

Full wwPDB X-ray Structure Validation Report (i)

Jan 2, 2024 – 07:21 pm GMT

PDB ID	:	5EYQ
Title	:	Racemic crystal structures of Pribnow box consensus promoter sequence
		(Pnna)
Authors	:	Mandal, P.K.; Collie, G.W.; Kauffmann, B.; Srivastava, S.C.; Huc, I.
Deposited on	:	2015-11-25
Resolution	:	2.30 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 (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
Xtriage (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)	:	2.36

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 2.30 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	Percentile Ranks	Value
Clashscore		76
Worse		Better
Percentile re	elative to all X-ray structures	
Percentile re	elative to X-ray structures of similar resolution	
	71 1 1	<u> </u>

Metric	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	5643 (2.30-2.30)

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%

Note EDS failed to run properly.

Mol	Chain	Length		Quality of chain	
1	А	12	17%	75%	8%
2	В	12		100%	



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 506 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 Pribnow box template strand.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	12	Total 243	C 117	N 45	O 70	Р 11	0	0	0

• Molecule 2 is a DNA chain called Complementary strand.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	12	Total 243	C 117	N 45	O 70	Р 11	0	0	0

• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Na 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	11	Total O 11 11	0	0
4	В	8	Total O 8 8	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: Pribnow box template strand

Chain A:	17%	75%	8%
C1 22 45 44 47 48 79 79 79 79 79 70 70 70 70 70 70 70 70 70 70 70 70 70	811 812 812		
• Molecule	2: Complementary strand		
Chain B:		100%	
C1 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3	610 611 612		



4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P n n a	Depositor	
Cell constants	28.91Å 68.45 Å 34.21 Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	34.23 - 2.30	Depositor	
% Data completeness	96.6 (34.23-2.30)	Depositor	
(in resolution range)		Depositor	
R _{merge}	0.04	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) >$	-	Xtriage	
Refinement program	REFMAC 5.8.0073	Depositor	
R, R_{free}	0.272 , 0.357	Depositor	
Wilson B-factor $(Å^2)$	(Not available)	Xtriage	
Anisotropy	(Not available)	Xtriage	
L-test for twinning ¹	L > = (Not available), $ L > =$ (Not available)	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	506	wwPDB-VP	
Average B, all atoms $(Å^2)$	39.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: (Not available)

¹Theoretical 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: NA

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	Bon	d lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.95	1/272~(0.4%)	1.12	1/418~(0.2%)	
2	В	0.93	1/272~(0.4%)	1.06	1/418~(0.2%)	
All	All	0.94	2/544~(0.4%)	1.09	2/836~(0.2%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
1	А	1	DC	O3'-P	-5.72	1.54	1.61
2	В	1	DC	O3'-P	-5.21	1.54	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	12	DG	O5'-P-OP1	-6.51	99.84	105.70
2	В	2	DG	O4'-C1'-C2'	-5.59	101.43	105.90

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	А	243	0	127	44	0
2	В	243	0	122	47	0

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\mathbf{Mol}	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
3	В	1	0	0	0	0		
4	А	11	0	0	0	0		
4	В	8	0	0	1	0		
All	All	506	0	249	$\overline{56}$	0		

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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 76.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic Clash			
Atom-1	Atom-2	distance (\AA)	overlap (Å)		
1:A:12:DG:H5'	2:B:12:DG:P	1.48	1.50		
1:A:12:DG:C5'	2:B:12:DG:O5'	1.75	1.32		
1:A:12:DG:H5'	2:B:12:DG:O5'	1.09	1.24		
1:A:12:DG:H5'	2:B:12:DG:C5'	1.75	1.15		
1:A:12:DG:C5'	2:B:12:DG:P	2.34	1.14		
1:A:12:DG:C5'	2:B:12:DG:C5'	2.23	1.03		
1:A:9:DT:H5'	2:B:8:DT:H1'	1.44	0.97		
1:A:8:DA:H1'	1:A:9:DT:H5'	1.57	0.85		
1:A:12:DG:C5'	2:B:12:DG:H5'	2.06	0.84		
1:A:6:DT:H5'	2:B:5:DT:C3'	2.06	0.84		
1:A:9:DT:H5'	2:B:8:DT:C1'	2.08	0.83		
1:A:11:DC:H41	2:B:11:DC:N4	1.35	0.82		
1:A:11:DC:N4	2:B:11:DC:N4	0.79	0.79		
1:A:6:DT:O4'	2:B:5:DT:H2"	1.86	0.75		
1:A:11:DC:H42	2:B:11:DC:H42	0.75	0.75		
1:A:6:DT:H5'	2:B:5:DT:O3'	1.30	0.75		
1:A:9:DT:H5'	2:B:8:DT:C2'	2.19	0.71		
1:A:11:DC:N4	2:B:11:DC:H42	0.68	0.71		
1:A:8:DA:H1'	1:A:9:DT:C5'	2.23	0.68		
2:B:3:DC:OP1	4:B:201:HOH:O	2.11	0.67		
2:B:6:DT:H2"	2:B:7:DA:C8	2.30	0.66		
1:A:9:DT:C5'	2:B:8:DT:H1'	2.25	0.64		
1:A:11:DC:H41	2:B:11:DC:H41	0.96	0.64		
1:A:12:DG:C4'	2:B:12:DG:O5'	2.25	0.64		
2:B:8:DT:H2"	2:B:9:DA:C8	2.33	0.64		
1:A:4:DT:H5'	2:B:3:DC:H2"	1.79	0.63		
2:B:7:DA:H1'	2:B:8:DT:H5'	1.80	0.63		
2:B:7:DA:H1'	2:B:8:DT:C5'	2.28	0.62		
1:A:8:DA:H2"	1:A:9:DT:H5'	1.81	0.61		
1:A:5:DA:H2"	1:A:6:DT:OP2	2.00	0.61		

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:DA:H2"	1:A:8:DA:OP2	2.00	0.60
1:A:11:DC:H2"	1:A:12:DG:C8	2.41	0.56
1:A:7:DA:O4'	2:B:6:DT:H2"	2.06	0.56
1:A:9:DT:H5'	2:B:9:DA:C8	2.41	0.55
1:A:7:DA:C8	2:B:6:DT:H2'	2.42	0.55
1:A:7:DA:C8	2:B:6:DT:C2'	2.90	0.54
1:A:11:DC:N4	2:B:11:DC:H41	1.09	0.53
2:B:8:DT:H2"	2:B:9:DA:H8	1.72	0.53
1:A:3:DC:O2	2:B:3:DC:O2	0.53	0.53
2:B:6:DT:H2"	2:B:7:DA:H8	1.75	0.51
2:B:12:DG:H5'	2:B:12:DG:C8	2.45	0.51
1:A:9:DT:H5'	2:B:8:DT:H2"	1.95	0.49
1:A:6:DT:H5"	2:B:6:DT:OP1	1.46	0.48
1:A:4:DT:H2"	1:A:5:DA:C8	2.49	0.48
2:B:5:DT:H2'	2:B:6:DT:H72	1.97	0.47
1:A:4:DT:C5'	2:B:3:DC:H2"	2.44	0.46
2:B:7:DA:H2"	2:B:8:DT:H5'	1.51	0.46
1:A:8:DA:C1'	1:A:9:DT:H5'	2.28	0.45
2:B:7:DA:H1'	2:B:8:DT:H5"	2.00	0.44
1:A:12:DG:H5'	2:B:12:DG:H5'	1.72	0.43
1:A:8:DA:C2'	1:A:9:DT:H5'	2.34	0.42
2:B:10:DG:H4'	2:B:11:DC:OP1	2.20	0.42
1:A:7:DA:H8	2:B:6:DT:H2'	1.84	0.41
1:A:12:DG:H4'	2:B:12:DG:O5'	2.01	0.40
1:A:3:DC:H2"	2:B:4:DA:C8	2.57	0.40
1:A:7:DA:H2"	2:B:7:DA:H2'	1.01	0.40

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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)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 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.

