



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 03:53 PM GMT

PDB ID : 1EUG  
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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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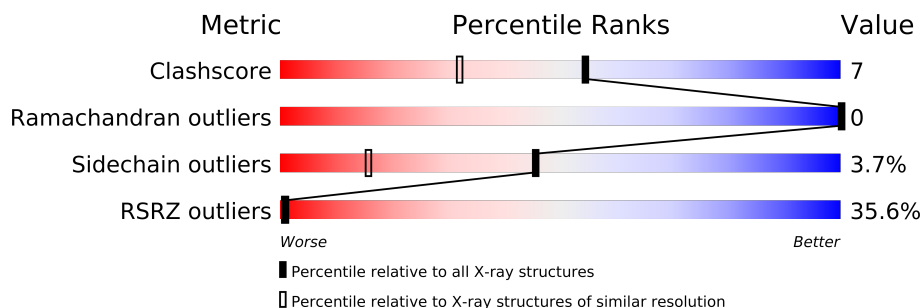
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
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 1.60 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	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.

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 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 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	MUTATION	UNP P12295

- Molecule 2 is water.

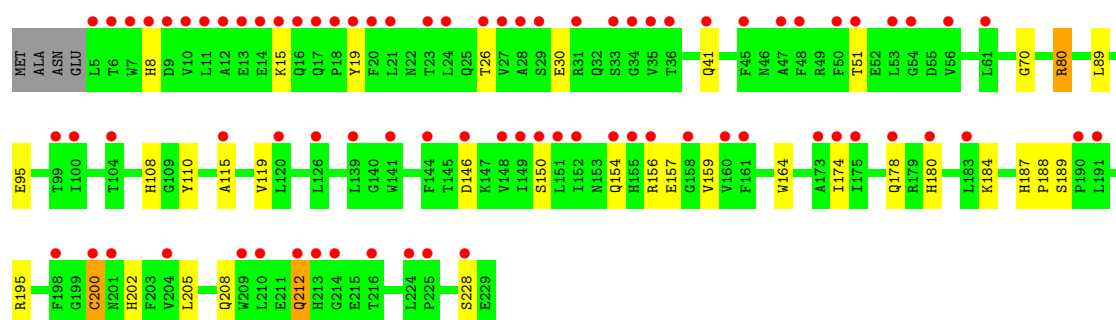
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	300	Total	O	0	0
			300	300		

### 3 Residue-property plots

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.

#### • Molecule 1: PROTEIN (GLYCOSYLASE)

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.13Å 61.32Å 64.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 1.60 44.41 – 1.44	Depositor EDS
% Data completeness (in resolution range)	92.5 (99.00-1.60) 71.6 (44.41-1.44)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 1.44Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.194 , 0.250 0.350 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	0.1	Xtriage
Anisotropy	7.013	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 66.4	EDS
Estimated twinning fraction	0.025 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	3 of 32709 reflections (0.009%)	Xtriage
$F_o, F_c$ correlation	0.67	EDS
Total number of atoms	2090	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.42	0/1847	1.10	8/2518 (0.3%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ARG	NE-CZ-NH2	-12.86	113.87	120.30
1	A	80	ARG	NE-CZ-NH1	12.05	126.32	120.30
1	A	80	ARG	CD-NE-CZ	11.17	139.24	123.60
1	A	200	CYS	C-N-CA	-9.79	97.22	121.70
1	A	195	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	A	200	CYS	O-C-N	-6.54	112.24	122.70
1	A	146	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	19	TYR	CB-CG-CD2	5.14	124.09	121.00

There are no chirality outliers.

There are no planarity outliers.

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

All (24) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:HB2	1:A:184:LYS:HE3	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:NE2	1:A:212:GLN:CA	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:HA	1:A:205:LEU:HD23	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%)	184 (96%)	7 (4%)	45	16

All (7) 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	178	GLN
1	A	189	SER
1	A	212	GLN
1	A	228	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	22	ASN
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 ⓘ

There are no RNA chains in this entry.



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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	225/229 (98%)	1.84	80 (35%) <b>1</b> <b>1</b>	5, 11, 26, 38	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	LEU	7.2
1	A	21	LEU	5.4
1	A	24	LEU	5.4
1	A	10	VAL	5.1
1	A	17	GLN	4.6
1	A	173	ALA	4.5
1	A	20	PHE	4.1
1	A	141	TRP	4.0
1	A	7	TRP	3.9
1	A	11	LEU	3.8
1	A	174	ILE	3.8
1	A	12	ALA	3.8
1	A	35	VAL	3.7
1	A	53	LEU	3.6
1	A	212	GLN	3.6
1	A	19	TYR	3.6
1	A	151	LEU	3.6
1	A	191	LEU	3.5
1	A	154	GLN	3.5
1	A	36	THR	3.4
1	A	175	ILE	3.3
1	A	6	THR	3.3
1	A	9	ASP	3.2
1	A	45	PHE	3.2
1	A	56	VAL	3.1
1	A	15	LYS	3.1
1	A	18	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	139	LEU	3.1
1	A	16	GLN	3.0
1	A	155	HIS	2.9
1	A	33	SER	2.9
1	A	51	THR	2.9
1	A	144	PHE	2.9
1	A	13	GLU	2.9
1	A	156	ARG	2.9
1	A	178	GLN	2.8
1	A	148	VAL	2.8
1	A	161	PHE	2.8
1	A	200	CYS	2.8
1	A	183	LEU	2.8
1	A	160	VAL	2.8
1	A	23	THR	2.8
1	A	54	GLY	2.8
1	A	41	GLN	2.7
1	A	8	HIS	2.7
1	A	214	GLY	2.7
1	A	213	HIS	2.6
1	A	126	LEU	2.6
1	A	28	ALA	2.6
1	A	201	ASN	2.6
1	A	204	VAL	2.6
1	A	225	PRO	2.5
1	A	152	ILE	2.5
1	A	216	THR	2.5
1	A	48	PHE	2.5
1	A	27	VAL	2.4
1	A	228	SER	2.4
1	A	100	ILE	2.4
1	A	149	ILE	2.4
1	A	50	PHE	2.4
1	A	99	THR	2.4
1	A	31	ARG	2.4
1	A	198	PHE	2.3
1	A	120	LEU	2.3
1	A	26	THR	2.3
1	A	224	LEU	2.2
1	A	190	PRO	2.2
1	A	158	GLY	2.2
1	A	14	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	34	GLY	2.2
1	A	150	SER	2.1
1	A	180	HIS	2.1
1	A	104	THR	2.1
1	A	115	ALA	2.1
1	A	209	TRP	2.1
1	A	47	ALA	2.1
1	A	210	LEU	2.1
1	A	146	ASP	2.0
1	A	29	SER	2.0
1	A	61	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.