

wwPDB NMR Structure Validation Summary Report (i)

Oct 13, 2022 – 02:01 PM EDT

PDB ID : 7SHX BMRB ID : 51127

Title : A functional SNP regulates E-cadherin expression by dynamically remodeling

the 3D structure of a promoter-associated non-coding RNA transcript, NMR,

minimized average structure

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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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity: 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

RCI : v 1n 11 5 13 A (Berjanski et al., 2005)

PANAV : Wang et al. (2010)

ShiftChecker : 2.31.2

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.31.2

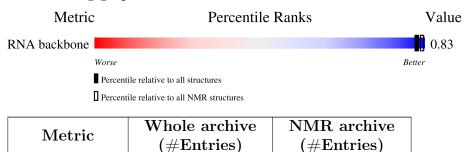
RNA backbone

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 66%.

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.



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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%

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Mol	Chain	Length	Quality of chain
1	Δ	94	100%
1	Λ	94	100%



2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3042 atoms, of which 1024 are hydrogens and 0 are deuteriums.

• Molecule 1 is a RNA chain called RNA (94-MER).

Mol	Chain	Residues			Aton	ıs			Trace
1	Λ	0.4	Total	С	Н	N	О	Р	0
1	A	94	3042	899	1024	376	650	93	U



4 Residue-property plots (i)

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: RNA (94-MER)

С	h	ai	n	A																					10	0%	ó																					
G1	d2	A3	5 5	90	A7	80 V	A10	C11	C12	C13	C15	C16	U17	A18	G19	A20	C21	C22	U24	A25	G26	1128	U29	C30	G31	G32	C33	A35	985	A37	2000	G40	U41	C42	A 44	C45	G46	C47	A 49	A50	A51	G52	C53	A55	G56	G28 G28	C29	095
G61			465	995	C67	895	025	U7.1	A72	674	U75	C76	C7.7	G78	623	080	C81	G83	G84	G85	985	A87	685	065	G91	U92	C93	F 00																				



Refinement protocol and experimental data overview (i) 5



The models were refined using the following method: simulated annealing.

Of the 10 calculated structures, 1 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 NIH	refinement	
X-PLOR NIH	structure calculation	

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1213
Number of shifts mapped to atoms	1213
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	66%



6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

N	Mol	Chain	Non-H	H(model)	H(added)	Clashes
	1	A	0	0	0	0
	All	All	0	0	0	-

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)

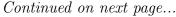
There are no protein molecules in this entry.

6.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

6.3.3 RNA (i)

Mol 0	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	93/94 (99%)	10 (11%)	0 (0%)	0.83





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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
All	All	93/94 (99%)	10 (11%)	0 (0%)	0.83

The overall RNA backbone suiteness is 0.83.

5 of 10 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	A
1	A	18	A
1	A	35	A
1	A	43	A
1	A	49	A

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 monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 66% for the well-defined parts and 66% for the entire structure.

7.1 Chemical shift list 1

File name: working cs.cif

Chemical shift list name: assigned_chemical_shifts_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	1213
Number of shifts mapped to atoms	1213
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 66%, i.e. 1189 atoms were assigned a chemical shift out of a possible 1797. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}{ m H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
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	1189/1797 (66%)	642/1045 (61%)	518/623 (83%)	29/129 (22%)

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_chemical_shifts_1). RCI is only applicable to proteins.

