Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 10:22 PM EDT

PDB ID	:	1JGR
Title	:	Crystal Structure Analysis of the B-DNA Dodecamer CGCGAATTCGCG with Thallium Ions.
Authors	:	Howerton, S.B.; Sines, C.C.; VanDerveer, D.; Williams, L.D.
Deposited on	:	2001-06-26
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 (i)) were used in the production of this report:

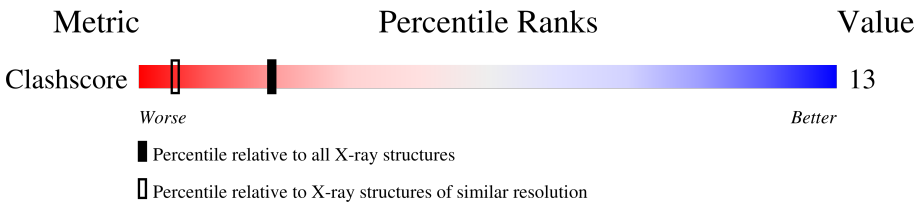
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1286 (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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	12	8% 75% 17%
1	B	12	25% 58% 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 640 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 5'-D(*CP*GP*CP*GP*AP*AP*TP*TP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	12	243	116	46	70	11	0	0	0
1	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
			Total	Mg		
2	A	1	1	1	0	0

- Molecule 3 is THALLIUM (I) ION (three-letter code: TL) (formula: Tl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Tl		
3	A	7	7	7	0	0
3	B	6	6	6	0	0

- Molecule 4 is water.

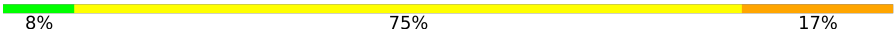
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	76	76	76	0	0
4	B	64	64	64	0	0

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. 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. 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.

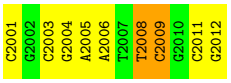
Note EDS was not executed.

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

Chain A: 

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

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	25.94Å 40.74Å 66.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.169 , 0.222	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	640	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

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: MG, TL

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	1.08	0/272	2.20	19/418 (4.5%)
1	B	1.00	0/272	1.95	9/418 (2.2%)
All	All	1.04	0/544	2.08	28/836 (3.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	5
All	All	0	8

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1004	DG	P-O3'-C3'	8.38	129.75	119.70
1	B	2004	DG	P-O3'-C3'	8.37	129.74	119.70
1	B	2006	DA	C2-N3-C4	8.04	114.62	110.60
1	A	1008	DT	P-O3'-C3'	7.84	129.11	119.70
1	A	1002	DG	P-O3'-C3'	7.55	128.76	119.70
1	A	1009	DC	N3-C4-C5	-7.18	119.03	121.90
1	B	2009	DC	P-O3'-C3'	7.14	128.27	119.70
1	A	1011	DC	C5-C6-N1	6.71	124.36	121.00
1	A	1001	DC	N3-C2-O2	-6.51	117.34	121.90
1	A	1006	DA	P-O3'-C3'	6.20	127.13	119.70
1	A	1009	DC	N3-C2-O2	-6.12	117.61	121.90
1	A	1011	DC	C6-N1-C2	-6.11	117.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2008	DT	N3-C2-O2	-5.95	118.73	122.30
1	A	1008	DT	N3-C2-O2	-5.83	118.80	122.30
1	A	1005	DA	P-O3'-C3'	5.76	126.62	119.70
1	B	2012	DG	N3-C4-C5	-5.76	125.72	128.60
1	A	1009	DC	P-O3'-C3'	5.75	126.60	119.70
1	A	1007	DT	N3-C2-O2	-5.72	118.87	122.30
1	A	1009	DC	C5-C4-N4	5.66	124.16	120.20
1	A	1001	DC	C2-N3-C4	-5.61	117.10	119.90
1	B	2006	DA	N1-C2-N3	-5.55	126.53	129.30
1	B	2001	DC	N3-C2-O2	-5.48	118.07	121.90
1	A	1007	DT	P-O3'-C3'	5.42	126.20	119.70
1	A	1010	DG	C5-C6-N1	5.41	114.21	111.50
1	B	2001	DC	C6-N1-C2	-5.32	118.17	120.30
1	A	1009	DC	C6-N1-C2	-5.26	118.19	120.30
1	B	2008	DT	P-O3'-C3'	5.08	125.79	119.70
1	A	1009	DC	C4-C5-C6	5.04	119.92	117.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1003	DC	Sidechain
1	A	1009	DC	Sidechain
1	A	1011	DC	Sidechain
1	B	2003	DC	Sidechain
1	B	2005	DA	Sidechain
1	B	2008	DT	Sidechain
1	B	2009	DC	Sidechain
1	B	2011	DC	Sidechain

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	A	243	0	136	0	0
1	B	243	0	136	0	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	7	0	0	0	0
3	B	6	0	0	1	0
4	A	76	0	0	1	0
4	B	64	0	0	0	0
All	All	640	0	272	1	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 13.

All (1) 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:A:3001:HOH:O	3:B:2106:TL:TL	0.49	0.45

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 14 ligands modelled in this entry, 14 are monoatomic - 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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.