



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:35 PM UTC

PDB ID : 6AQX / pdb_00006aqx
Title : Crystal Structure of Z-DNA with 6-fold Twinning_Z4B
Authors : Luo, Z.; Dauter, Z.; Gilski, M.
Deposited on : 2017-08-21
Resolution : 1.55 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

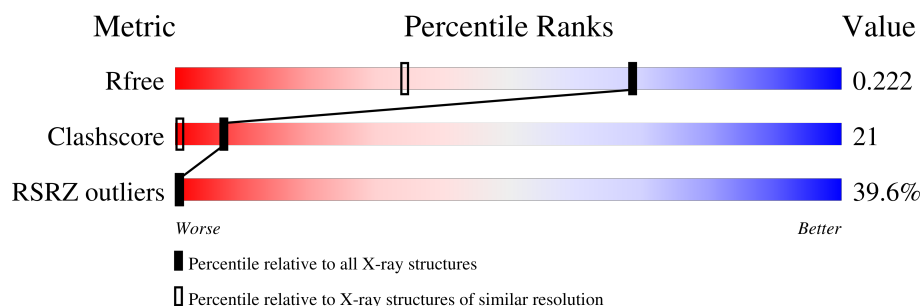
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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))
R_{free}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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 $\leq 5\%$. 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	6	
1	B	6	
1	C	6	
1	D	6	
1	E	6	
1	F	6	
1	G	6	

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Mol	Chain	Length	Quality of chain
1	H	6	67% 67% 33%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1001 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(*CP*GP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	6	Total	C	N	O	P	0	0	0
			120	57	24	34	5			
1	B	6	Total	C	N	O	P	0	0	0
			120	57	24	34	5			
1	C	6	Total	C	N	O	P	0	0	0
			120	57	24	34	5			
1	D	6	Total	C	N	O	P	0	0	0
			120	57	24	34	5			
1	E	6	Total	C	N	O	P	0	0	0
			120	57	24	34	5			
1	F	6	Total	C	N	O	P	0	0	0
			120	57	24	34	5			
1	G	6	Total	C	N	O	P	0	0	0
			120	57	24	34	5			
1	H	6	Total	C	N	O	P	0	0	0
			120	57	24	34	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	O	0	0
			4	4		
2	B	6	Total	O	0	0
			6	6		
2	C	6	Total	O	0	0
			6	6		
2	D	6	Total	O	0	0
			6	6		
2	E	4	Total	O	0	0
			4	4		
2	F	6	Total	O	0	0
			6	6		

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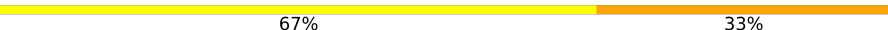
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	4	Total 4	O 4	0	0
2	H	5	Total 5	O 5	0	0

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 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(*CP*GP*CP*GP*CP*G)-3')

Chain A: 

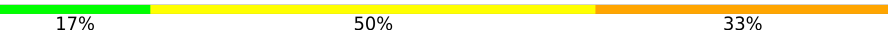


- Molecule 1: DNA (5'-D(*CP*GP*CP*GP*CP*G)-3')

Chain B: 



- Molecule 1: DNA (5'-D(*CP*GP*CP*GP*CP*G)-3')

Chain C: 



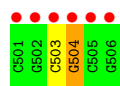
- Molecule 1: DNA (5'-D(*CP*GP*CP*GP*CP*G)-3')

Chain D: 



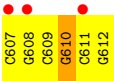
- Molecule 1: DNA (5'-D(*CP*GP*CP*GP*CP*G)-3')

Chain E: 

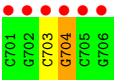


- Molecule 1: DNA (5'-D(*CP*GP*CP*GP*CP*G)-3')

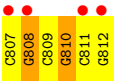
Chain F: 



● Molecule 1: DNA (5'-D(*CP*GP*CP*GP*CP*G)-3')



● Molecule 1: DNA (5'-D(*CP*GP*CP*GP*CP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	35.20Å 42.22Å 35.21Å 90.00° 119.83° 90.00°	Depositor
Resolution (Å)	30.54 – 1.55 30.54 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.54-1.55) 99.8 (30.54-1.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.54Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.209 , 0.227 0.211 , 0.222	Depositor DCC
R_{free} test set	657 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 89.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.101 for -h-l,k,h 0.101 for l,k,-h-l 0.096 for h,-k,-h-l 0.108 for -h-l,-k,l 0.469 for l,-k,h	Xtriage
Reported twinning fraction	0.354 for H, K, L 0.375 for L, -K, H 0.073 for -H, -K, H+L 0.082 for L, K, -H-L 0.061 for -H-L, K, H 0.055 for H+L, -K, -L	Depositor
Outliers	0 of 13133 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	1001	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 90.08 % 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 2.6527e-08. The detected translational NCS is most*

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.

likely also responsible for the elevated intensity ratio.

5 Model quality

5.1 Standard geometry

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	0.51	0/134	1.43	3/205 (1.5%)
1	B	0.51	0/134	1.15	2/205 (1.0%)
1	C	0.51	0/134	1.44	4/205 (2.0%)
1	D	0.51	0/134	1.16	2/205 (1.0%)
1	E	0.39	0/134	1.25	1/205 (0.5%)
1	F	0.58	0/134	1.20	2/205 (1.0%)
1	G	0.42	0/134	1.24	1/205 (0.5%)
1	H	0.52	0/134	1.18	2/205 (1.0%)
All	All	0.50	0/1072	1.26	17/1640 (1.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	304	DG	C2'-C3'-O3'	-9.17	97.74	111.50
1	A	104	DG	C2'-C3'-O3'	-9.15	97.77	111.50
1	E	504	DG	C2'-C3'-O3'	6.99	121.98	111.50
1	C	301	DC	C2'-C3'-O3'	-6.87	101.19	111.50
1	G	704	DG	C2'-C3'-O3'	6.86	121.78	111.50
1	H	810	DG	C4'-C3'-O3'	-6.81	99.79	110.00
1	C	303	DC	C2'-C3'-O3'	-6.71	101.43	111.50
1	F	610	DG	C2'-C3'-O3'	6.64	121.46	111.50
1	A	103	DC	C2'-C3'-O3'	-6.63	101.56	111.50
1	A	101	DC	C2'-C3'-O3'	-6.61	101.59	111.50
1	B	212	DG	C2'-C3'-O3'	-6.14	102.29	111.50
1	D	412	DG	C2'-C3'-O3'	-5.97	102.55	111.50
1	D	411	DC	C4'-C3'-O3'	-5.83	101.25	110.00
1	B	211	DC	C4'-C3'-O3'	-5.65	101.52	110.00
1	H	808	DG	C2'-C3'-O3'	-5.41	103.38	111.50
1	C	304	DG	C4'-C3'-O3'	5.24	117.85	110.00
1	F	610	DG	C4'-C3'-O3'	-5.18	102.23	110.00

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	120	0	68	4	0
1	B	120	0	68	7	0
1	C	120	0	68	7	0
1	D	120	0	68	0	0
1	E	120	0	68	1	0
1	F	120	0	68	7	1
1	G	120	0	68	6	0
1	H	120	0	68	6	1
2	A	4	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
2	E	4	0	0	0	0
2	F	6	0	0	0	0
2	G	4	0	0	0	0
2	H	5	0	0	0	0
All	All	1001	0	544	29	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 21.

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:DG:H4'	1:G:704:DG:H5'	1.41	1.02
1:H:810:DG:H2'	1:H:811:DC:C5	2.18	0.78
1:F:610:DG:H2'	1:F:611:DC:C5	2.18	0.78
1:F:608:DG:N3	1:F:608:DG:H2'	2.03	0.72
1:H:810:DG:H2'	1:H:811:DC:H5	1.54	0.71
1:F:610:DG:H2'	1:F:611:DC:H5	1.56	0.70
1:B:210:DG:H4'	1:G:704:DG:C5'	2.24	0.66
1:B:210:DG:H1'	1:G:703:DC:OP1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:808:DG:H2'	1:H:808:DG:N3	2.14	0.63
1:F:608:DG:H2''	1:F:609:DC:OP1	2.01	0.61
1:H:808:DG:H2''	1:H:809:DC:OP1	2.04	0.56
1:C:303:DC:H5''	1:F:610:DG:H1'	1.88	0.55
1:G:703:DC:H4'	1:G:704:DG:O5'	2.10	0.51
1:B:208:DG:O5'	1:C:306:DG:H1'	2.14	0.48
1:B:208:DG:H1'	1:C:305:DC:OP2	2.14	0.46
1:F:609:DC:H4'	1:F:610:DG:O5'	2.17	0.45
1:C:303:DC:OP1	1:F:610:DG:H1'	2.16	0.45
1:C:303:DC:H4'	1:C:304:DG:O5'	2.17	0.45
1:B:210:DG:C5'	1:G:704:DG:H4'	2.47	0.45
1:A:103:DC:H4'	1:A:104:DG:O5'	2.18	0.44
1:E:503:DC:H4'	1:E:504:DG:O5'	2.18	0.43
1:C:304:DG:H2'	1:C:305:DC:C5	2.54	0.43
1:C:305:DC:O4'	1:C:306:DG:C2	2.73	0.42
1:A:104:DG:H2'	1:A:105:DC:C5	2.55	0.42
1:H:808:DG:N3	1:H:808:DG:C2'	2.83	0.41
1:A:105:DC:O4'	1:A:106:DG:C2	2.74	0.41
1:H:809:DC:H4'	1:H:810:DG:O5'	2.21	0.41
1:A:102:DG:H2'	1:A:103:DC:C6	2.56	0.40
1:B:210:DG:C1'	1:G:703:DC:OP1	2.68	0.40

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)
1:H:807:DC:O5'	1:H:812:DG:O3'[2_556]	2.09	0.11
1:F:607:DC:O5'	1:F:612:DG:O3'[2_655]	2.10	0.10

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 oligosaccharides 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, 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%)	0.03	0  100  100	22, 28, 29, 30	0
1	B	6/6 (100%)	-0.02	0  100  100	22, 24, 28, 31	0
1	C	6/6 (100%)	-0.13	0  100  100	21, 27, 29, 29	0
1	D	6/6 (100%)	0.13	0  100  100	22, 24, 27, 31	0
1	E	6/6 (100%)	2.67	6 (100%)  0  0	38, 45, 49, 51	0
1	F	6/6 (100%)	2.02	3 (50%)  0  0	32, 40, 42, 57	0
1	G	6/6 (100%)	2.77	6 (100%)  0  0	38, 43, 53, 59	0
1	H	6/6 (100%)	2.36	4 (66%)  0  0	35, 40, 59, 68	0
All	All	48/48 (100%)	1.23	19 (39%)  1  0	21, 31, 57, 68	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	808	DG	3.7
1	G	703	DC	3.3
1	G	702	DG	3.2
1	F	608	DG	3.2
1	E	503	DC	3.0
1	H	807	DC	2.8
1	G	701	DC	2.7
1	E	502	DG	2.7
1	E	506	DG	2.7
1	E	501	DC	2.7
1	E	505	DC	2.7
1	H	811	DC	2.6
1	G	704	DG	2.6
1	G	705	DC	2.5
1	G	706	DG	2.4
1	F	611	DC	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	812	DG	2.4
1	E	504	DG	2.3
1	F	607	DC	2.1

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 oligosaccharides 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.