



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2022 – 02:10 PM EDT

PDB ID : 4TS2
Title : Crystal structure of the Spinach RNA aptamer in complex with DFHBI, magnesium ions
Authors : Warner, K.D.; Chen, M.C.; Song, W.; Strack, R.L.; Thorn, A.; Jaffrey, S.R.; Ferre-D'Amare, A.R.
Deposited on : 2014-06-18
Resolution : 2.88 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

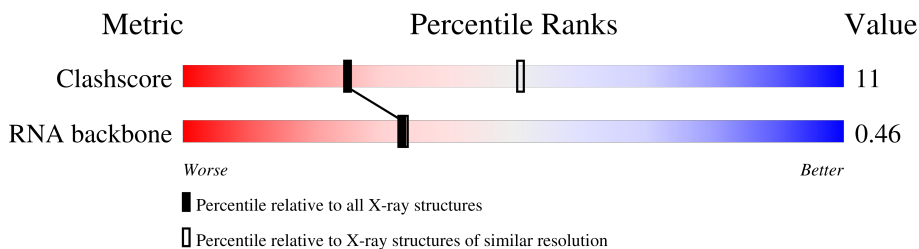
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 Å.

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2947 (2.90-2.86)
RNA backbone	3102	1121 (3.16-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	X	44	
2	Y	47	
3	A	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CCC	X	44	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 1972 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called Spinach aptamer RNA, bimolecular construct.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	X	44	933	415	176	298	44	0	0	0

- Molecule 2 is a RNA chain called Spinach aptamer RNA, bimolecular construct.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	Y	47	989	439	173	330	47	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	A	2	23	12	11	0	0	0

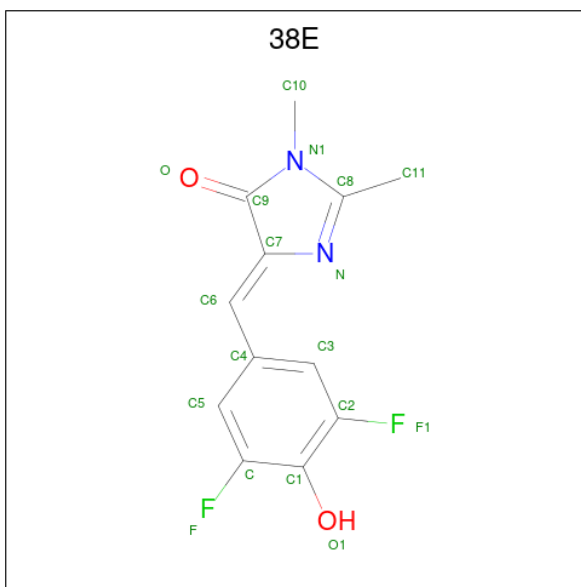
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	1	Total	Mg	0	0
			1	1		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	Y	3	Total	K	0	0
			3	3		

- Molecule 6 is (5Z)-5-(3,5-difluoro-4-hydroxybenzylidene)-2,3-dimethyl-3,5-dihydro-4H-imidazol-4-one (three-letter code: 38E) (formula: C₁₂H₁₀F₂N₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
6	Y	1	18	12	2	2	2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	X	2	Total O 2 2	0	0
7	Y	3	Total O 3 3	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

- Molecule 1: Spinach aptamer RNA, bimolecular construct

Chain X: 



- Molecule 2: Spinach aptamer RNA, bimolecular construct

Chain Y: 



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain A: 



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	39.88Å 49.40Å 188.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.88	Depositor
% Data completeness (in resolution range)	99.3 (50.00-2.88)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.213 , 0.257	Depositor
Wilson B-factor (Å ²)	94.7	Xtrriage
Anisotropy	0.406	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1972	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, CCC, MG, FRU, 38E, K

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 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	X	0.51	1/1022 (0.1%)	0.97	6/1595 (0.4%)
2	Y	0.53	1/1079 (0.1%)	0.85	2/1682 (0.1%)
All	All	0.52	2/2101 (0.1%)	0.91	8/3277 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	10	G	O3'-P	-6.39	1.53	1.61
2	Y	59	U	O3'-P	5.04	1.67	1.61

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	20	G	O5'-P-OP2	-9.42	97.22	105.70
2	Y	71	U	O5'-P-OP2	-8.65	97.92	105.70
1	X	19	G	O5'-P-OP2	6.40	118.38	110.70
1	X	17	A	O5'-P-OP1	-5.83	100.45	105.70
1	X	19	G	O5'-P-OP1	-5.75	100.53	105.70
1	X	24	A	O5'-P-OP2	-5.43	100.81	105.70
2	Y	86	U	O5'-P-OP2	-5.42	100.82	105.70
1	X	25	G	O5'-P-OP2	5.23	116.98	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	933	0	470	18	0
2	Y	989	0	496	14	0
3	A	23	0	21	1	0
4	X	1	0	0	0	0
5	Y	3	0	0	0	0
6	Y	18	0	9	1	0
7	X	2	0	0	0	0
7	Y	3	0	0	0	0
All	All	1972	0	996	31	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 11.

All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1:G:H2'	1:X:2:A:C8	2.11	0.85
2:Y:94:U:H2'	2:Y:101:CCC:O4'	1.90	0.71
1:X:26:G:H4'	1:X:27:A:H5''	1.74	0.69
2:Y:76:G:H2'	2:Y:77:C:H5'	1.79	0.65
1:X:43:G:C2	1:X:44:CCC:C2	2.82	0.63
2:Y:74:G:H2'	2:Y:75:A:H5'	1.81	0.63
2:Y:76:G:C2'	2:Y:77:C:H5'	2.29	0.63
2:Y:76:G:O2'	3:A:1:GLC:H62	2.02	0.58
1:X:43:G:H3'	1:X:44:CCC:H6	1.85	0.58
1:X:43:G:O3'	1:X:44:CCC:O4'	2.22	0.57
1:X:1:G:H2'	1:X:2:A:H8	1.67	0.57
2:Y:74:G:C2'	2:Y:75:A:H5'	2.34	0.57
1:X:43:G:C2	1:X:44:CCC:N3	2.73	0.56
1:X:1:G:H22	2:Y:101:CCC:C2	2.25	0.50
2:Y:78:U:H2'	2:Y:79:C:C6	2.47	0.49
2:Y:67:A:H4'	2:Y:68:G:OP2	2.14	0.48
1:X:43:G:N2	1:X:44:CCC:O2	2.47	0.48
1:X:43:G:H2'	1:X:43:G:N3	2.30	0.47
1:X:43:G:H3'	1:X:44:CCC:C6	2.45	0.46
2:Y:79:C:H2'	2:Y:80:C:C6	2.51	0.45
2:Y:93:G:H2'	2:Y:94:U:C6	2.51	0.45
2:Y:94:U:H6	2:Y:94:U:O5'	2.01	0.43
1:X:7:A:H2'	1:X:8:C:H6	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:79:C:H2'	2:Y:80:C:H6	1.84	0.43
1:X:26:G:H4'	1:X:27:A:C5'	2.46	0.42
2:Y:65:G:H3'	2:Y:65:G:N3	2.34	0.42
1:X:7:A:H2'	1:X:8:C:C6	2.55	0.42
1:X:32:U:H2'	1:X:33:C:O4'	2.20	0.41
1:X:43:G:C5	1:X:44:CCC:C4	3.03	0.41
1:X:31:G:O6	6:Y:204:38E:H4	2.21	0.41
1:X:43:G:C6	1:X:44:CCC:N4	2.89	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	43/44 (97%)	7 (16%)	0
2	Y	46/47 (97%)	11 (23%)	0
All	All	89/91 (97%)	18 (20%)	0

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	12	A
1	X	13	U
1	X	27	A
1	X	28	C
1	X	42	U
1	X	43	G
1	X	44	CCC
2	Y	58	U

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Mol	Chain	Res	Type
2	Y	66	U
2	Y	67	A
2	Y	68	G
2	Y	72	G
2	Y	73	U
2	Y	75	A
2	Y	77	C
2	Y	83	A
2	Y	94	U
2	Y	101	CCC

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

2 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

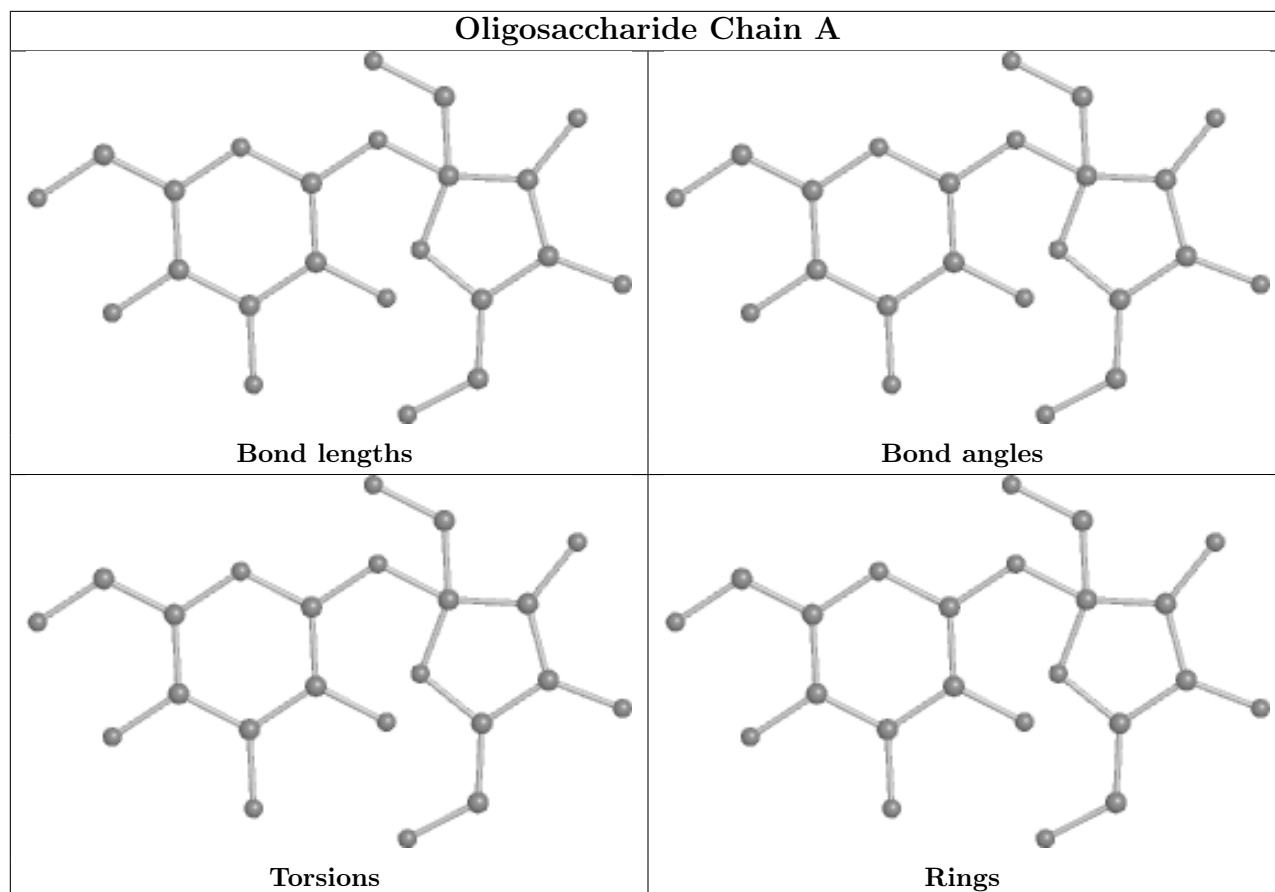
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.