



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 06:23 AM EDT

PDB ID : 1XUW
Title : Structural rationalization of a large difference in RNA affinity despite a small difference in chemistry between two 2'-O-modified nucleic acid analogs
Authors : Pattanayek, R.; Sethaphong, L.; Pan, C.; Prhavy, M.; Prakash, T.P.; Manoharan, M.; Egli, M.
Deposited on : unknown
Resolution : 1.25 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

<http://wwpdb.org/validation/2016/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 : **FAILED**
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

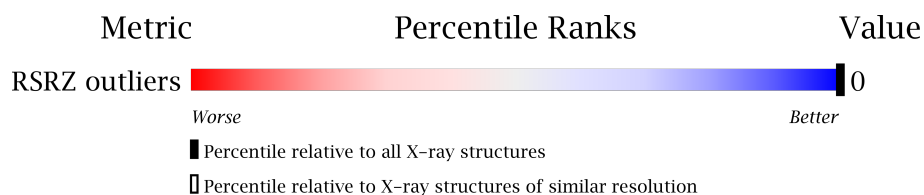
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.25 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))
RSRZ outliers	101464	1693 (1.30-1.22)

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2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 569 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 DNA chain called DNA (5'-D(*GP*CP*GP*TP*AP*(NMT)P*AP*CP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	10	Total	C	N	O	P	0	1	0
			209	100	40	60	9			
1	B	10	Total	C	N	O	P	0	0	0
			207	99	39	60	9			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	81	Total	O	0	0
			81	81		
2	B	72	Total	O	0	0
			72	72		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	24.60 Å 44.88 Å 46.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.25 9.97 – 1.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.25) 90.4 (9.97-1.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 1.25 Å)	Xtriage
Refinement program	CNS, SHELXL-97	Depositor
R, R_{free}	0.153 , 0.221 0.163 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	569	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.27% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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

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4.5 Carbohydrates [i](#)

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4.6 Ligand geometry [i](#)

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4.7 Other polymers [i](#)

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4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	9/10 (90%)	-0.42	0 100 100	16, 17, 26, 32	0
1	B	9/10 (90%)	-0.38	0 100 100	18, 20, 26, 29	0
All	All	18/20 (90%)	-0.40	0 100 100	16, 20, 29, 32	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	NMT	A	6[A]	25/26	0.96	0.07	-	17,20,36,51	2
1	NMT	A	6[B]	25/26	0.96	0.07	-	17,20,38,51	2
1	NMT	B	116	25/26	0.93	0.09	-	21,32,52,59	0

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers

There are no such residues in this entry.