



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:21 AM UTC

PDB ID : 1EUG / pdb_00001eug
Title : CRYSTAL STRUCTURE OF ESCHERICHIA COLI URACIL DNA GLYCOSYLASE AND ITS COMPLEXES WITH URACIL AND GLYCEROL: STRUCTURE AND GLYCOSYLASE MECHANISM REVISITED
Authors : Xiao, G.; Tordova, M.; Jagadeesh, J.; Drohat, A.C.; Stivers, J.T.; Gilliland, G.L.
Deposited on : 1998-10-12
Resolution : 1.60 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

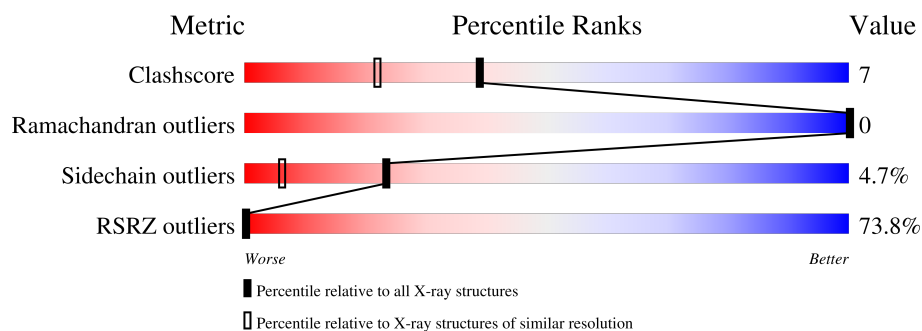
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	229	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2090 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 PROTEIN (GLYCOSYLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1790	1151	318	318	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	HIS	ARG	engineered mutation	UNP P12295

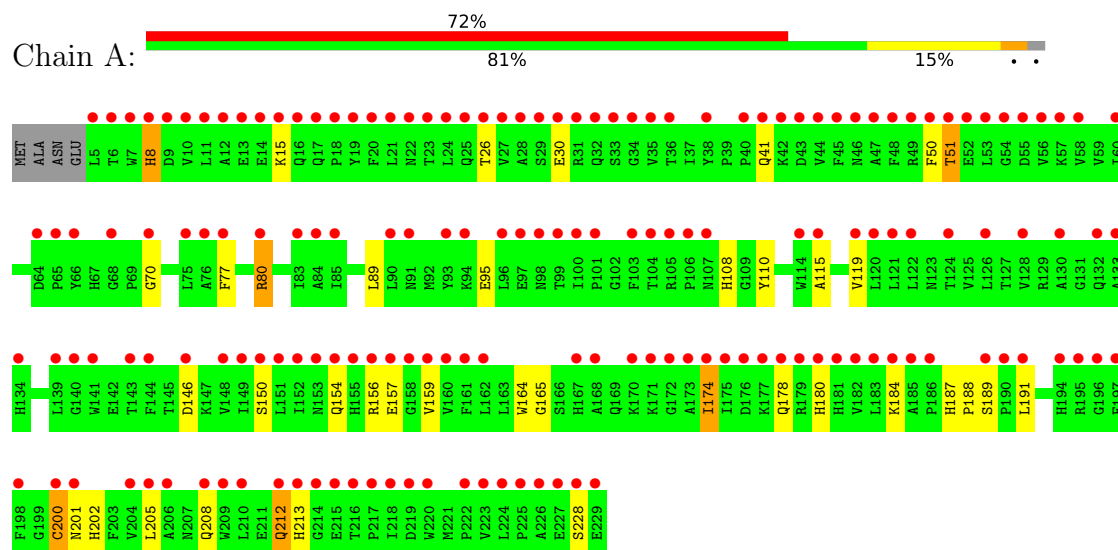
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	300	Total	O	0	0
			300	300		

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 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.

• Molecule 1: PROTEIN (GLYCOSYLASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.13Å 61.32Å 64.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 1.60 99.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	92.5 (99.00-1.60) 91.9 (99.00-1.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.44Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.194 , 0.250 0.328 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	0.1	Xtriage
Anisotropy	7.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 76.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.025 for -h,l,k	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	2090	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 9.34% 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.

5 Model quality

5.1 Standard geometry

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	0.53	1/1847 (0.1%)	1.39	15/2518 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	ASN	N-CA	7.29	1.55	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	CYS	CA-C-N	-12.73	97.22	121.54
1	A	200	CYS	C-N-CA	-12.73	97.22	121.54
1	A	201	ASN	CA-CB-CG	10.72	123.32	112.60
1	A	80	ARG	CD-NE-CZ	10.60	139.24	124.40
1	A	200	CYS	O-C-N	-9.00	112.24	122.86
1	A	51	THR	CA-C-O	7.17	129.28	120.25
1	A	213	HIS	CA-CB-CG	-6.50	107.30	113.80
1	A	165	GLY	CA-C-O	-6.07	118.05	122.23
1	A	80	ARG	NE-CZ-NH2	-5.92	113.87	119.20
1	A	200	CYS	N-CA-C	-5.86	102.25	110.50
1	A	50	PHE	CA-C-N	-5.35	114.69	122.44
1	A	50	PHE	C-N-CA	-5.35	114.69	122.44
1	A	146	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	77	PHE	CA-CB-CG	-5.19	108.61	113.80
1	A	8	HIS	CA-CB-CG	-5.04	108.76	113.80

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	1790	0	1747	24	0
2	A	300	0	0	3	0
All	All	2090	0	1747	24	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 7.

All (24) 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:164:TRP:HE1	1:A:202:HIS:HD2	1.31	0.78
1:A:212:GLN:N	1:A:212:GLN:HE21	1.82	0.77
1:A:159:VAL:H	1:A:180:HIS:HD2	1.31	0.75
1:A:108:HIS:HD2	1:A:110:TYR:H	1.38	0.71
1:A:212:GLN:HE21	1:A:212:GLN:CA	2.05	0.68
1:A:164:TRP:HE1	1:A:202:HIS:CD2	2.15	0.64
1:A:150:SER:O	1:A:154:GLN:HG3	1.99	0.62
1:A:208:GLN:O	1:A:212:GLN:NE2	2.42	0.52
1:A:70:GLY:O	1:A:80:ARG:HG3	2.12	0.50
1:A:108:HIS:CD2	1:A:110:TYR:H	2.23	0.50
1:A:174:ILE:HG12	2:A:416:HOH:O	2.12	0.48
1:A:184:LYS:HE3	1:A:184:LYS:HB2	1.51	0.48
1:A:159:VAL:H	1:A:180:HIS:CD2	2.20	0.48
1:A:8:HIS:HD2	1:A:15:LYS:NZ	2.13	0.47
1:A:212:GLN:CA	1:A:212:GLN:NE2	2.77	0.46
1:A:156:ARG:NH2	2:A:399:HOH:O	2.48	0.46
1:A:95:GLU:OE2	1:A:200:CYS:O	2.34	0.45
1:A:156:ARG:NH1	2:A:468:HOH:O	2.49	0.45
1:A:187:HIS:CG	1:A:188:PRO:HD2	2.52	0.45
1:A:156:ARG:NH1	1:A:157:GLU:H	2.18	0.42
1:A:26:THR:O	1:A:30:GLU:HG3	2.20	0.41
1:A:159:VAL:N	1:A:180:HIS:HD2	2.07	0.41
1:A:115:ALA:HA	1:A:119:VAL:O	2.21	0.40
1:A:205:LEU:HD23	1:A:205:LEU:HA	1.97	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	223/229 (97%)	215 (96%)	8 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	191/194 (98%)	182 (95%)	9 (5%)	23	6

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	51	THR
1	A	89	LEU
1	A	174	ILE
1	A	178	GLN
1	A	189	SER
1	A	191	LEU
1	A	212	GLN
1	A	228	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	16	GLN
1	A	22	ASN
1	A	41	GLN
1	A	108	HIS
1	A	167	HIS
1	A	178	GLN
1	A	180	HIS
1	A	202	HIS
1	A	212	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	225/229 (98%)	2.93	166 (73%) 0 0	5, 11, 26, 38	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	LEU	8.6
1	A	191	LEU	7.4
1	A	174	ILE	6.5
1	A	35	VAL	6.4
1	A	173	ALA	6.1
1	A	154	GLN	6.1
1	A	16	GLN	6.0
1	A	24	LEU	5.9
1	A	209	TRP	5.8
1	A	34	GLY	5.7
1	A	10	VAL	5.7
1	A	28	ALA	5.6
1	A	11	LEU	5.6
1	A	12	ALA	5.5
1	A	213	HIS	5.4
1	A	8	HIS	5.2
1	A	214	GLY	5.2
1	A	212	GLN	5.2
1	A	151	LEU	5.1
1	A	21	LEU	5.0
1	A	51	THR	5.0
1	A	17	GLN	5.0
1	A	175	ILE	4.9
1	A	18	PRO	4.9
1	A	13	GLU	4.8
1	A	7	TRP	4.7
1	A	141	TRP	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	20	PHE	4.7
1	A	19	TYR	4.6
1	A	223	VAL	4.6
1	A	178	GLN	4.6
1	A	15	LYS	4.5
1	A	45	PHE	4.5
1	A	41	GLN	4.5
1	A	9	ASP	4.4
1	A	216	THR	4.4
1	A	170	LYS	4.3
1	A	14	GLU	4.2
1	A	32	GLN	4.2
1	A	54	GLY	4.2
1	A	180	HIS	4.2
1	A	139	LEU	4.2
1	A	36	THR	4.2
1	A	225	PRO	4.1
1	A	23	THR	4.0
1	A	48	PHE	4.0
1	A	200	CYS	4.0
1	A	100	ILE	3.9
1	A	6	THR	3.9
1	A	204	VAL	3.8
1	A	42	LYS	3.8
1	A	56	VAL	3.7
1	A	53	LEU	3.7
1	A	155	HIS	3.7
1	A	27	VAL	3.6
1	A	149	ILE	3.6
1	A	160	VAL	3.6
1	A	153	ASN	3.5
1	A	130	ALA	3.5
1	A	215	GLU	3.5
1	A	198	PHE	3.5
1	A	158	GLY	3.5
1	A	183	LEU	3.5
1	A	148	VAL	3.5
1	A	107	ASN	3.4
1	A	144	PHE	3.4
1	A	105	ARG	3.4
1	A	228	SER	3.4
1	A	103	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	205	LEU	3.4
1	A	33	SER	3.4
1	A	210	LEU	3.3
1	A	49	ARG	3.3
1	A	201	ASN	3.3
1	A	40	PRO	3.3
1	A	168	ALA	3.3
1	A	152	ILE	3.3
1	A	50	PHE	3.3
1	A	177	LYS	3.3
1	A	126	LEU	3.3
1	A	114	TRP	3.2
1	A	99	THR	3.2
1	A	196	GLY	3.1
1	A	128	VAL	3.1
1	A	106	PRO	3.1
1	A	133	ALA	3.1
1	A	30	GLU	3.1
1	A	44	VAL	3.0
1	A	120	LEU	3.0
1	A	83	ILE	3.0
1	A	143	THR	3.0
1	A	55	ASP	3.0
1	A	47	ALA	3.0
1	A	189	SER	2.9
1	A	29	SER	2.9
1	A	181	HIS	2.9
1	A	38	TYR	2.8
1	A	115	ALA	2.8
1	A	58	VAL	2.8
1	A	96	LEU	2.8
1	A	156	ARG	2.8
1	A	220	TRP	2.8
1	A	161	PHE	2.8
1	A	227	GLU	2.8
1	A	146	ASP	2.8
1	A	22	ASN	2.7
1	A	85	ILE	2.7
1	A	76	ALA	2.7
1	A	150	SER	2.6
1	A	197	PHE	2.6
1	A	182	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	52	GLU	2.6
1	A	122	LEU	2.6
1	A	224	LEU	2.6
1	A	132	GLN	2.6
1	A	26	THR	2.6
1	A	208	GLN	2.6
1	A	43	ASP	2.5
1	A	104	THR	2.5
1	A	66	TYR	2.5
1	A	190	PRO	2.5
1	A	167	HIS	2.5
1	A	80	ARG	2.5
1	A	157	GLU	2.5
1	A	70	GLY	2.5
1	A	194	HIS	2.5
1	A	94	LYS	2.5
1	A	98	ASN	2.5
1	A	179	ARG	2.5
1	A	97	GLU	2.4
1	A	84	ALA	2.4
1	A	119	VAL	2.4
1	A	65	PRO	2.4
1	A	184	LYS	2.4
1	A	60	ILE	2.4
1	A	101	PRO	2.3
1	A	64	ASP	2.3
1	A	57	LYS	2.3
1	A	121	LEU	2.3
1	A	162	LEU	2.3
1	A	159	VAL	2.3
1	A	25	GLN	2.2
1	A	206	ALA	2.2
1	A	176	ASP	2.2
1	A	217	PRO	2.2
1	A	90	LEU	2.2
1	A	93	TYR	2.2
1	A	226	ALA	2.2
1	A	46	ASN	2.2
1	A	222	PRO	2.2
1	A	219	ASP	2.1
1	A	186	PRO	2.1
1	A	218	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	31	ARG	2.1
1	A	124	THR	2.1
1	A	68	GLY	2.1
1	A	171	LYS	2.1
1	A	195	ARG	2.1
1	A	77	PHE	2.1
1	A	140	GLY	2.0
1	A	172	GLY	2.0
1	A	75	LEU	2.0
1	A	134	HIS	2.0
1	A	229	GLU	2.0
1	A	91	ASN	2.0
1	A	185	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.