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Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:40 AM GMT

PDB ID   :   28DN
Title   :   CRYSTAL STRUCTURE ANALYSIS OF AN A(DNA) OCTAMER
D(GTACGTAC)
Authors   :   Courseille, C.; Dautant, A.; Hospital, M.; Langlois D'Estaintot, B.; Precigoux,
G.; Molko, D.; Teoule, R.
Deposited on   :   1990-05-03
Resolution   :   2.40 Å(reported)

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

MolProbity	:	4.02b-467
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

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.40 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		28
RSRZ outliers		0

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
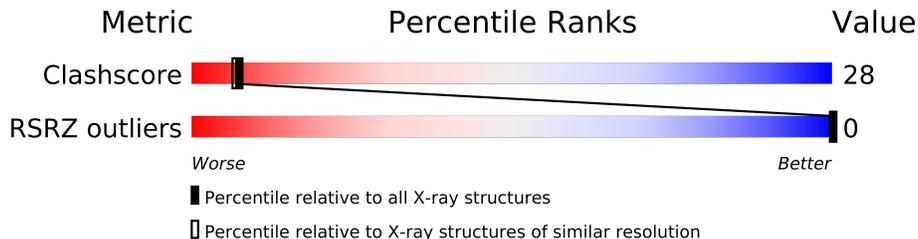
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2789 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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.

Mol	Chain	Length	Quality of chain
1	A	8	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 217 atoms, of which 0 are hydrogen 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 DNA chain called DNA (5'-D(*GP*TP*AP*CP*GP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	8	Total	C	N	O	P	0	0	0
			161	78	30	46	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	56	Total	O	0	0
			56	56		

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.

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

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	42.50Å　42.50Å　24.79Å 90.00°　90.00°　90.00°	Depositor
Resolution (Å)	(Not available) – 2.40 21.41 – 2.43	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40) 97.3 (21.41-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.170　,　(Not available) 0.163　,　(Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 59.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.45, < L^2 > = 0.29$	Xtriage
Outliers	0 of 973 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	217	wwPDB-VP
Average B, all atoms (Å^2)	12.0	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 23.90 % 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 4.2590e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	2.14	4/180 (2.2%)	3.31	23/276 (8.3%)

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	1	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	DT	C5-C6	16.09	1.45	1.34
1	A	1	DG	C6-N1	-7.04	1.34	1.39
1	A	5	DG	C6-N1	-6.79	1.34	1.39
1	A	6	DT	N3-C4	-6.54	1.33	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	DC	O4'-C4'-C3'	-24.45	91.33	106.00
1	A	5	DG	O4'-C1'-N9	11.21	115.85	108.00
1	A	6	DT	O4'-C1'-N1	10.89	115.62	108.00
1	A	2	DT	O4'-C4'-C3'	-9.91	100.05	106.00
1	A	6	DT	C5-C6-N1	-8.55	118.57	123.70
1	A	8	DC	O4'-C1'-N1	8.53	113.97	108.00
1	A	3	DA	O4'-C1'-N9	8.23	113.76	108.00
1	A	2	DT	O4'-C1'-N1	8.05	113.63	108.00
1	A	1	DG	N3-C4-C5	-7.40	124.90	128.60
1	A	6	DT	C4-C5-C6	7.21	122.33	118.00
1	A	4	DC	N3-C4-C5	-7.00	119.10	121.90
1	A	6	DT	N1-C2-N3	6.95	118.77	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4	DC	O4'-C1'-C2'	-6.72	100.53	105.90
1	A	4	DC	N3-C2-O2	-6.59	117.29	121.90
1	A	3	DA	O4'-C1'-C2'	-6.46	100.73	105.90
1	A	8	DC	P-O5'-C5'	-6.18	111.01	120.90
1	A	2	DT	N3-C2-O2	-5.78	118.83	122.30
1	A	3	DA	P-O5'-C5'	-5.58	111.97	120.90
1	A	2	DT	C2-N3-C4	5.51	130.51	127.20
1	A	3	DA	N1-C6-N6	-5.47	115.31	118.60
1	A	6	DT	N3-C4-O4	5.15	122.99	119.90
1	A	6	DT	C6-C5-C7	-5.14	119.81	122.90
1	A	4	DC	C1'-O4'-C4'	5.08	115.18	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	DG	C3'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	DT	Sidechain
1	A	3	DA	Sidechain
1	A	4	DC	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	161	0	91	7	0
2	A	56	0	0	0	0
All	All	217	0	91	7	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

All (7) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:3:DA:H8	1:A:3:DA:H5'	1.28	0.97
1:A:3:DA:C8	1:A:3:DA:H5'	2.07	0.89
1:A:7:DA:C2'	1:A:8:DC:H5'	2.03	0.87
1:A:7:DA:H2"	1:A:8:DC:H5'	1.56	0.86
1:A:2:DT:C2'	1:A:3:DA:H5"	2.20	0.71
1:A:2:DT:H2'	1:A:3:DA:H5"	1.84	0.59
1:A:2:DT:H2'	1:A:3:DA:C5'	2.42	0.49

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

There are no protein chains in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein chains in this entry.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

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	8/8 (100%)	-0.88	0	100	100	3, 5, 6, 7	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.