

Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2023 – 03:03 AM EDT

PDB ID	:	6XEK
Title	:	Self-assembly of a 3D DNA crystal lattice (4x5 junction version) containing
		the J14 immobile Holliday junction
Authors	:	Simmons, C.R.; MacCulloch, T.; Stephanopoulos, N.; Yan, H.
Deposited on		
Resolution	:	2.85 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:

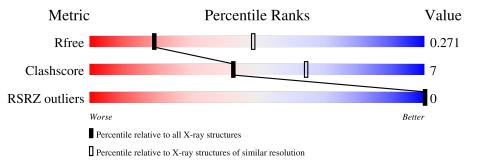
Refmac CCP4	: : : :	 1.13 2.35.1 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove)
Ideal geometry (proteins) Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	:	Parkinson et al. (1996)

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 2.85 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	73%	27%						
2	В	10	60%	30% 10%						
3	С	5	60%	40%						
4	D	16	38%	62%						



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 855 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*CP*TP*G)-3').

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	А	11	Total 229	C 108	N 51	O 60	Р 10	0	0	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	10	Total 197	С 94	N 35	O 58	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 17	O 32	Р 5	0	0	0

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

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
4	D	16	Total 326	C 156	N 57	O 98	Р 15	0	0	0



E C E S

<mark>8 5 5 5 5 5 5 5 5</mark>

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*CP*TP*G)-3')

Chain A:	73%	27%	
6 <mark>6 88</mark>			
• Molecule 2: DNA	(5'-D(P*AP*CP*TP*CP))	P*CP*AP*CP*TP*CP*	*A)-3')
Chain B:	60%	30%	10%
A12 C13 A17 A21 A21			
• Molecule 3: DNA	A (5'-D(P*CP*AP*AP*GI	P*T)-3')	
Chain C:	60%	40%	
1 2 3 3 1 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4			
• Molecule 4: DNA 3')	(5'-D(*TP*CP*TP*GP))	*AP*GP*TP*GP*GP*	GP*GP*TP*CP*T
Chain D:	38%	62%	



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	68.91Å 68.91 Å 62.09 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 - 2.85	Depositor
Resolution (A)	34.45 - 2.85	EDS
% Data completeness	99.6 (50.00-2.85)	Depositor
(in resolution range)	99.7 (34.45-2.85)	EDS
R _{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.18 (at 2.85 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
D D.	0.241 , 0.263	Depositor
R, R_{free}	0.248 , 0.271	DCC
R_{free} test set	227 reflections (5.41%)	wwPDB-VP
Wilson B-factor $(Å^2)$	89.5	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.24 , 73.5	EDS
L-test for twinning ²	$< L >=0.52, < L^2>=0.36$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	855	wwPDB-VP
Average B, all atoms $(Å^2)$	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 16.72% 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)

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		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.61	0/259	0.92	0/399	
2	В	0.95	1/219~(0.5%)	1.15	2/333~(0.6%)	
3	С	1.32	2/114~(1.8%)	1.73	5/174~(2.9%)	
4	D	0.83	1/364~(0.3%)	1.09	3/561~(0.5%)	
All	All	0.88	4/956~(0.4%)	1.16	10/1467~(0.7%)	

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	9	DG	O3'-P	-6.31	1.53	1.61
2	В	17	DA	O3'-P	-6.08	1.53	1.61
3	С	1	DC	O3'-P	-5.68	1.54	1.61
3	С	2	DT	O3'-P	-5.54	1.54	1.61

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	С	1	DC	O5'-P-OP2	-11.02	95.78	105.70
3	С	4	DG	O5'-P-OP1	7.53	119.73	110.70
3	С	4	DG	O4'-C4'-C3'	-6.72	101.81	104.50
4	D	9	DG	C1'-O4'-C4'	-6.13	103.97	110.10
2	В	12	DA	C1'-O4'-C4'	-6.06	104.04	110.10
3	С	2	DT	C4'-C3'-O3'	-5.79	95.22	109.70
2	В	18	DC	C1'-O4'-C4'	-5.61	104.49	110.10
3	С	2	DT	C1'-O4'-C4'	-5.57	104.53	110.10
4	D	9	DG	O4'-C1'-C2'	-5.54	101.47	105.90
4	D	9	DG	O5'-P-OP1	-5.15	101.06	105.70

All (10) bond angle outliers are listed below:

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	229	0	123	1	2
2	В	197	0	112	1	2
3	С	103	0	58	1	3
4	D	326	0	183	6	0
All	All	855	0	476	9	5

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 7.

All (9) 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)	
2:B:12:DA:H2"	2:B:13:DC:O4'	1.89	0.72	
4:D:14:DT:H2"	4:D:15:DG:C8	2.37	0.60	
4:D:2:DC:H2"	4:D:3:DT:O5'	2.05	0.55	
3:C:2:DT:H2"	3:C:3:DG:OP1	2.07	0.55	
4:D:11:DG:H2'	4:D:12:DT:C6	2.42	0.55	
4:D:15:DG:H1'	4:D:16:DC:C6	2.46	0.50	
4:D:3:DT:H2"	4:D:4:DG:N7	2.32	0.44	
1:A:7:DA:H2"	1:A:8:DC:O5'	2.18	0.43	
4:D:1:DT:H2"	4:D:2:DC:H6	1.86	0.40	

All (5) 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:A:11:DG:O3'	2:B:12:DA:OP1[3_565]	1.51	0.69	
3:C:1:DC:OP1	3:C:5:DT:O3'[3_565]	1.58	0.62	
3:C:1:DC:OP2	3:C:5:DT:O3'[3_565]	1.95	0.25	
3:C:1:DC:P	3:C:5:DT:O3'[3_565]	1.98	0.22	
1:A:11:DG:O3'	2:B:12:DA:P[3_565]	2.02	0.18	



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	<RSRZ $>$	$\#RSRZ{>}2$		LZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	11/11 (100%)	-0.30	0	100	100	82, 101, 114, 117	0
2	В	10/10~(100%)	-0.37	0	100	100	73, 82, 101, 103	0
3	С	5/5~(100%)	-0.25	0	100	100	60, 65, 72, 72	0
4	D	16/16~(100%)	-0.26	0	100	100	69, 96, 114, 140	0
All	All	42/42~(100%)	-0.30	0	100	100	60, 87, 114, 140	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.

