



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 01:13 pm BST

PDB ID : 9DNA
Title : CRYSTAL STRUCTURE ANALYSIS OF AN A-DNA FRAGMENT AT 1.8
ANGSTROMS RESOLUTION. D(GCCCGGGC)
Authors : Heinemann, U.
Deposited on : 1987-07-10
Resolution : 1.80 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 : 2.11
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) : 2.11

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 195 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*CP*CP*GP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	8	161	76	32	46	7	0	0	0

- Molecule 2 is water.

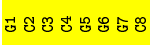
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	34	Total	O	0	0
			34	34		

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 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*CP*CP*GP*GP*GP*C)-3')

Chain A:  100%

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4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	43.25Å 43.25Å 24.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.80 21.62 – 1.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-1.80) 63.9 (21.62-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 1.79Å)	Xtrriage
Refinement program	NUCLSQ	Depositor
R, R_{free}	0.171 , (Not available) 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtrriage
Anisotropy	0.209	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	195	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.06 % 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 5.0305e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	1.93	2/180 (1.1%)	3.50	40/276 (14.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	DC	P-OP1	7.09	1.61	1.49
1	A	6	DG	P-OP2	-5.10	1.40	1.49

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	DC	O5'-P-OP2	13.81	127.27	110.70
1	A	7	DG	P-O3'-C3'	12.43	134.62	119.70
1	A	6	DG	O5'-P-OP2	10.92	123.81	110.70
1	A	5	DG	C5-C6-N1	10.80	116.90	111.50
1	A	5	DG	P-O3'-C3'	10.03	131.74	119.70
1	A	1	DG	C5-C6-N1	9.57	116.29	111.50
1	A	1	DG	C6-N1-C2	-9.22	119.57	125.10
1	A	8	DC	N1-C2-O2	8.78	124.17	118.90
1	A	8	DC	O4'-C1'-N1	8.50	113.95	108.00
1	A	4	DC	OP1-P-OP2	-8.40	106.99	119.60
1	A	8	DC	O4'-C4'-C3'	-8.26	101.04	106.00
1	A	5	DG	C6-N1-C2	-7.50	120.60	125.10
1	A	8	DC	N3-C2-O2	-7.47	116.67	121.90
1	A	4	DC	N3-C4-C5	-7.27	118.99	121.90
1	A	3	DC	P-O3'-C3'	7.08	128.19	119.70
1	A	1	DG	N1-C2-N3	7.04	128.12	123.90
1	A	7	DG	O4'-C1'-C2'	6.86	111.39	105.90
1	A	7	DG	O5'-P-OP2	-6.78	99.59	105.70
1	A	8	DC	C5-C4-N4	6.54	124.78	120.20
1	A	5	DG	P-O5'-C5'	6.36	131.08	120.90
1	A	1	DG	N1-C6-O6	-6.32	116.11	119.90
1	A	8	DC	C5-C6-N1	6.15	124.07	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	DC	O4'-C1'-N1	5.92	112.15	108.00
1	A	4	DC	O4'-C1'-N1	5.92	112.14	108.00
1	A	8	DC	C6-N1-C1'	5.87	127.84	120.80
1	A	2	DC	N3-C4-N4	5.86	122.11	118.00
1	A	8	DC	C6-N1-C2	-5.73	118.01	120.30
1	A	3	DC	O3'-P-O5'	5.54	114.53	104.00
1	A	2	DC	O5'-P-OP1	5.54	117.35	110.70
1	A	7	DG	P-O5'-C5'	-5.52	112.07	120.90
1	A	6	DG	C5-C6-N1	5.43	114.21	111.50
1	A	5	DG	C5-C6-O6	-5.42	125.35	128.60
1	A	3	DC	P-O5'-C5'	-5.39	112.27	120.90
1	A	7	DG	C1'-O4'-C4'	-5.37	104.73	110.10
1	A	5	DG	O4'-C4'-C3'	-5.32	102.37	104.50
1	A	5	DG	N3-C2-N2	-5.32	116.18	119.90
1	A	6	DG	O4'-C1'-N9	5.28	111.70	108.00
1	A	5	DG	O3'-P-O5'	-5.23	94.06	104.00
1	A	7	DG	O4'-C1'-N9	-5.21	104.35	108.00
1	A	4	DC	O5'-P-OP1	-5.12	101.09	105.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	161	0	90	0	0
2	A	34	0	0	0	0
All	All	195	0	90	0	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 0.

There are no clashes within the asymmetric unit.

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 carbohydrates 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 [i](#)

6.1 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	8/8 (100%)	-0.83	0 100 100	21, 23, 27, 28	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.