



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2023 – 12:16 PM EDT

PDB ID : 6GN3
Title : Racemic crystal structure of A-DNA duplex formed from d(CCCGGG) in space group P21/n
Authors : Mandal, P.K.; Collie, G.W.; Kauffmann, B.; Huc, I.
Deposited on : 2018-05-29
Resolution : 2.80 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 ⓘ 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 ⓘ](#)) 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 : **FAILED**
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

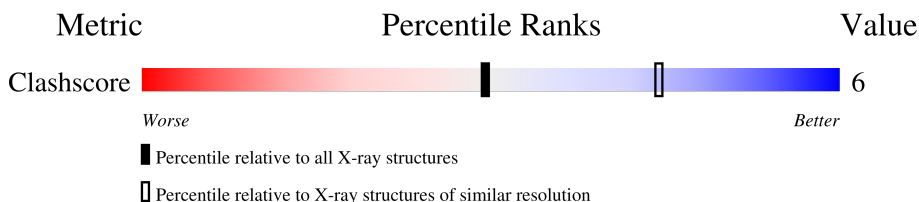
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

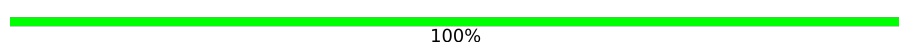
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)

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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	6	 100%
1	B	6	 33% 67%
1	C	6	 67% 33%
1	D	6	 100%
1	E	6	 67% 33%
1	F	6	 100%

2 Entry composition [i](#)

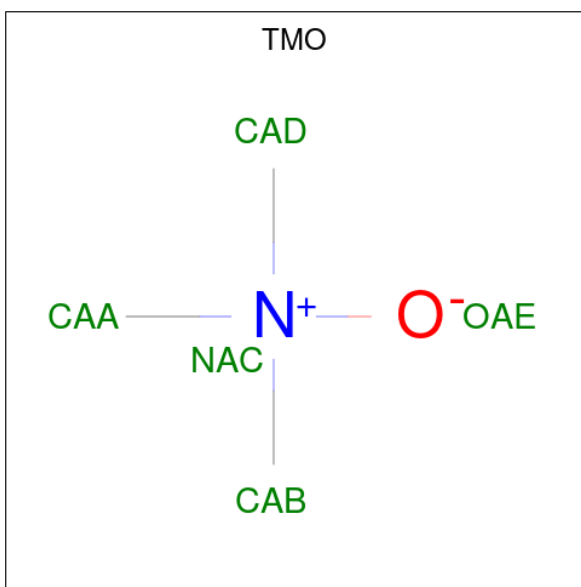
There are 5 unique types of molecules in this entry. The entry contains 751 atoms, of which 0 are hydrogens and 0 are deuteriums.

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*CP*CP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	6	Total 120	C 57	N 24	O 34	P 5	0	0	0
1	B	6	Total 120	C 57	N 24	O 34	P 5	0	0	0
1	C	6	Total 120	C 57	N 24	O 34	P 5	0	0	0
1	D	6	Total 120	C 57	N 24	O 34	P 5	0	0	0
1	E	6	Total 120	C 57	N 24	O 34	P 5	0	0	0
1	F	6	Total 120	C 57	N 24	O 34	P 5	0	0	0

- Molecule 2 is trimethylamine oxide (three-letter code: TMO) (formula: C₃H₉NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	3	1	1		
2	A	1	Total	C	N	O	0	0
			5	3	1	1		
2	B	1	Total	C	N	O	0	0
			5	3	1	1		
2	F	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Co	0	0
			1	1		
3	D	1	Total	Co	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	1	Total	O	0	0
			1	1		
5	C	2	Total	O	0	0
			2	2		
5	D	1	Total	O	0	0
			1	1		
5	E	2	Total	O	0	0
			2	2		
5	F	1	Total	O	0	0
			1	1		

3 Residue-property plots

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 failed to run properly.

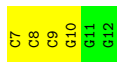
- Molecule 1: DNA (5'-D(*CP*CP*CP*GP*GP*G)-3')

Chain A:  100%

There are no outlier residues recorded for this chain.

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

Chain B:  33% 67%



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

Chain C:  67% 33%



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

Chain D:  100%

There are no outlier residues recorded for this chain.

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

Chain E:  67% 33%



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

Chain F:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21/n 1	Depositor
Cell constants a, b, c, α , β , γ	48.88Å 41.43Å 71.96Å 90.00° 97.47° 90.00°	Depositor
Resolution (Å)	31.49 - 2.80	Depositor
% Data completeness (in resolution range)	98.8 (31.49-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.280 , 0.318	Depositor
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	751	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO, CL, TMO

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	0.47	0/134	0.71	0/205
1	B	0.53	0/134	0.75	0/205
1	C	0.51	0/134	0.73	0/205
1	D	0.71	0/134	0.74	0/205
1	E	0.71	0/134	0.82	0/205
1	F	0.58	0/134	0.76	0/205
All	All	0.60	0/804	0.75	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

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	120	0	68	0	0
1	B	120	0	68	4	0
1	C	120	0	68	2	0
1	D	120	0	68	0	0
1	E	120	0	68	1	0
1	F	120	0	68	0	0
2	A	10	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	9	1	0
2	F	5	0	9	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	C	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
All	All	751	0	444	7	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 6.

The worst 5 of 7 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:9:DC:H2'	1:B:10:DG:H8	1.72	0.54
1:C:2:DC:H2'	1:C:3:DC:C6	2.47	0.49
1:B:7:DC:H41	2:B:102:TMO:HADB	1.82	0.44
1:B:8:DC:H2'	1:B:9:DC:C6	2.53	0.44
1:C:2:DC:H2'	1:C:3:DC:H6	1.81	0.44

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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TMO	A	101	-	4,4,4	1.84	1 (25%)	6,6,6	0.22	0
2	TMO	B	102	-	4,4,4	1.89	2 (50%)	6,6,6	0.24	0
2	TMO	F	101	-	4,4,4	1.90	2 (50%)	6,6,6	0.22	0
2	TMO	A	102	-	4,4,4	1.89	3 (75%)	6,6,6	0.22	0

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	101	TMO	CAA-NAC	-2.06	1.45	1.48
2	B	102	TMO	CAB-NAC	-2.05	1.45	1.48
2	B	102	TMO	CAD-NAC	-2.05	1.45	1.48
2	A	102	TMO	CAD-NAC	-2.05	1.45	1.48
2	F	101	TMO	CAD-NAC	-2.04	1.45	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	102	TMO	1	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

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.