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wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2M39
Title	:	The solution structure of 3',5'-LINKED 2'-O-(2-METHOXYETHYL)-RNA DUPLEX
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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 (i)) were used in the production of this report:

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	FAILED
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
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 is 7%.

There are no percentiles available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis (i)

This entry contains 9 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 1024 atoms, of which 418 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called RNA (5'-R(*(C5L)P*(G48)P*(C5L)P*(G48)P*(A44)P*(A44)P*(T39)P*(T39)P*(C5L)P*(G48)P*(C5L)P*DG)-3').

Mol	Chain	Residues	Atoms							Trace
1	A	12	Total	C	H	Ho	N	O	P	0
			512	153	209	1	46	92	11	
1	B	12	Total	C	H	Ho	N	O	P	0
			512	153	209	1	46	92	11	

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: RNA (5'-R(*(C5L)P*(G48)P*(C5L)P*(G48)P*(A44)P*(A44)P*(T39)P*(T39)P*(C5L)P*(G48)P*(C5L)P*DG)-3')

Chain A: ━━━━━━━━━━━━━━━━━ 100%

There are no outlier residues in this chain.

• Molecule 1: RNA (5'-R(*(C5L)P*(G48)P*(C5L)P*(G48)P*(A44)P*(A44)P*(T39)P*(T39)P*(C5L)P*(G48)P*(C5L)P*DG)-3')

Chain B: ━━━━━━━━━━━━━━━━━ 100%

There are no outlier residues in this chain.

4.2 Residue scores for the representative (author defined) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

• Molecule 1: RNA (5'-R(*(C5L)P*(G48)P*(C5L)P*(G48)P*(A44)P*(A44)P*(T39)P*(T39)P*(C5L)P*(G48)P*(C5L)P*DG)-3')

Chain A: ━━━━━━━━━━━━━━━━━ 100%

There are no outlier residues in this chain.

• Molecule 1: RNA (5'-R(*(C5L)P*(G48)P*(C5L)P*(G48)P*(A44)P*(A44)P*(T39)P*(T39)P*(C5L)P*(G48)P*(C5L)P*DG)-3')

Chain B: ━━━━━━━━━━━━━━━━━ 100%

There are no outlier residues in this chain.

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing, energy minimization*.

Of the 50 calculated structures, 9 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
AMBER	structure solution	7
AMBER	refinement	7

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)	2m39_cs.str
Number of chemical shift lists	1
Total number of shifts	173
Number of shifts mapped to atoms	173
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	7%

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)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts (i)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA (i)

MolProbity failed to run properly - this section will have to be empty.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates (i)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry (i)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers (i)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 7% for the well-defined parts and 7% for the entire structure.

7.1 Chemical shift list 1

File name: 2m39_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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	173
Number of shifts mapped to atoms	173
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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 7%, i.e. 3 atoms were assigned a chemical shift out of a possible 42. 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	3/42 (7%)	3/26 (12%)	0/12 (0%)	0/4 (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.