



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 05:53 AM GMT

PDB ID : 310D
Title : Crystal structure of 2'-O-Me(CGCGCG)₂: an RNA duplex at 1.3 Å resolution.
Hydration pattern of 2'-O-methylated RNA
Authors : Adamiak, D.A.; Milecki, J.; Adamiak, R.W.; Dauter, Z.; Rypniewski, W.R.
Deposited on : 1996-05-25
Resolution : 1.30 Å(reported)

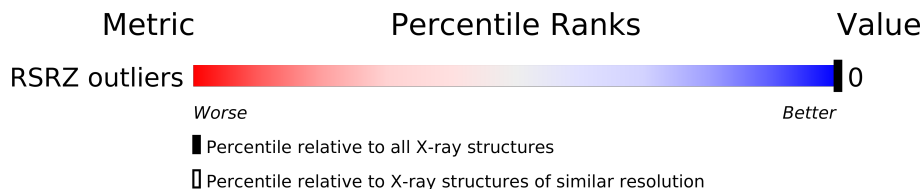
This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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

MolProbity : **FAILED**
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

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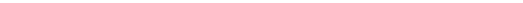
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
RSRZ outliers	66119	1025 (1.34-1.26)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note MolProbity failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	6	
1	B	6	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 464 atoms, of which 154 are hydrogens and 0 are deuterium.

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 RNA (5'-R(*(OMC)P*(OMG)P*(OMC)P*(OMG)P*(OMC)P*(OMG))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	6	Total	C	H	N	O	P	0	0	0
			208	63	76	24	40	5			
1	B	6	Total	C	H	N	O	P	0	0	0
			210	63	78	24	40	5			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	B	19	Total	O	0	0
			19	19		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note MolProbity failed to run properly.

- Molecule 1: RNA (5'-R(* (OMC)P*(OMG)P*(OMC)P*(OMG)P*(OMC)P*(OMG))-3')

Chain A: 

There are no outlier residues recorded for this chain.

- Molecule 1: RNA (5'-R(* (OMC)P*(OMG)P*(OMC)P*(OMG)P*(OMC)P*(OMG))-3')

Chain B: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	26.27Å 26.27Å 160.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 1.30 22.75 – 1.32	Depositor EDS
% Data completeness (in resolution range)	95.3 (8.00-1.30) 95.9 (22.75-1.32)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 1.32Å)	Xtriage
Refinement program	SHELXL-96	Depositor
R, R_{free}	0.172 , (Not available) 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 104.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 8236 reflections (0.024%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	464	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.27 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.8008e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.2 Close contacts ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.3.2 Protein sidechains ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.3.3 RNA ⓘ

MolProbity failed to run properly - this section will therefore be empty.

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

MolProbity failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

MolProbity failed to run properly - this section will therefore be empty.

5.8 Polymer linkage issues

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, 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	6/6 (100%)	0.62	0 100 100	18, 22, 28, 28	0
1	B	6/6 (100%)	0.75	0 100 100	17, 20, 31, 38	0
All	All	12/12 (100%)	0.69	0 100 100	17, 22, 31, 38	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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	OMC	A	3	21/22	0.09	-	20,24,45,45	0
1	OMG	B	10	24/25	0.07	-	15,18,31,31	0
1	OMG	A	6	24/25	0.07	-	17,21,53,53	0
1	OMG	A	2	24/25	0.09	-	19,30,51,51	0
1	OMG	B	8	24/25	0.09	-	19,34,57,57	0
1	OMC	A	1	18/22	0.10	-	21,29,46,46	0
1	OMC	B	11	21/22	0.08	-	14,17,26,26	0
1	OMC	B	7	18/22	0.09	-	28,41,66,66	0
1	OMC	A	5	21/22	0.06	-	15,18,26,26	0
1	OMG	A	4	24/25	0.06	-	15,18,30,30	0
1	OMC	B	9	21/22	0.08	-	19,27,44,44	0
1	OMG	B	12	24/25	0.07	-	16,20,47,47	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	B	13	1/1	0.28	-	19,19,19,19	1
2	MG	A	14	1/1	0.07	-	29,29,29,29	1

6.5 Other polymers

There are no such residues in this entry.