



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 04:59 AM EDT

PDB ID : 3QI5 / pdb_00003qi5
Title : Crystal structure of human alkyladenine DNA glycosylase in complex with 3,N4-ethenocytosine containing duplex DNA
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Deposited on : 2011-01-26
Resolution : 2.20 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 ⓘ 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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.20 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4516 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 DNA-3-methyladenine glycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	1	0
			1616	1019	296	291	10			
1	B	210	Total	C	N	O	S	0	0	0
			1642	1034	304	294	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	GLY	-	expression tag	UNP P29372
A	81	PRO	-	expression tag	UNP P29372
A	82	HIS	-	expression tag	UNP P29372
A	83	MET	-	expression tag	UNP P29372
B	80	GLY	-	expression tag	UNP P29372
B	81	PRO	-	expression tag	UNP P29372
B	82	HIS	-	expression tag	UNP P29372
B	83	MET	-	expression tag	UNP P29372

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*AP*CP*AP*TP*GP*(EDC)P*TP*TP*GP*CP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	P	0	0	0
			263	128	45	78	12			
2	E	13	Total	C	N	O	P	0	0	0
			263	128	45	78	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	13	Total	C	N	O	P	0	0	0
			249	117	48	72	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	13	Total	C	N	O	P	0	0	0
			249	117	48	72	12			

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mn	0	0
			1	1		
4	F	1	Total	Mn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	77	Total	O	0	0
			77	77		
5	B	88	Total	O	0	0
			88	88		
5	C	19	Total	O	0	0
			19	19		
5	D	16	Total	O	0	0
			16	16		
5	E	17	Total	O	0	0
			17	17		
5	F	15	Total	O	0	0
			15	15		

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

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.23Å 41.22Å 82.14Å 81.23° 88.40° 89.15°	Depositor
Resolution (Å)	81.00 – 2.20	Depositor
% Data completeness (in resolution range)	96.2 (81.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.236 , 0.284	Depositor
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.054	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
Total number of atoms	4516	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
2	EDC	C	7	2	20,23,24	1.66	4 (20%)	25,33,36	2.19	8 (32%)
2	EDC	E	7	2	20,23,24	1.64	4 (20%)	25,33,36	2.23	8 (32%)

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
2	EDC	C	7	2	-	0/7/21/22	0/3/3/3
2	EDC	E	7	2	-	0/7/21/22	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	7	EDC	C2-N3	-3.67	1.34	1.40
2	E	7	EDC	C2-N3	-3.47	1.35	1.40
2	C	7	EDC	C4-N3	-3.19	1.34	1.39
2	E	7	EDC	C4-N3	-3.12	1.35	1.39
2	C	7	EDC	C8-N3	-3.02	1.34	1.39
2	E	7	EDC	C2-N1	2.97	1.42	1.38
2	E	7	EDC	C8-N3	-2.93	1.34	1.39
2	C	7	EDC	C2-N1	2.71	1.42	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	7	EDC	N3-C2-N1	7.38	120.51	114.11
2	E	7	EDC	N3-C2-N1	7.35	120.49	114.11
2	E	7	EDC	C6-N1-C2	-4.02	118.51	121.80
2	C	7	EDC	C6-N1-C2	-3.59	118.86	121.80
2	C	7	EDC	N3-C4-N4	-2.98	108.75	111.02
2	E	7	EDC	C8-C7-N4	-2.89	106.96	110.74
2	E	7	EDC	N3-C4-N4	-2.88	108.83	111.02
2	C	7	EDC	C8-C7-N4	-2.84	107.02	110.74
2	E	7	EDC	O2-C2-N3	-2.80	118.90	123.28
2	E	7	EDC	C7-C8-N3	2.76	108.00	105.02
2	C	7	EDC	O2-C2-N3	-2.73	119.02	123.28
2	C	7	EDC	C7-C8-N3	2.58	107.81	105.02
2	E	7	EDC	C1'-N1-C2	2.44	121.76	116.97
2	E	7	EDC	C7-N4-C4	2.21	108.30	104.75
2	C	7	EDC	C7-N4-C4	2.21	108.30	104.75
2	C	7	EDC	C1'-N1-C2	2.04	120.98	116.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

4.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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.

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

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

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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