



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 8THV / pdb_00008thv
BMRB ID : 31099
Title : FARFAR-NMR ensemble of HIV-1 TAR with apical loop capturing ground and excited conformational states
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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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Ensemble composition and analysis

This entry contains 20 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 925 atoms, of which 311 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called RNA (29-MER).

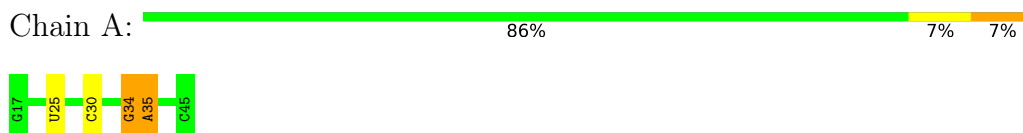
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	29	925	275	311	109	202	28	0

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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.

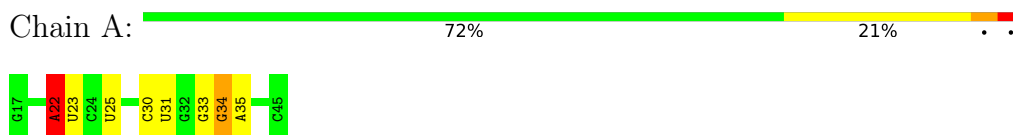
- Molecule 1: RNA (29-MER)



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 (29-MER)



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
Rosetta	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	503
Number of shifts mapped to atoms	500
Number of unparsed shifts	0
Number of shifts with mapping errors	3
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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	0.37±0.16	0±0/685 (0.0± 0.0%)	0.54±0.18	0±1/1067 (0.0± 0.1%)
All	All	0.40	1/13700 (0.0%)	0.57	8/21340 (0.0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	34	G	O3'-P	-5.53	1.52	1.61	18	1

5 of 8 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	25	U	C2'-C3'-O3'	-9.52	99.42	113.70	19	1
1	A	22	A	P-O3'-C3'	7.34	131.20	120.20	1	1
1	A	22	A	O3'-P-O5'	6.93	114.40	104.00	1	1
1	A	22	A	C2'-C3'-O3'	-6.85	103.42	113.70	5	1
1	A	23	U	O3'-P-O5'	6.25	113.38	104.00	19	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
1	A	614	311	312	5±2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	12280	6220	6240	109

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:G:O2'	1:A:35:A:OP1	1.18	1.60	2	2
1:A:33:G:O4'	1:A:33:G:OP1	1.16	1.62	15	1
1:A:30:C:O2'	1:A:31:U:OP2	1.16	1.61	7	1
1:A:34:G:O2'	1:A:35:A:OP2	1.07	1.69	18	1
1:A:24:C:O2'	1:A:25:U:OP2	1.04	1.71	4	1

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	28/29 (97%)	2±0 (7±0%)	1±1 (3±3%)	0.66±0.00
All	All	560/580 (97%)	40 (7%)	19 (3%)	0.66

The overall RNA backbone suiteness is 0.66.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	34	G	20
1	A	35	A	20

5 of 9 unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	34	G	3
1	A	24	C	3
1	A	23	U	3
1	A	22	A	2
1	A	29	C	2

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 oligosaccharides 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 75% for the well-defined parts and 75% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *chemical_shifts*

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	503
Number of shifts mapped to atoms	500
Number of unparsed shifts	0
Number of shifts with mapping errors	3
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.

- No matching atom found in the structure. All 3 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	17	G	H5'	4.283	0.002	.
1	A	17	G	H5''	4.407	0.002	.
1	A	17	G	P	-1.889	0.004	1

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 75%, i.e. 425 atoms were assigned a chemical shift out of a possible 563. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Sugar	312/319 (98%)	168/174 (97%)	144/145 (99%)	0/0 (—%)
Base	113/244 (46%)	50/143 (35%)	41/48 (85%)	22/53 (42%)
Overall	425/563 (75%)	218/317 (69%)	185/193 (96%)	22/53 (42%)

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. RCI is only applicable to proteins

8 NMR restraints analysis

No restraints data found

9 Distance violation analysis

No distance restraints data found

10 Dihedral-angle violation analysis

No dihedral-angle restraints found