

Full wwPDB X-ray Structure Validation Report (i)

Jan 30, 2024 - 07:24 PM EST

PDB ID	:	1FQ2
Title	:	CRYSTAL STRUCTURE ANALYSIS OF THE POTASSIUM FORM OF B-
		DNA DODECAMER CGCGAATTCGCG
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Deposited on		
Resolution	:	1.20 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:

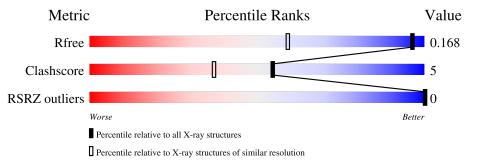
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.20 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	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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 c	hain
1	А	12	92%	8%
1	В	12	8% 50%	42%



1FQ2

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 681 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.

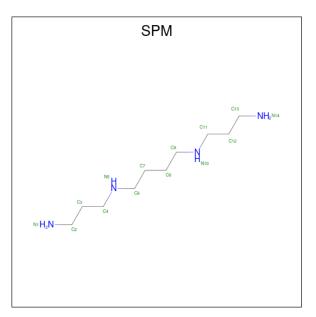
• Molecule 1 is a DNA chain called DNA (5'-D(*CP*GP*CP*GP*AP*AP*TP*TP*CP*GP* CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	12	Total	С	Ν	Ο	Р	0	0	0
	I A	12	243	116	46	70	11	0	0	0
1	В	12	Total	С	Ν	Ο	Р	0	0	0
	I B	12	243	116	46	70	11	0	0	0

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Mg 1 1	0	0

• Molecule 3 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).





Ν	ſol	Chain	Residues	Ate	oms		ZeroOcc	AltConf
	3	В	1	Total 7	$\begin{array}{c} \mathrm{C} \\ 5 \end{array}$	N 2	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	97	Total O 97 97	0	0
4	В	90	Total O 90 90	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*AP*AP*TP*TP*CP*GP*CP*G)-3')

□ 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Chain A:	92%	8%	6
	C1 G2 G2 G3 G4 A6 A6 A6 C3 C11 C11 C11 C12			
Chain B: 8% 50% 42%	• Molecule 1: DNA (5	o'-D(*CP*GP*CP*GP	*AP*AP*TP*TP*CP*GP*C	P*G)-3')
	Chain B: 8%	50%	42%	-



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	25.59Å 40.82 Å 66.67 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 - 1.20	Depositor
Resolution (A)	9.76 - 1.20	EDS
% Data completeness	86.0 (10.00-1.20)	Depositor
(in resolution range)	85.5 (9.76-1.20)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$12.01 (at 1.20 \text{\AA})$	Xtriage
Refinement program	SHELXL-97	Depositor
D D.	0.139 , 0.215	Depositor
R, R_{free}	0.152 , 0.168	DCC
R_{free} test set	1933 reflections (9.98%)	wwPDB-VP
Wilson B-factor $(Å^2)$	13.2	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.63, 132.9	EDS
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	681	wwPDB-VP
Average B, all atoms $(Å^2)$	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 11.31% 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: SPM, MG

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		
10101	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.59	2/272~(0.7%)	2.64	31/418~(7.4%)	
1	В	1.65	3/272~(1.1%)	2.74	30/418~(7.2%)	
All	All	1.62	5/544~(0.9%)	2.69	61/836~(7.3%)	

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	8	DT	O4'-C1'	6.73	1.50	1.42
1	А	11	DC	O4'-C1'	5.45	1.48	1.42
1	А	7	DT	O4'-C1'	5.39	1.48	1.42
1	В	5	DA	O4'-C1'	5.16	1.48	1.42
1	В	9	DC	N1-C6	5.16	1.40	1.37

All (61)	bond angle	outliers ar	e listed	below:
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	4	DG	P-O3'-C3'	12.02	134.12	119.70
1	В	8	DT	O4'-C1'-N1	-10.56	100.61	108.00
1	А	11	DC	O4'-C1'-N1	-10.14	100.91	108.00
1	В	1	DC	N3-C2-O2	-9.86	115.00	121.90
1	А	2	DG	P-O3'-C3'	9.56	131.18	119.70
1	В	4	DG	O4'-C1'-N9	8.86	114.20	108.00
1	В	4	DG	P-O3'-C3'	8.72	130.17	119.70
1	В	8	DT	P-O3'-C3'	8.53	129.94	119.70
1	А	7	DT	C6-N1-C2	-7.98	117.31	121.30
1	В	1	DC	N1-C2-O2	7.77	123.56	118.90
1	В	9	DC	O4'-C1'-N1	-7.71	102.61	108.00
1	А	12	DG	C5-C6-N1	7.69	115.34	111.50
1	В	1	DC	O4'-C1'-N1	-7.62	102.66	108.00
1	В	4	DG	C8-N9-C4	-7.37	103.45	106.40

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Mol	nued fron Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	9	DC	O4'-C1'-N1	-7.18	102.97	108.00
1	В	5	DA	O4'-C1'-N9	-7.05	103.06	108.00
1	В	12	DG	C2-N3-C4	7.01	115.41	111.90
1	В	12	DG	N3-C4-C5	-6.97	125.11	128.60
1	В	3	DC	O4'-C1'-N1	-6.85	103.21	108.00
1	В	8	DT	C6-C5-C7	-6.77	118.84	122.90
1	А	1	DC	C2-N3-C4	-6.74	116.53	119.90
1	А	5	DA	O4'-C1'-N9	-6.67	103.33	108.00
1	В	4	DG	N9-C4-C5	6.46	107.98	105.40
1	В	7	DT	C6-C5-C7	-6.35	119.09	122.90
1	А	12	DG	C1'-O4'-C4'	6.32	116.42	110.10
1	В	8	DT	N1-C1'-C2'	6.27	124.52	112.60
1	В	6	DA	P-O3'-C3'	6.23	127.17	119.70
1	В	1	DC	C2-N3-C4	-6.20	116.80	119.90
1	А	6	DA	P-O3'-C3'	6.19	127.13	119.70
1	А	8	DT	N3-C2-O2	-6.19	118.59	122.30
1	В	9	DC	N3-C4-C5	-6.18	119.43	121.90
1	В	11	DC	C4-C5-C6	6.16	120.48	117.40
1	А	1	DC	N3-C2-O2	-6.13	117.61	121.90
1	А	2	DG	O4'-C1'-C2'	-6.03	101.07	105.90
1	А	10	DG	P-O3'-C3'	6.00	126.90	119.70
1	А	11	DC	N1-C1'-C2'	5.98	123.96	112.60
1	В	8	DT	O4'-C1'-C2'	-5.85	101.22	105.90
1	А	7	DT	N3-C2-O2	-5.81	118.82	122.30
1	В	1	DC	P-O3'-C3'	5.79	126.65	119.70
1	А	2	DG	C6-N1-C2	-5.79	121.62	125.10
1	В	8	DT	N1-C2-N3	5.77	118.06	114.60
1	А	7	DT	C5-C6-N1	5.71	127.12	123.70
1	А	8	DT	P-O3'-C3'	5.69	126.53	119.70
1	А	12	DG	O4'-C1'-N9	-5.65	104.04	108.00
1	А	8	DT	O4'-C1'-N1	-5.64	104.05	108.00
1	А	4	DG	N1-C6-O6	-5.57	116.56	119.90
1	А	12	DG	N1-C6-O6	-5.54	116.57	119.90
1	В	2	DG	N9-C4-C5	5.50	107.60	105.40
1	В	7	DT	P-O3'-C3'	5.50	126.30	119.70
1	В	5	DA	C6-N1-C2	-5.40	115.36	118.60
1	А	9	DC	O4'-C1'-C2'	-5.32	101.64	105.90
1	А	7	DT	O4'-C1'-N1	-5.32	104.28	108.00
1	А	3	DC	O4'-C1'-N1	-5.24	104.33	108.00
1	А	10	DG	C3'-C2'-C1'	-5.19	96.27	102.50
1	А	5	DA	P-O3'-C3'	5.13	125.86	119.70
1	В	9	DC	P-O3'-C3'	5.11	125.83	119.70

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	5	DA	C4-C5-C6	5.06	119.53	117.00
1	А	9	DC	N1-C1'-C2'	5.06	122.22	112.60
1	А	8	DT	C1'-O4'-C4'	-5.04	105.06	110.10
1	В	6	DA	O4'-C1'-C2'	-5.02	101.89	105.90
1	А	12	DG	C6-N1-C2	-5.00	122.10	125.10

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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	243	0	136	1	0
1	В	243	0	136	3	0
2	А	1	0	0	0	0
3	В	7	0	11	2	0
4	А	97	0	0	0	0
4	В	90	0	0	0	0
All	All	681	0	283	4	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 5.

All (4) 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:2:DG:N7	3:B:1026:SPM:H62	2.10	0.66	
1:A:10:DG:O6	3:B:1026:SPM:H61	2.10	0.52	
1:B:11:DC:H2'	1:B:12:DG:C8	2.52	0.43	
1:B:3:DC:H2'	1:B:4:DG:C8	2.54	0.43	

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, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Mol Type Chain Res	Link	B	Bond lengths			Bond angles			
IVIOI	туре	Unam	nes	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	SPM	В	1026	-	$6,\!6,\!13$	0.73	0	$5,\!5,\!12$	1.66	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SPM	В	1026	-	-	3/4/4/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	В	1026	SPM	C3-C4-N5	-2.89	104.34	112.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	В	1026	SPM	C7-C6-N5-C4
3	В	1026	SPM	C3-C4-N5-C6
3	В	1026	SPM	N1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes	
3	В	1026	SPM	2	0	

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		2Z>2	$OWAB(Å^2)$	Q < 0.9
1	А	12/12~(100%)	-0.44	0	100	100	13, 14, 21, 25	0
1	В	12/12~(100%)	-0.20	0	100	100	13, 14, 21, 22	0
All	All	24/24~(100%)	-0.32	0	100	100	13, 14, 21, 25	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.

Mo	l Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
3	SPM	В	1026	7/14	0.91	0.10	24,27,47,96	0
2	MG	А	1025	1/1	1.00	0.02	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.

