Full wwPDB NMR Structure Validation Report (i)

Jun 7, 2020 – 02:46 am BST

PDB ID	:	6GZK
Title	:	Solution NMR structure of the tetramethylrhodamine (TMR) aptamer 3 in complex with 5-TAMRA
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Deposited on	:	2018-07-04

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
https://www.wwpdb.org/validation/2017/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:

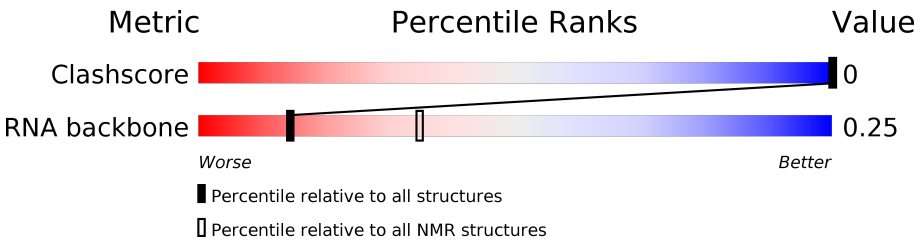
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 84%.

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	158937	12864
RNA backbone	4643	676

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	48	69% 31%

2 Ensemble composition and analysis (i)

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.

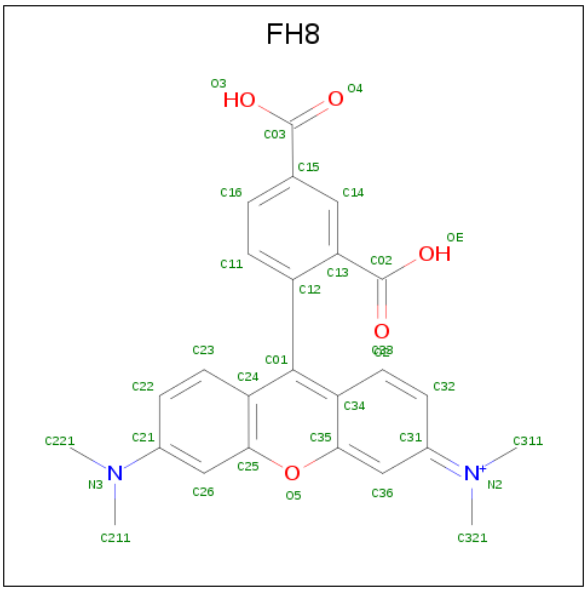
3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1599 atoms, of which 539 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called TMR3 (48-MER).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	48	1546	458	518	186	336	48	0

- Molecule 2 is 5-carboxy methylrhodamine (three-letter code: FH8) (formula: $C_{25}H_{23}N_2O_5$).



Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
2	A	1	53	25	21	2	5

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: TMR3 (48-MER)

Chain A: 69% 31%

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

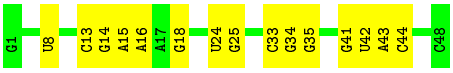
- Molecule 1: TMR3 (48-MER)

Chain A: 69% 31%

4.2.2 Score per residue for model 2

- Molecule 1: TMR3 (48-MER)

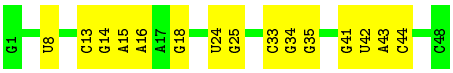
Chain A: 69% 31%



4.2.3 Score per residue for model 3

- Molecule 1: TMR3 (48-MER)

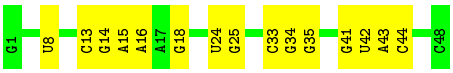
Chain A: 69% 31%



4.2.4 Score per residue for model 4

- Molecule 1: TMR3 (48-MER)

Chain A: 69% 31%



4.2.5 Score per residue for model 5

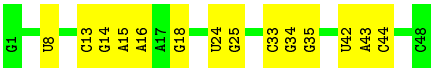
- Molecule 1: TMR3 (48-MER)

Chain A: 69% 31%

4.2.6 Score per residue for model 6

- Molecule 1: TMR3 (48-MER)

Chain A: 71% 29%



4.2.7 Score per residue for model 7

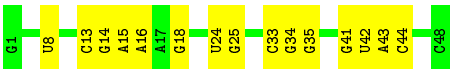
- Molecule 1: TMR3 (48-MER)

Chain A: 75% 25%

4.2.8 Score per residue for model 8

- Molecule 1: TMR3 (48-MER)

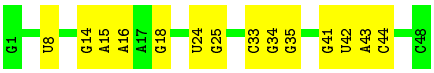
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: TMR3 (48-MER)

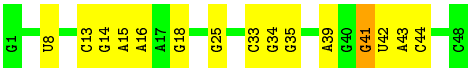
Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: TMR3 (48-MER)

Chain A:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	refinement	3.97
CYANA	structure calculation	3.97

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	957
Number of shifts mapped to atoms	957
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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

COVALENT-GEOMETRY INFOmissingINFO

5.1 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
All	All	10600	5390	5190	-

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.

5.2 Torsion angles (i)

5.2.1 Protein backbone (i)

There are no protein molecules in this entry.

5.2.2 Protein sidechains (i)

There are no protein molecules in this entry.

5.2.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	47/48 (98%)	13±1 (27±2%)	0±0 (0±0%)	0.25±0.01
All	All	470/480 (98%)	125 (27%)	0 (0%)	0.25

The overall RNA backbone suiteness is 0.25.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	18	G	10
1	A	14	G	10
1	A	16	A	10
1	A	8	U	10
1	A	15	A	10
1	A	25	G	10
1	A	35	G	10
1	A	43	A	10
1	A	42	U	10
1	A	44	C	9
1	A	13	C	9
1	A	24	U	8
1	A	41	G	8
1	A	39	A	1

There are no RNA pucker outliers to report.

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

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

5.4 Carbohydrates (i)

There are no carbohydrates in this entry.

LIGAND-GEOMETRY INFOmissingINFO

5.5 Other polymers (i)

There are no such molecules in this entry.

5.6 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 84% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

6.1.1 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	957
Number of shifts mapped to atoms	957
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	28

6.1.2 Chemical shift referencing (i)

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

6.1.3 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 84%, i.e. 789 atoms were assigned a chemical shift out of a possible 940. 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	789/940 (84%)	404/524 (77%)	293/320 (92%)	92/96 (96%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 789 atoms were assigned a chemical shift out of a possible 940. 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	789/940 (84%)	404/524 (77%)	293/320 (92%)	92/96 (96%)

6.1.4 Statistically unusual chemical shifts (i)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	4	C	C4	151.05	173.92 – 160.32	-11.8
1	A	11	A	C6	157.65	156.32 – 154.32	11.6
1	A	43	A	C6	157.63	156.32 – 154.32	11.6
1	A	3	A	C6	157.41	156.32 – 154.32	10.5
1	A	10	A	C6	157.40	156.32 – 154.32	10.4
1	A	26	G	C5	119.45	117.74 – 114.54	10.3
1	A	25	G	C5	119.40	117.74 – 114.54	10.2
1	A	39	A	C6	157.34	156.32 – 154.32	10.1
1	A	18	G	C5	119.19	117.74 – 114.54	9.5
1	A	6	A	C6	157.19	156.32 – 154.32	9.4
1	A	42	U	H4'	3.19	5.04 – 3.74	-9.2
1	A	35	G	C5	119.05	117.74 – 114.54	9.1
1	A	14	G	C5	118.95	117.74 – 114.54	8.8
1	A	19	G	C5	118.89	117.74 – 114.54	8.6
1	A	45	G	C5	118.84	117.74 – 114.54	8.4
1	A	37	A	C6	156.96	156.32 – 154.32	8.2
1	A	34	G	C5	118.67	117.74 – 114.54	7.9
1	A	2	G	C5	118.63	117.74 – 114.54	7.8
1	A	38	G	C5	118.58	117.74 – 114.54	7.6
1	A	9	G	C5	118.56	117.74 – 114.54	7.6
1	A	1	G	C5	118.55	117.74 – 114.54	7.5
1	A	17	A	C6	156.79	156.32 – 154.32	7.3
1	A	29	G	C5	118.48	117.74 – 114.54	7.3
1	A	5	G	C5	118.03	117.74 – 114.54	5.9
1	A	33	C	H5"	2.68	5.47 – 2.87	-5.7
1	A	18	G	H1'	3.61	7.41 – 3.81	-5.6
1	A	40	G	C5	117.91	117.74 – 114.54	5.5
1	A	15	A	C6	156.33	156.32 – 154.32	5.0

6.1.5 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.