wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2023 – 10:26 PM 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.; Prhavc, M.; Prakash, T.P.; Manoharan, M.; Egli, M.
Deposited on	:	2004-10-26
Resolution	:	1.25 Å(reported)

This is a wwPDB X-ray 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/XrayValidationReportHelp
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 (1)) were used in the production of this report:

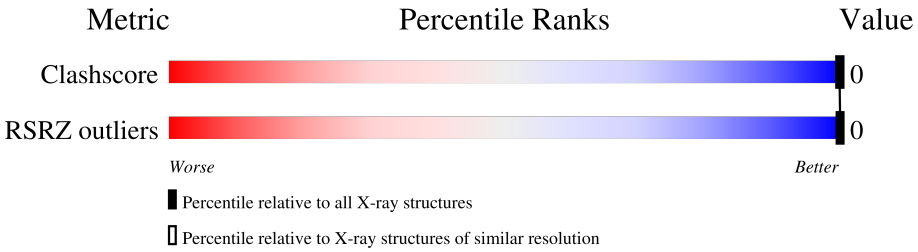
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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))
Clashscore	141614	1060 (1.28-1.24)
RSRZ outliers	127900	1004 (1.28-1.24)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	10	10% 90%
1	B	10	10% 90%

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	NMT	A	6[A]	X	-	-	-
1	NMT	A	6[B]	X	-	-	-
1	NMT	B	116	X	-	-	-

2 Entry composition (i)

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.

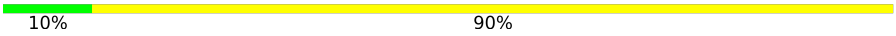
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	81	Total	O	0	0
			81	81		
2	B	72	Total	O	0	0
			72	72		

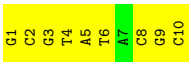
3 Residue-property plots (i)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

- Molecule 1: DNA (5'-D(*GP*CP*GP*TP*AP*(NMT)P*AP*CP*GP*C)-3')

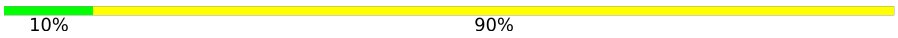
Chain A:





- Molecule 1: DNA (5'-D(*GP*CP*GP*TP*AP*(NMT)P*AP*CP*GP*C)-3')

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	24.60Å 44.88Å 46.30Å 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
$< I/\sigma(I) >$ [1]	3.03 (at 1.25Å)	Xtriage
Refinement program	SHELXL-97, CNS	Depositor
R, R_{free}	0.153 , 0.221 0.163 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NMT

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	A	2.20	8/203 (3.9%)	2.42	21/309 (6.8%)
1	B	2.25	11/203 (5.4%)	2.51	18/309 (5.8%)
All	All	2.23	19/406 (4.7%)	2.47	39/618 (6.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	0
1	B	1	0
All	All	3	0

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	119	DG	C2'-C1'	-10.87	1.41	1.52
1	A	3	DG	C2'-C1'	-10.08	1.42	1.52
1	B	120	DC	C2'-C1'	-9.43	1.42	1.52
1	A	4	DT	C2'-C1'	-9.29	1.43	1.52
1	A	9	DG	C2'-C1'	-8.51	1.43	1.52

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	119	DG	O4'-C1'-N9	-12.06	99.56	108.00
1	A	5	DA	O4'-C4'-C3'	-8.68	100.79	106.00
1	B	120	DC	O4'-C1'-N1	-8.67	101.93	108.00
1	A	3	DG	O4'-C1'-N9	-8.60	101.98	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	118	DC	O4'-C4'-C3'	-7.92	101.25	106.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	6[A]	NMT	C7'
1	A	6[B]	NMT	C7'
1	B	116	NMT	C7'

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	A	209	0	110	0	0
1	B	207	0	117	0	0
2	A	81	0	0	0	2
2	B	72	0	0	0	1
All	All	569	0	227	0	2

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 0.

There are no clashes within the asymmetric unit.

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1032:HOH:O	2:B:1066:HOH:O[4_565]	1.99	0.21
2:A:1086:HOH:O	2:A:1095:HOH:O[3_655]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein molecules in this entry.

5.3.2 Protein sidechains

There are no protein molecules in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	NMT	A	6[B]	-	22,26,27	2.02	3 (13%)	29,37,40	1.49	7 (24%)
1	NMT	B	116	1	22,26,27	1.98	4 (18%)	29,37,40	1.43	4 (13%)
1	NMT	A	6[A]	-	22,26,27	2.02	3 (13%)	29,37,40	1.45	6 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NMT	A	6[B]	-	1/1/6/7	0/9/31/32	0/2/2/2
1	NMT	B	116	1	1/1/6/7	0/9/31/32	0/2/2/2
1	NMT	A	6[A]	-	1/1/6/7	0/9/31/32	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6[A]	NMT	O7'-C7'	-7.92	1.20	1.40
1	A	6[B]	NMT	O7'-C7'	-7.92	1.20	1.40
1	B	116	NMT	O7'-C7'	-7.41	1.22	1.40
1	B	116	NMT	C2'-C1'	-3.25	1.44	1.53
1	A	6[A]	NMT	C2'-C1'	-2.88	1.45	1.53

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	116	NMT	C9'-N8'-C7'	4.12	120.39	114.38
1	B	116	NMT	O4'-C1'-N1	-3.08	101.32	108.36
1	A	6[B]	NMT	C9'-N8'-C7'	2.72	118.35	114.38
1	A	6[A]	NMT	O4'-C1'-C2'	2.52	110.98	106.57
1	A	6[B]	NMT	O4'-C1'-C2'	2.52	110.98	106.57

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	6[A]	NMT	C7'
1	A	6[B]	NMT	C7'
1	B	116	NMT	C7'

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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.

6.2 Non-standard residues in protein, DNA, RNA chains

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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
1	NMT	B	116	25/26	0.93	0.09	21,32,52,59	0
1	NMT	A	6[B]	25/26	0.96	0.07	17,20,38,51	2
1	NMT	A	6[A]	25/26	0.96	0.07	17,20,36,51	2

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.