wwPDB NMR Structure Validation Summary Report

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PDB ID	:	1K5I
Title	:	NMR Structure of a Ribosomal RNA Hairpin Containing a Conserved CUCAA Pentaloop
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Deposited on	:	2001-10-10

This is a wwPDB NMR Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

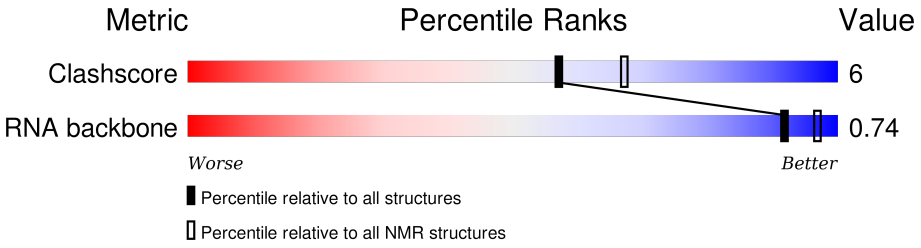
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	23	83% 17%

2 Ensemble composition and analysis (i)

This entry contains 10 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 (i)

There is only 1 type of molecule in this entry. The entry contains 740 atoms, of which 250 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	23	740	218	250	88	161	23	0

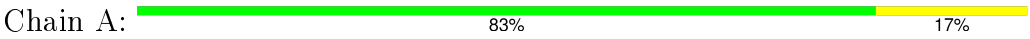
4 Residue-property plots (i)

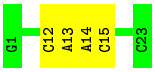
4.1 Average score per residue in the NMR ensemble

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: 5'-R(P*GP*GP*AP*CP*CP*CP*GP*GP*GP*CP*UP*CP*AP*AP*CP*CP*UP*GP*GP*GP*UP*CP*C)-3'

Chain A:



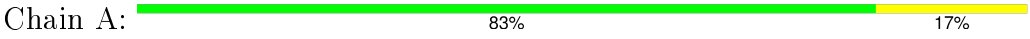


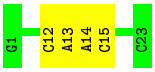
4.2 Residue scores for the first model from the NMR ensemble

No representative models were identified. Colouring as in section 4.1 above.

• Molecule 1: 5'-R(P*GP*GP*AP*CP*CP*CP*GP*GP*GP*CP*UP*CP*AP*AP*CP*CP*UP*GP*GP*GP*UP*CP*C)-3'

Chain A:





5 Refinement protocol and experimental data overview

The models were refined using the following method: *Distance Geometry, Simulated Annealing, Restrained Molecular Dynamics.*

Of the 33 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
X-PLOR	refinement	3.1

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

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	490	250	251	5±1
All	All	4900	2500	2510	46

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 6.

5 of 9 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:C:H2'	1:A:11:U:O4'	0.72	1.84	10	2
1:A:13:A:H2'	1:A:14:A:O4'	0.67	1.89	1	9
1:A:14:A:O2'	1:A:15:C:H5'	0.64	1.92	9	9
1:A:14:A:H2'	1:A:15:C:O4'	0.56	2.00	6	9
1:A:14:A:C2	1:A:15:C:C2	0.52	2.97	3	3

6.3 Torsion angles

6.3.1 Protein backbone

There are no protein molecules in this entry.

6.3.2 Protein sidechains

There are no protein molecules in this entry.

6.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	22/23 (96%)	1±0 (5±2%)	0±0 (1±2%)	0.74±0.03
All	All	220/230 (96%)	12 (5%)	2 (1%)	0.74

The overall RNA backbone suiteness is 0.74.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	12	C	10
1	A	14	A	1
1	A	11	U	1

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	11	U	2

6.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

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

No chemical shift data were provided