

# wwPDB X-ray Structure Validation Summary Report (i)

#### Sep 26, 2023 – 04:54 AM EDT

PDB ID	:	6AQV
Title	:	Crystal Structure of Z-DNA with 6-fold Twinning_Z3B
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Deposited on	:	2017-08-21
Resolution	:	1.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

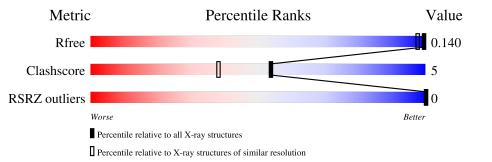
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.30 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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% 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	А	6	83%	17%
1	В	6	100%	
1	С	6	100%	
1	D	6	50%	50%
1	Е	6	83%	17%
1	F	6	100%	



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 797 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.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	А	6	Total	С	Ν	Ο	Р	0	0	0
	A	0	120	57	24	34	5	0	0	0
1	В	6	Total	С	Ν	Ο	Р	0	0	0
1	D	0	120	57	24	34	5	0	0	0
1	С	6	Total	С	Ν	Ο	Р	0	0	0
	U	0	120	57	24	34	5	0	0	0
1	D	6	Total	С	Ν	Ο	Р	0	0	0
1	D	0	120	57	24	34	5	0	0	0
1	Е	6	Total	С	Ν	Ο	Р	0	0	0
1	Ľ	0	120	57	24	34	5	0	0	0
1	F	6	Total	С	Ν	Ο	Р	0	0	0
	Г	U	120	57	24	34	5		0	0

• Molecule 1 is a DNA chain called DNA (5'-D(\*CP\*GP\*CP\*GP\*CP\*G)-3').

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	17	Total O 17 17	0	0
2	В	19	Total         O           19         19	0	0
2	С	9	Total O 9 9	0	0
2	D	10	Total O 10 10	0	0
2	Ε	9	Total O 9 9	0	0
2	F	13	Total         O           13         13	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:	83%	17%
C101 G106		
• Molecule	1: DNA (5'-D(*CP*GP*CP*GP*CP*G)-3')	
Chain B:	100%	
There are a	no outlier residues recorded for this chain.	
• Molecule	1: DNA (5'-D(*CP*GP*CP*GP*CP*G)-3')	
Chain C:	100%	
There are a	no outlier residues recorded for this chain.	
• Molecule	1: DNA (5'-D(*CP*GP*CP*GP*CP*G)-3')	
Chain D:	50%	50%
C407 6408 C409 6412		
• Molecule	1: DNA (5'-D(*CP*GP*CP*GP*CP*G)-3')	
Chain E:	83%	17%
C501 C505 G506		
• Molecule	1: DNA (5'-D(*CP*GP*CP*GP*CP*G)-3')	
Chain F:	100%	

There are no outlier residues recorded for this chain.



## 4 Data and refinement statistics (i)

Property	Value	Source		
Space group	P 1 21 1	Depositor		
Cell constants	30.84Å $42.57$ Å $30.84$ Å	Depositor		
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $120.05^{\circ}$ $90.00^{\circ}$	Depositor		
Resolution (Å)	26.71 - 1.30	Depositor		
Resolution (A)	$26.71 \ - \ 1.30$	EDS		
% Data completeness	99.0 (26.71-1.30)	Depositor		
(in resolution range)	99.0 (26.71-1.30)	EDS		
R <sub>merge</sub>	0.06	Depositor		
R <sub>sym</sub>	(Not available)	Depositor		
$\frac{R_{sym}}{< I/\sigma(I) > 1}$	1.40 (at 1.30Å)	Xtriage		
Refinement program	REFMAC 5.8.0135	Depositor		
D D	0.131 , $0.147$	Depositor		
$R, R_{free}$	0.132 , $0.140$	DCC		
$R_{free}$ test set	873 reflections $(5.13%)$	wwPDB-VP		
Wilson B-factor $(Å^2)$	16.3	Xtriage		
Anisotropy	0.322	Xtriage		
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.24,76.6	EDS		
L-test for twinning <sup>2</sup>	$<  L  > = 0.45, < L^2 > = 0.28$	Xtriage		
	0.470 for -h-l,k,h			
	0.470 for l,k,-h-l			
Estimated twinning fraction	0.439 for l,-k,h	Xtriage		
	0.446 for h,-k,-h-l			
	0.447 for -h-l,-k,l			
	0.164 for H, K, L			
	0.203 for L, -K, H			
Departed twinning fraction	0.161 for H+L, -K, -L	Deperitor		
Reported twinning fraction	0.210 for -H, -K, H+L	Depositor		
	0.119 for L, K, -H-L			
	0.144 for -H-L, K, H			
Outliers	0 of 17033 reflections	Xtriage		
$F_o, F_c$ correlation	0.98	EDS		
Total number of atoms	797	wwPDB-VP		
Average B, all atoms $(Å^2)$	28.0	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 34.71 % 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 6.5379e-04. The detected translational NCS is most

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for a centric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

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	
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.88	0/134	1.06	0/205
1	В	0.98	0/134	1.18	0/205
1	С	0.79	0/134	1.08	0/205
1	D	0.68	0/134	0.91	0/205
1	Е	0.85	0/134	1.01	0/205
1	F	0.85	0/134	0.97	0/205
All	All	0.84	0/804	1.04	0/1230

There are no bond length outliers.

There are no bond angle outliers.

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	120	0	68	1	0
1	В	120	0	68	0	0
1	С	120	0	68	0	0
1	D	120	0	68	5	0
1	Е	120	0	68	1	0
1	F	120	0	68	0	0
2	А	17	0	0	0	0
2	В	19	0	0	0	0
2	С	9	0	0	0	0
2	D	10	0	0	1	0

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Mol	0	1	H(model)	H(added)	Clashes	Symm-Clashes
2	Е	9	0	0	0	0
2	F	13	0	0	0	0
All	All	797	0	408	6	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 5.

The worst 5 of 6 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:D:409:DC:P	2:D:501:HOH:O	2.53	0.65
1:D:408:DG:H1'	1:E:505:DC:OP2	2.00	0.61
1:D:408:DG:H2'	1:D:409:DC:C5	2.54	0.43
1:D:407:DC:H4'	1:D:408:DG:C5'	2.48	0.43
1:A:106:DG:N3	1:A:106:DG:H2'	2.34	0.42

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)

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,  $95^{th}$  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	$\langle RSRZ \rangle$	# RSRZ > 2		$OWAB(A^2)$	Q < 0.9
1	А	6/6~(100%)	0.07	0 100	100	22, 25, 29, 31	0
1	В	6/6~(100%)	-0.08	0 100	100	18, 23, 25, 25	0
1	С	6/6~(100%)	-0.02	0 100	100	24, 27, 30, 34	0
1	D	6/6~(100%)	0.10	0 100	100	26, 29, 33, 34	0
1	Ε	6/6~(100%)	0.23	0 100	100	24, 31, 32, 34	0
1	F	6/6~(100%)	0.20	0 100	100	27, 31, 32, 32	0
All	All	36/36~(100%)	0.08	0 100	100	18, 28, 34, 34	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 monosaccharides 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.

