

Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 10:53 PM EDT

PDB ID	:	6XGK
Title	:	Self-assembly of a 3D DNA crystal lattice (4x5 junction version) containing
		the J35 immobile Holliday junction
Authors	:	Simmons, C.R.; MacCulloch, T.; Stephanopoulos, N.; Yan, H.
Deposited on		
Resolution	:	3.06 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:

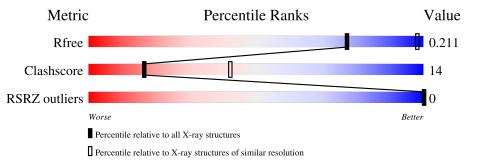
Refmac CCP4	: : : :	 1.13 2.35.1 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove)
Ideal geometry (proteins) Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	:	Parkinson et al. (1996)

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 3.06 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	11	27%	55%		18%		
2	В	10	30%	30%	40%			
3	С	5		40%				
4	D	16	50%	12%				



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 857 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*AP*GP*CP*AP*GP*AP*CP*AP*TP* G)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	11	Total 227	C 108	N 48	O 61	Р 10	0	0	0

• Molecule 2 is a DNA chain called DNA (5'-D(P*AP*CP*TP*GP*CP*AP*CP*TP*CP*A)-3').

Mo	l Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	10	Total 201	C 96	N 36	O 59	Р 10	0	0	0

• Molecule 3 is a DNA chain called DNA (5'-D(P*CP*AP*AP*GP*T)-3').

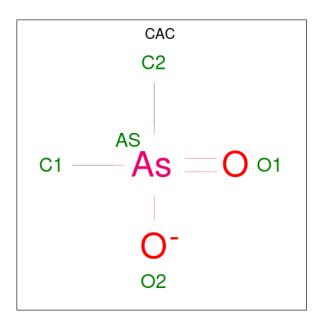
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	С	5	Total 103	C 49	N 20	O 29	Р 5	0	0	0

• Molecule 4 is a DNA chain called DNA (5'-D(*TP*CP*TP*GP*AP*GP*TP*GP*CP*TP*GP*CP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
4	D	16	Total 324	C 156	N 54	O 99	Р 15	0	0	0

• Molecule 5 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	1	Total As 1 1	0	0
5	D	1	Total As 1 1	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(*GP*AP*GP*CP*AP*GP*AP*CP*AP*TP*G)-3')

Chain A:	27%	55%		18%		
G1 645 66 66 67 89 710 611						
• Molecule 2:	DNA (5'-D(P*.	AP*CP*TP*GP*CP*A	AP*CP*TP*CF	P *A)-3')		
Chain B:	30%	30%	40%			
A12 C13 T14 G15 C16 A17 C18 T19 T19 T19 A21						
• Molecule 3:	DNA (5'-D(P*	CP*AP*AP*GP*T)-3')			
Chain C:	60	%	40%			
C1 A2 A3 G4 T5						
• Molecule 4: 3')	DNA (5'-D(*T	P*CP*TP*GP*AP*G	P*TP*GP*CP	*TP*GP	*TP*CP*TP*GP*(C)-
Chain D:	50%		38%	12%		
11 64 65 65 68 68 68 63 710 611	016 016					



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants	68.67Å 68.67 Å 60.12 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.34 - 3.06	Depositor
Resolution (A)	34.34 - 3.06	EDS
% Data completeness	89.9 (34.34-3.06)	Depositor
(in resolution range)	89.9(34.34-3.06)	EDS
R _{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.56 (at 3.06 Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
D D	0.197 , 0.211	Depositor
R, R_{free}	0.197 , 0.211	DCC
R_{free} test set	258 reflections $(4.81%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	107.9	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.14, 34.2	EDS
L-test for twinning ²	$< L > = 0.48, < L^2 > = 0.31$	Xtriage
	0.045 for -h,-k,l	
Estimated twinning fraction	0.094 for h,-h-k,-l	Xtriage
	0.085 for -k,-h,-l	
$\mathbf{F}_o, \mathbf{F}_c$ correlation	0.97	EDS
Total number of atoms	857	wwPDB-VP
Average B, all atoms $(Å^2)$	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.70% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: CAC

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	1.02	1/256~(0.4%)	0.99	1/394~(0.3%)	
2	В	1.40	3/224~(1.3%)	1.26	2/342~(0.6%)	
3	С	2.14	4/115~(3.5%)	1.91	4/175~(2.3%)	
4	D	1.21	1/361~(0.3%)	1.33	3/556~(0.5%)	
All	All	1.36	9/956~(0.9%)	1.32	10/1467~(0.7%)	

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	С	3	DA	N7-C5	-7.33	1.34	1.39
2	В	12	DA	C3'-O3'	-6.21	1.35	1.44
2	В	19	DT	C3'-O3'	-6.12	1.35	1.44
2	В	18	DC	C3'-O3'	-5.99	1.36	1.44
3	С	3	DA	N3-C4	-5.86	1.31	1.34
4	D	9	DC	C3'-O3'	-5.34	1.37	1.44
3	С	5	DT	C3'-O3'	-5.13	1.37	1.44
1	А	9	DA	C3'-O3'	-5.13	1.37	1.44
3	С	3	DA	N9-C8	-5.09	1.33	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
4	D	11	DG	O4'-C4'-C3'	-9.16	100.50	106.00
3	С	5	DT	O4'-C4'-C3'	-8.62	100.83	106.00
3	С	4	DG	O4'-C4'-C3'	-8.03	101.18	106.00
3	С	1	DC	C1'-O4'-C4'	-7.06	103.04	110.10
4	D	8	DG	O4'-C4'-C3'	-6.49	101.91	104.50
2	В	18	DC	C1'-O4'-C4'	-5.69	104.41	110.10
3	С	3	DA	O4'-C1'-N9	-5.51	104.14	108.00
4	D	12	DT	C1'-O4'-C4'	-5.17	104.94	110.10

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	10	DT	N3-C4-O4	5.11	122.96	119.90
2	В	14	DT	N3-C4-O4	5.05	122.93	119.90

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	227	0	124	6	0
2	В	201	0	113	5	0
3	С	103	0	57	4	0
4	D	324	0	184	6	0
5	С	1	0	0	0	0
5	D	1	0	0	0	0
All	All	857	0	478	18	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 14.

All (18) 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)
4:D:8:DG:C8	4:D:8:DG:H5'	2.25	0.72
2:B:12:DA:H2'	2:B:13:DC:O4'	1.98	0.64
2:B:18:DC:H2'	2:B:19:DT:C6	2.35	0.62
3:C:1:DC:H2'	3:C:2:DA:C8	2.40	0.57
3:C:2:DA:H2"	4:D:10:DT:H5'	1.87	0.56
3:C:3:DA:H5'	4:D:9:DC:H2"	1.86	0.55
2:B:16:DC:H2"	2:B:17:DA:OP2	2.08	0.54
1:A:6:DG:H2'	1:A:7:DA:H8	1.76	0.51
1:A:6:DG:H2'	1:A:7:DA:C8	2.48	0.47
3:C:3:DA:C8	4:D:9:DC:C2	3.02	0.47
1:A:4:DC:H2"	1:A:5:DA:C8	2.50	0.46
2:B:13:DC:H2'	2:B:14:DT:C6	2.52	0.44

Continued on next page...



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:DT:H2"	1:A:11:DG:C8	2.54	0.43
1:A:5:DA:H2"	1:A:6:DG:O4'	2.18	0.42
1:A:8:DC:H2"	1:A:9:DA:OP2	2.17	0.42
4:D:7:DT:H4'	4:D:8:DG:OP1	2.19	0.42
2:B:17:DA:H2"	2:B:18:DC:O5'	2.20	0.41
4:D:4:DG:H2"	4:D:5:DA:C8	2.56	0.40

Continued from previous page...

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 2 ligands modelled in this entry, 2 are modelled with single atom - 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)

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		RZ>2	$OWAB(A^2)$	Q < 0.9
1	А	11/11 (100%)	-1.33	0	100	100	94, 139, 158, 159	0
2	В	10/10~(100%)	-1.33	0	100	100	87, 94, 127, 140	0
3	С	5/5~(100%)	-1.09	0	100	100	68, 68, 74, 76	0
4	D	16/16~(100%)	-1.33	0	100	100	67, 133, 160, 161	0
All	All	42/42 (100%)	-1.30	0	100	100	67, 110, 158, 161	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
5	CAC	D	101	1/5	0.96	0.06	140,140,140,140	0
5	CAC	С	101	1/5	0.98	0.18	154,154,154,154	0



6.5 Other polymers (i)

There are no such residues in this entry.

