



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 05:05 pm BST

PDB ID : 1EH8
Title : BENZYLATED HUMAN O6-ALKYLGUANINE-DNA ALKYLTRANSFERASE
Authors : Daniels, D.S.; Tainer, J.A.
Deposited on : 2000-02-18
Resolution : 2.50 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 ⓘ symbol.

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) : **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) : 2.11

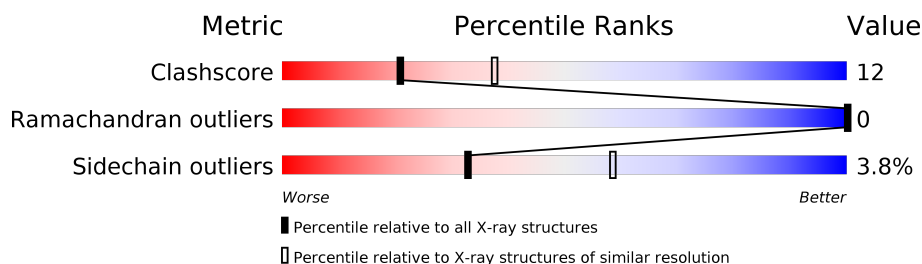
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 on 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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	207	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1354 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 protein called O6-ALKYLGUANINE-DNA ALKYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1267	817	222	220	8			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total	O	0	0
			86	86		

Note EDS was not executed.

[illegible]

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.60 Å 71.60 Å 76.04 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.50	Depositor
% Data completeness (in resolution range)	99.3 (19.95-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.194 , 0.230	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1354	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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: ZN, BCS

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	0.35	0/1286	0.62	1/1745 (0.1%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ILE	N-CA-C	-5.11	97.21	111.00

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	A	1267	0	1279	31	0
2	A	1	0	0	0	0
3	A	86	0	0	2	0
All	All	1354	0	1279	31	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 12.

All (31) 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:A:134:MET:HE2	1:A:148:VAL:HG21	1.44	0.96
1:A:134:MET:HE2	1:A:148:VAL:CG2	2.16	0.76
1:A:59:LEU:O	1:A:63:THR:HG22	1.86	0.75
1:A:123:ASN:OD1	1:A:125:LYS:HD2	1.98	0.63
1:A:134:MET:HE1	1:A:145:BCS:HA	1.80	0.63
1:A:144:PRO:HB2	1:A:147:ARG:HD2	1.81	0.63
1:A:158:TYR:HB2	1:A:165:LYS:HD2	1.83	0.61
1:A:47:PRO:HG3	1:A:71:HIS:CG	2.38	0.58
1:A:94:PHE:O	1:A:98:VAL:HG23	2.04	0.58
1:A:107:LYS:HE2	1:A:110:GLU:OE2	2.08	0.53
1:A:157:ASN:ND2	1:A:158:TYR:H	2.06	0.53
1:A:101:LYS:HG3	1:A:120:LEU:HD23	1.92	0.51
1:A:177:GLY:O	1:A:179:PRO:HD3	2.11	0.50
1:A:145:BCS:HZ2	1:A:158:TYR:CZ	2.47	0.49
1:A:61:GLN:NE2	3:A:237:HOH:O	2.41	0.48
1:A:108:PHE:CZ	1:A:172:GLU:HG2	2.49	0.47
1:A:107:LYS:HG2	1:A:110:GLU:CD	2.36	0.46
1:A:113:SER:HA	1:A:149:VAL:O	2.15	0.46
1:A:16:LEU:O	1:A:33:LEU:HD11	2.16	0.45
1:A:95:THR:O	1:A:99:LEU:HD22	2.16	0.45
1:A:9:ARG:HH11	1:A:9:ARG:HG3	1.81	0.45
1:A:72:GLN:N	1:A:73:PRO:CD	2.80	0.44
1:A:102:LEU:HD21	1:A:145:BCS:HA	1.98	0.44
1:A:108:PHE:CE1	1:A:172:GLU:HG2	2.52	0.43
1:A:144:PRO:CB	1:A:147:ARG:HD2	2.48	0.43
1:A:134:MET:CE	1:A:145:BCS:HA	2.49	0.42
1:A:130:VAL:O	1:A:134:MET:HG2	2.20	0.42
1:A:16:LEU:HD11	1:A:167:TRP:CE3	2.55	0.41
1:A:107:LYS:NZ	3:A:273:HOH:O	2.52	0.41
1:A:18:LYS:HD2	1:A:34:LEU:HD12	2.02	0.41
1:A:60:MET:HA	1:A:63:THR:CG2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	161/207 (78%)	156 (97%)	5 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	131/154 (85%)	126 (96%)	5 (4%)	33	58

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	63	THR
1	A	99	LEU
1	A	107	LYS
1	A	125	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	61	GLN
1	A	72	GLN
1	A	90	GLN
1	A	157	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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$
1	BCS	A	145	1	12,13,14	0.58	0	11,15,17	3.31	8 (72%)

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
1	BCS	A	145	1	-	2/6/8/10	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	BCS	CD-CE-CZ2	5.16	130.99	120.86
1	A	145	BCS	CH-CT1-CZ1	-4.33	113.60	120.19
1	A	145	BCS	CH-CT2-CZ2	-4.32	113.60	120.19
1	A	145	BCS	CT2-CH-CT1	3.57	126.57	119.93
1	A	145	BCS	CT1-CZ1-CE	3.49	125.98	120.63
1	A	145	BCS	CT2-CZ2-CE	3.38	125.82	120.63
1	A	145	BCS	CD-CE-CZ1	-3.21	114.58	120.86
1	A	145	BCS	CZ2-CE-CZ1	-2.38	114.43	118.17

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	145	BCS	SG-CD-CE-CZ2
1	A	145	BCS	SG-CD-CE-CZ1

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	145	BCS	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.