



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 07:11 PM GMT

PDB ID : 1PU7
Title : Crystal structure of H.pylori 3-methyladenine DNA glycosylase (MagIII)
bound to 3,9-dimethyladenine
Authors : Eichman, B.F.; O'Rourke, E.J.; Radicella, J.P.; Ellenberger, T.
Deposited on : 2003-06-24
Resolution : 1.93 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

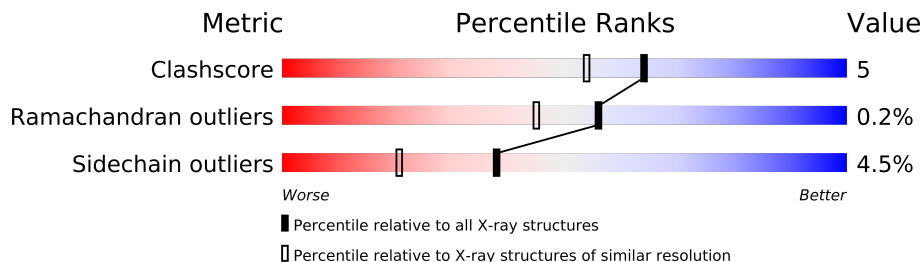
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **FAILED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.93 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	79885	2281 (1.96-1.92)
Ramachandran outliers	78287	2255 (1.96-1.92)
Sidechain outliers	78261	2255 (1.96-1.92)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	218	
1	B	218	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3871 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

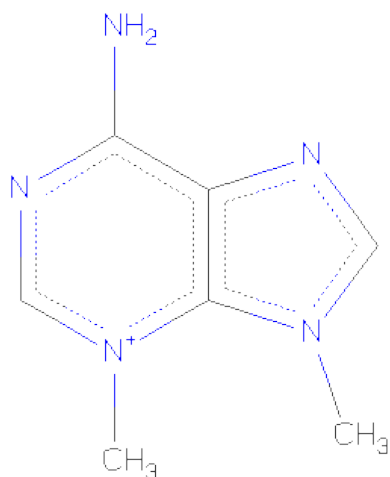
- Molecule 1 is a protein called 3-METHYLADENINE DNA GLYCOSYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	1	3	0
			1736	1131	278	323	4			
1	B	216	Total	C	N	O	S	0	4	1
			1741	1134	274	329	4			

There are 10 discrepancies between the modelled and reference sequences:

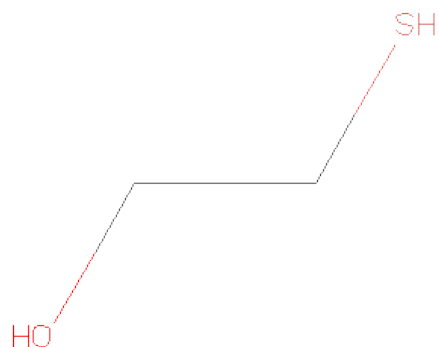
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	MET	SEE REMARK 999	UNP O25323
A	102	GLY	LYS	SEE REMARK 999	UNP O25323
A	120	ARG	LYS	SEE REMARK 999	UNP O25323
A	141	ALA	VAL	SEE REMARK 999	UNP O25323
A	205	KCX	LYS	MODIFIED RESIDUE	UNP O25323
B	1	VAL	MET	SEE REMARK 999	UNP O25323
B	102	GLY	LYS	SEE REMARK 999	UNP O25323
B	120	ARG	LYS	SEE REMARK 999	UNP O25323
B	141	ALA	VAL	SEE REMARK 999	UNP O25323
B	205	KCX	LYS	MODIFIED RESIDUE	UNP O25323

- Molecule 2 is 6-AMINO-3,9-DIMETHYL-9H-PURIN-3-IUM (three-letter code: 39A) (formula: C₇H₁₀N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			12	7	5		
2	B	1	Total	C	N	0	0
			12	7	5		

- Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	183	Total 183	O 183	0	0
4	B	179	Total 179	O 179	0	0

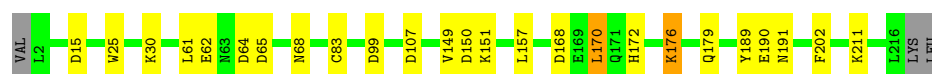
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS failed to run properly.

- Molecule 1: 3-METHYLADENINE DNA GLYCOSYLASE

Chain A: 



- Molecule 1: 3-METHYLADENINE DNA GLYCOSYLASE

Chain B: 



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.60Å 44.40Å 81.52Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	50.00 – 1.93	Depositor
% Data completeness (in resolution range)	93.5 (50.00-1.93)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.183 , 0.222	Depositor
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.524	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 35777 reflections	Xtriage
Total number of atoms	3871	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.98 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.4601e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 39A, KCX, BME

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	0.69	0/1777	0.77	7/2397 (0.3%)
1	B	0.70	0/1782	0.76	4/2404 (0.2%)
All	All	0.69	0/3559	0.76	11/4801 (0.2%)

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	B	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	150	ASP	CB-CG-OD2	8.59	126.03	118.30
1	B	64	ASP	CB-CG-OD2	7.01	124.61	118.30
1	A	64	ASP	CB-CG-OD2	6.83	124.44	118.30
1	A	168	ASP	CB-CG-OD2	6.78	124.40	118.30
1	B	150	ASP	CB-CG-OD2	6.45	124.10	118.30
1	A	61	LEU	CA-CB-CG	5.73	128.47	115.30
1	A	99	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	65	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	166	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	107	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	125	ASP	CB-CG-OD2	5.07	122.86	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	190	GLU	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1736	0	1713	11	0
1	B	1741	0	1716	17	0
2	A	12	0	10	8	0
2	B	12	0	10	7	0
3	A	4	0	5	1	0
3	B	4	0	5	1	0
4	A	183	0	0	2	0
4	B	179	0	0	1	0
All	All	3871	0	3459	38	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (38) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:62:GLU:H	1:B:68:ASN:HD21	1.06	0.96
1:B:62:GLU:H	1:B:68:ASN:ND2	1.82	0.77
1:B:25:TRP:CD2	2:B:220:39A:H8	2.27	0.69
1:A:83:CYS:HA	3:A:983:BME:H12	1.74	0.69
1:A:25:TRP:CD2	2:A:219:39A:H8	2.28	0.67
2:B:220:39A:C3M	2:B:220:39A:C9M	2.73	0.66
1:A:62:GLU:H	1:A:68:ASN:HD21	1.44	0.65
1:B:58:ALA:O	1:B:59:PHE:HB2	1.99	0.63
2:A:219:39A:C3M	2:A:219:39A:C9M	2.78	0.62
1:B:2:LEU:HD23	1:B:162:ILE:HD12	1.86	0.56
1:A:176:LYS:NZ	4:A:366:HOH:O	2.39	0.56
2:B:220:39A:H9M3	2:B:220:39A:H3M2	1.87	0.55
1:B:158:LYS:HG3	1:B:163[B]:GLU:HG3	1.88	0.54
2:B:220:39A:H9M2	2:B:220:39A:H3M3	1.89	0.53
2:A:219:39A:H9M3	2:A:219:39A:H3M2	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:172:HIS:O	1:A:176:LYS:HG2	2.12	0.50
2:A:219:39A:H3M3	2:A:219:39A:H9M2	1.94	0.49
1:A:149:VAL:HB	1:A:170:LEU:HD13	1.94	0.49
1:B:25:TRP:CH2	2:B:220:39A:H9M1	2.48	0.49
1:B:149:VAL:HB	1:B:170:LEU:HD13	1.92	0.49
1:A:25:TRP:CH2	2:A:219:39A:H9M1	2.49	0.48
1:B:160:LEU:HD21	1:B:216:LEU:HB3	1.96	0.48
1:A:62:GLU:H	1:A:68:ASN:ND2	2.11	0.48
1:B:157:LEU:HD22	1:B:162:ILE:HB	1.96	0.46
2:B:220:39A:C3M	2:B:220:39A:H9M2	2.45	0.46
1:B:83:CYS:HA	3:B:983:BME:H22	1.97	0.46
2:B:220:39A:C3M	2:B:220:39A:H9M3	2.44	0.46
1:A:25:TRP:CE3	2:A:219:39A:H8	2.52	0.44
1:A:189:TYR:O	1:A:190:GLU:CB	2.64	0.44
1:B:176:LYS:O	1:B:180:GLU:HG3	2.18	0.43
1:B:36:GLY:HA3	4:B:309:HOH:O	2.17	0.43
1:B:157:LEU:HD12	1:B:170:LEU:CD2	2.49	0.43
1:B:5:PHE:CE1	1:B:9:LYS:HE2	2.53	0.43
2:A:219:39A:H9M2	4:A:326:HOH:O	2.19	0.42
1:A:176:LYS:HA	1:A:179:GLN:HE21	1.84	0.42
1:B:46:GLU:CD	1:B:46:GLU:H	2.22	0.42
2:A:219:39A:C3M	2:A:219:39A:H9M2	2.49	0.42
1:B:29:LEU:HD22	1:B:143:ALA:HB2	2.02	0.41

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	215/218 (99%)	210 (98%)	5 (2%)	0	100	100
1	B	217/218 (100%)	208 (96%)	8 (4%)	1 (0%)	38	22
All	All	432/436 (99%)	418 (97%)	13 (3%)	1 (0%)	56	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	190	GLU

5.3.2 Protein sidechains ⓘ

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	182/190 (96%)	172 (94%)	10 (6%)	30	14
1	B	182/190 (96%)	174 (96%)	8 (4%)	39	21
All	All	364/380 (96%)	346 (95%)	18 (5%)	38	17

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	30	LYS
1	A	151[A]	LYS
1	A	151[B]	LYS
1	A	157	LEU
1	A	170	LEU
1	A	176	LYS
1	A	191	ASN
1	A	202	PHE
1	A	211	LYS
1	B	46	GLU
1	B	49	LEU
1	B	147	MET
1	B	163[A]	GLU
1	B	163[B]	GLU
1	B	170	LEU
1	B	213	LYS
1	B	216	LEU

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	68	ASN
1	A	179	GLN

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Mol	Chain	Res	Type
1	B	27	ASN
1	B	68	ASN
1	B	179	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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
1	KCX	A	205	1	11,11,12	5.47	2 (18%)	10,12,14	1.93	5 (50%)
1	KCX	B	205	1	11,11,12	5.81	1 (9%)	10,12,14	1.97	3 (30%)

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	KCX	A	205	1	-	0/8/10/12	0/0/0/0
1	KCX	B	205	1	-	0/8/10/12	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	KCX	O-C	18.99	1.24	1.11
1	A	205	KCX	O-C	17.86	1.23	1.11
1	A	205	KCX	CA-C	2.11	1.52	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	KCX	OQ2-CX-NZ	3.93	121.23	116.33
1	A	205	KCX	OQ2-CX-NZ	3.11	120.20	116.33
1	B	205	KCX	OQ2-CX-OQ1	-2.95	118.49	122.17
1	A	205	KCX	OQ1-CX-NZ	-2.82	120.25	124.94
1	B	205	KCX	OQ1-CX-NZ	-2.81	120.26	124.94
1	A	205	KCX	CE-NZ-CX	-2.77	116.94	121.99
1	A	205	KCX	C-CA-N	-2.22	111.61	113.83
1	A	205	KCX	OQ2-CX-OQ1	-2.09	119.55	122.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands 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	39A	A	219	-	13,13,13	1.28	1 (7%)	18,19,19	1.46	4 (22%)
3	BME	A	983	1	3,3,3	0.52	0	2,2,2	0.69	0
2	39A	B	220	-	13,13,13	1.48	1 (7%)	18,19,19	1.65	4 (22%)
3	BME	B	983	1	3,3,3	0.29	0	2,2,2	2.48	1 (50%)

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	39A	A	219	-	-	0/0/0/0	0/0/2/2
3	BME	A	983	1	-	0/1/1/1	0/0/0/0
2	39A	B	220	-	-	0/0/0/0	0/0/2/2
3	BME	B	983	1	-	0/1/1/1	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	220	39A	C4-N9	-3.97	1.30	1.38
2	A	219	39A	C4-N9	-3.65	1.31	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	220	39A	C9M-N9-C8	4.53	135.06	125.33
2	A	219	39A	C9M-N9-C8	4.04	133.99	125.33
3	B	983	BME	C1-C2-S2	-3.33	107.30	113.03
2	B	220	39A	C9M-N9-C4	-2.76	118.23	124.62
2	B	220	39A	N6-C6-N1	2.68	124.63	119.36
2	A	219	39A	N6-C6-N1	2.44	124.16	119.36
2	A	219	39A	C9M-N9-C4	-2.26	119.39	124.62
2	B	220	39A	C2-N1-C6	2.08	125.07	119.68
2	A	219	39A	C5-C6-N6	-2.07	116.03	120.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.