1	145.1	0.05	1
UNMAPPED	11	G	H8	7.848	0.005	1
UNMAPPED	27	G	H8	7.849	0.005	1
UNMAPPED	9	A	N3	213.7	0.05	1
UNMAPPED	10	U	H3'	4.577	0.005	1
UNMAPPED	18	A	N3	214.8	0.05	1
UNMAPPED	8	U	H4'	4.431	0.005	1
UNMAPPED	15	U	H3'	4.437	0.005	1
UNMAPPED	17	A	H2	7.743	0.005	1
UNMAPPED	30	C	C5	97.25	0.05	1
UNMAPPED	28	U	H5	5.563	0.005	1
UNMAPPED	18	A	H4'	4.332	0.005	1
UNMAPPED	17	A	H8	8.317	0.005	1
UNMAPPED	18	A	H1'	5.473	0.005	1
UNMAPPED	10	U	H5''	4.091	0.005	1
UNMAPPED	19	A	H5''	4.285	0.005	1
UNMAPPED	35	C	N3	198.0	0.05	1
UNMAPPED	24	C	H5	5.127	0.005	1
UNMAPPED	34	U	H1'	5.641	0.005	1
UNMAPPED	10	U	H1'	5.52	0.005	1
UNMAPPED	4	G	H2'	4.565	0.005	1
UNMAPPED	29	A	C2	153.3	0.05	1
UNMAPPED	2	G	H8	7.564	0.005	1
UNMAPPED	7	G	H22	5.946	0.005	1
UNMAPPED	29	A	N3	212.1	0.05	1
UNMAPPED	9	A	C2	153.8	0.05	1
UNMAPPED	30	C	H3'	4.486	0.005	1
UNMAPPED	35	C	H1'	5.571	0.005	1
UNMAPPED	19	A	H3'	4.962	0.005	1
UNMAPPED	19	A	C2	155.5	0.05	1
UNMAPPED	16	G	H3'	4.7	0.005	1
UNMAPPED	10	U	C5	104.1	0.05	1
UNMAPPED	31	G	H2'	4.644	0.005	1
UNMAPPED	12	C	H5'	4.415	0.005	1
UNMAPPED	2	G	H2'	4.644	0.005	1
UNMAPPED	7	G	H1'	5.694	0.005	1
UNMAPPED	4	G	H5'	4.367	0.005	1
UNMAPPED	31	G	H3'	4.544	0.005	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	24	C	C6	140.3	0.05	1
UNMAPPED	14	A	H4'	4.474	0.005	1
UNMAPPED	21	U	C6	141.5	0.05	1
UNMAPPED	31	G	H1	12.47	0.005	1
UNMAPPED	28	U	C6	142.2	0.05	1
UNMAPPED	1	G	H1'	5.81	0.005	1
UNMAPPED	1	G	C4'	85.49	0.05	1
UNMAPPED	26	C	H3'	4.493	0.005	1
UNMAPPED	2	G	H3'	4.667	0.005	1
UNMAPPED	12	C	H6	7.627	0.005	1
UNMAPPED	9	A	H3'	4.568	0.005	1
UNMAPPED	14	A	H3'	4.511	0.005	1
UNMAPPED	31	G	N1	146.5	0.05	1
UNMAPPED	3	A	N1	221.5	0.05	1
UNMAPPED	8	U	H5''	4.079	0.005	1
UNMAPPED	22	C	N3	196.9	0.05	1
UNMAPPED	13	G	H8	7.469	0.005	1
UNMAPPED	6	C	C5	97.76	0.05	1
UNMAPPED	6	C	C6	140.9	0.05	1
UNMAPPED	25	A	N3	214.5	0.05	1
UNMAPPED	4	G	C8	136.3	0.05	1
UNMAPPED	9	A	H5''	4.155	0.005	1
UNMAPPED	7	G	N1	147.0	0.05	1
UNMAPPED	25	A	H5'	4.449	0.005	1
UNMAPPED	1	G	C5'	67.87	0.05	1
UNMAPPED	15	U	C3'	72.11	0.05	1
UNMAPPED	22	C	H1'	5.541	0.005	1
UNMAPPED	13	G	C8	136.2	0.05	1
UNMAPPED	20	G	N1	144.3	0.05	1
UNMAPPED	6	C	H6	7.687	0.005	1
UNMAPPED	21	U	H2'	4.374	0.005	1
UNMAPPED	32	G	H4'	4.456	0.005	1
UNMAPPED	3	A	H61	7.924	0.005	1
UNMAPPED	19	A	H5'	4.541	0.005	1
UNMAPPED	1	G	N1	146.7	0.05	1
UNMAPPED	29	A	H3'	4.709	0.005	1
UNMAPPED	26	C	H1'	5.589	0.005	1
UNMAPPED	34	U	H5''	4.091	0.005	1
UNMAPPED	21	U	H6	7.724	0.005	1
UNMAPPED	11	G	H2'	4.6	0.005	1
UNMAPPED	23	G	H1'	5.617	0.005	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	19	A	H4'	4.467	0.005	1
UNMAPPED	24	C	H6	7.45	0.005	1
UNMAPPED	25	A	H4'	4.405	0.005	1
UNMAPPED	19	A	C1'	91.47	0.05	1
UNMAPPED	5	C	C6	141.6	0.05	1
UNMAPPED	6	C	H42	6.833	0.005	1
UNMAPPED	15	U	H4'	4.357	0.005	1
UNMAPPED	28	U	H2'	4.508	0.005	1
UNMAPPED	18	A	H3'	4.634	0.005	1
UNMAPPED	13	G	H2'	4.59	0.005	1
UNMAPPED	8	U	H6	7.726	0.005	1
UNMAPPED	2	G	H1	12.5	0.005	1
UNMAPPED	32	G	N1	148.3	0.05	1
UNMAPPED	12	C	H1'	5.479	0.005	1
UNMAPPED	9	A	H2	7.274	0.005	1
UNMAPPED	12	C	H5''	4.106	0.005	1
UNMAPPED	18	A	H8	7.959	0.005	1
UNMAPPED	17	A	H4'	4.147	0.005	1
UNMAPPED	36	C	H5	5.482	0.005	1
UNMAPPED	9	A	H62	6.484	0.005	1
UNMAPPED	29	A	C3'	73.04	0.05	1
UNMAPPED	29	A	H2	7.232	0.005	1
UNMAPPED	18	A	H2	7.697	0.005	1
UNMAPPED	27	G	C8	139.5	0.05	1
UNMAPPED	19	A	N3	215.9	0.05	1
UNMAPPED	12	C	H41	8.336	0.005	1
UNMAPPED	34	U	H5	5.617	0.005	1
UNMAPPED	7	G	C8	136.2	0.05	1
UNMAPPED	17	A	H1'	5.65	0.005	1
UNMAPPED	34	U	H3	14.47	0.005	1
UNMAPPED	1	G	C3'	75.9	0.05	1
UNMAPPED	27	G	C4'	83.44	0.05	1
UNMAPPED	31	G	H22	5.889	0.005	1
UNMAPPED	5	C	H2'	4.313	0.005	1
UNMAPPED	27	G	H1'	5.63	0.005	1
UNMAPPED	15	U	C4'	82.11	0.05	1
UNMAPPED	28	U	C5	104.2	0.05	1
UNMAPPED	17	A	C2	154.4	0.05	1
UNMAPPED	31	G	H8	7.487	0.005	1
UNMAPPED	30	C	H41	8.166	0.005	1
UNMAPPED	15	U	H1'	5.335	0.005	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	17	A	C8	142.2	0.05	1
UNMAPPED	9	A	C4'	82.55	0.05	1
UNMAPPED	35	C	H3'	4.425	0.005	1
UNMAPPED	16	G	H2'	4.489	0.005	1
UNMAPPED	9	A	H5'	4.446	0.005	1
UNMAPPED	25	A	H5''	4.055	0.005	1
UNMAPPED	5	C	H1'	5.515	0.005	1
UNMAPPED	15	U	N3	154.5	0.05	1
UNMAPPED	12	C	H5	5.182	0.005	1
UNMAPPED	3	A	C3'	73.3	0.05	1
UNMAPPED	26	C	H5''	4.042	0.005	1
UNMAPPED	20	G	H1	11.51	0.005	1
UNMAPPED	30	C	H2'	4.384	0.005	1
UNMAPPED	19	A	C3'	73.94	0.05	1
UNMAPPED	35	C	C4'	82.21	0.05	1
UNMAPPED	11	G	C8	139.0	0.05	1
UNMAPPED	14	A	H5''	4.105	0.005	1
UNMAPPED	23	G	C8	136.1	0.05	1
UNMAPPED	34	U	C5	103.6	0.05	1
UNMAPPED	28	U	H4'	4.623	0.005	1
UNMAPPED	35	C	H5''	4.081	0.005	1
UNMAPPED	6	C	H5	5.48	0.005	1
UNMAPPED	12	C	N3	196.6	0.05	1
UNMAPPED	25	A	C3'	71.97	0.05	1
UNMAPPED	18	A	C8	140.7	0.05	1
UNMAPPED	15	U	H6	7.4	0.005	1
UNMAPPED	18	A	C2	154.5	0.05	1

7.1.2 Chemical shift referencing [i](#)

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

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 643. 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 (—%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Sidechain	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	0/643 (0%)	0/371 (0%)	0/227 (0%)	0/45 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 643. 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	0/643 (0%)	0/371 (0%)	0/227 (0%)	0/45 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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.