



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:07 AM GMT

PDB ID : 2ZHX
Title : Crystal structure of Uracil-DNA Glycosylase from Mycobacterium tuberculosis
in complex with a proteinaceous inhibitor
Authors : Kaushal, P.S.; Talawar, R.K.; Krishna, P.D.V.; Varshney, U.; Vijayan, M.
Deposited on : 2008-02-11
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

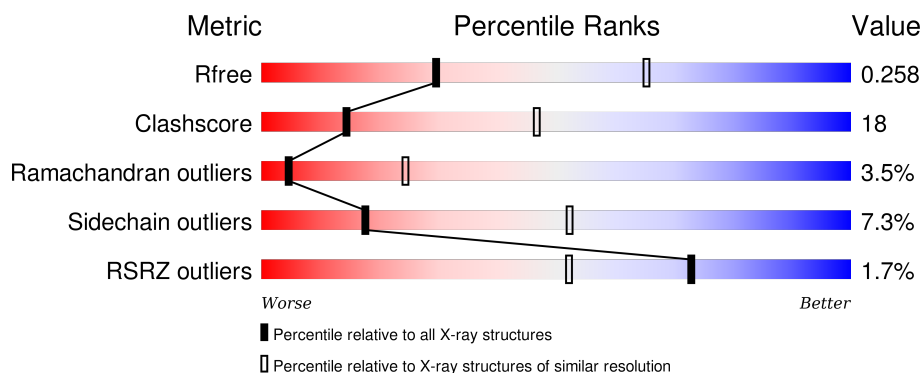
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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. 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	238	 61% 28% 5% • 5%
1	C	238	 61% 29% 5% • 5%
1	E	238	 64% 24% 5% • 6%
1	G	238	 66% 24% 5% 5%
1	I	238	 2% 58% 32% 5% 5%

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Mol	Chain	Length	Quality of chain
1	K	238	<div><div><div></div><div></div><div></div></div><div>2%</div><div>58%</div><div>31%</div><div>• • 5%</div></div>
1	M	238	<div><div><div></div><div></div><div></div></div><div>%</div><div>60%</div><div>29%</div><div>5% • 5%</div></div>
2	B	84	<div><div><div></div><div></div><div></div></div><div></div><div>71%</div><div>21%</div><div>5% •</div></div>
2	D	84	<div><div><div></div><div></div><div></div></div><div></div><div>69%</div><div>25%</div><div>• •</div></div>
2	F	84	<div><div><div></div><div></div><div></div></div><div>%</div><div>62%</div><div>33%</div><div>• •</div></div>
2	H	84	<div><div><div></div><div></div><div></div></div><div>2%</div><div>75%</div><div>19%</div><div>• •</div></div>
2	J	84	<div><div><div></div><div></div><div></div></div><div>15%</div><div>76%</div><div>20%</div><div>• •</div></div>
2	L	84	<div><div><div></div><div></div><div></div></div><div></div><div>74%</div><div>21%</div><div>• •</div></div>
2	N	84	<div><div><div></div><div></div><div></div></div><div>11%</div><div>68%</div><div>27%</div><div>• • •</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16840 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 Uracil-DNA glycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1715	1095	313	302	5			
1	C	225	Total	C	N	O	S	0	0	0
			1709	1092	310	302	5			
1	E	224	Total	C	N	O	S	0	0	0
			1704	1089	309	301	5			
1	G	225	Total	C	N	O	S	0	0	0
			1707	1091	312	299	5			
1	I	225	Total	C	N	O	S	0	0	0
			1705	1090	310	300	5			
1	K	225	Total	C	N	O	S	0	0	0
			1705	1090	309	301	5			
1	M	225	Total	C	N	O	S	0	0	0
			1701	1088	309	299	5			

There are 77 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	INITIATING METHIONINE	UNP P67071
A	-9	HIS	-	EXPRESSION TAG	UNP P67071
A	-8	HIS	-	EXPRESSION TAG	UNP P67071
A	-7	HIS	-	EXPRESSION TAG	UNP P67071
A	-6	HIS	-	EXPRESSION TAG	UNP P67071
A	-5	HIS	-	EXPRESSION TAG	UNP P67071
A	-4	HIS	-	EXPRESSION TAG	UNP P67071
A	-3	GLY	-	EXPRESSION TAG	UNP P67071
A	-2	MET	-	EXPRESSION TAG	UNP P67071
A	-1	ALA	-	EXPRESSION TAG	UNP P67071
A	0	SER	-	EXPRESSION TAG	UNP P67071
C	-10	MET	-	INITIATING METHIONINE	UNP P67071
C	-9	HIS	-	EXPRESSION TAG	UNP P67071
C	-8	HIS	-	EXPRESSION TAG	UNP P67071
C	-7	HIS	-	EXPRESSION TAG	UNP P67071

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	HIS	-	EXPRESSION TAG	UNP P67071
C	-5	HIS	-	EXPRESSION TAG	UNP P67071
C	-4	HIS	-	EXPRESSION TAG	UNP P67071
C	-3	GLY	-	EXPRESSION TAG	UNP P67071
C	-2	MET	-	EXPRESSION TAG	UNP P67071
C	-1	ALA	-	EXPRESSION TAG	UNP P67071
C	0	SER	-	EXPRESSION TAG	UNP P67071
E	-10	MET	-	INITIATING METHIONINE	UNP P67071
E	-9	HIS	-	EXPRESSION TAG	UNP P67071
E	-8	HIS	-	EXPRESSION TAG	UNP P67071
E	-7	HIS	-	EXPRESSION TAG	UNP P67071
E	-6	HIS	-	EXPRESSION TAG	UNP P67071
E	-5	HIS	-	EXPRESSION TAG	UNP P67071
E	-4	HIS	-	EXPRESSION TAG	UNP P67071
E	-3	GLY	-	EXPRESSION TAG	UNP P67071
E	-2	MET	-	EXPRESSION TAG	UNP P67071
E	-1	ALA	-	EXPRESSION TAG	UNP P67071
E	0	SER	-	EXPRESSION TAG	UNP P67071
G	-10	MET	-	INITIATING METHIONINE	UNP P67071
G	-9	HIS	-	EXPRESSION TAG	UNP P67071
G	-8	HIS	-	EXPRESSION TAG	UNP P67071
G	-7	HIS	-	EXPRESSION TAG	UNP P67071
G	-6	HIS	-	EXPRESSION TAG	UNP P67071
G	-5	HIS	-	EXPRESSION TAG	UNP P67071
G	-4	HIS	-	EXPRESSION TAG	UNP P67071
G	-3	GLY	-	EXPRESSION TAG	UNP P67071
G	-2	MET	-	EXPRESSION TAG	UNP P67071
G	-1	ALA	-	EXPRESSION TAG	UNP P67071
G	0	SER	-	EXPRESSION TAG	UNP P67071
I	-10	MET	-	INITIATING METHIONINE	UNP P67071
I	-9	HIS	-	EXPRESSION TAG	UNP P67071
I	-8	HIS	-	EXPRESSION TAG	UNP P67071
I	-7	HIS	-	EXPRESSION TAG	UNP P67071
I	-6	HIS	-	EXPRESSION TAG	UNP P67071
I	-5	HIS	-	EXPRESSION TAG	UNP P67071
I	-4	HIS	-	EXPRESSION TAG	UNP P67071
I	-3	GLY	-	EXPRESSION TAG	UNP P67071
I	-2	MET	-	EXPRESSION TAG	UNP P67071
I	-1	ALA	-	EXPRESSION TAG	UNP P67071
I	0	SER	-	EXPRESSION TAG	UNP P67071
K	-10	MET	-	INITIATING METHIONINE	UNP P67071
K	-9	HIS	-	EXPRESSION TAG	UNP P67071

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-8	HIS	-	EXPRESSION TAG	UNP P67071
K	-7	HIS	-	EXPRESSION TAG	UNP P67071
K	-6	HIS	-	EXPRESSION TAG	UNP P67071
K	-5	HIS	-	EXPRESSION TAG	UNP P67071
K	-4	HIS	-	EXPRESSION TAG	UNP P67071
K	-3	GLY	-	EXPRESSION TAG	UNP P67071
K	-2	MET	-	EXPRESSION TAG	UNP P67071
K	-1	ALA	-	EXPRESSION TAG	UNP P67071
K	0	SER	-	EXPRESSION TAG	UNP P67071
M	-10	MET	-	INITIATING METHIONINE	UNP P67071
M	-9	HIS	-	EXPRESSION TAG	UNP P67071
M	-8	HIS	-	EXPRESSION TAG	UNP P67071
M	-7	HIS	-	EXPRESSION TAG	UNP P67071
M	-6	HIS	-	EXPRESSION TAG	UNP P67071
M	-5	HIS	-	EXPRESSION TAG	UNP P67071
M	-4	HIS	-	EXPRESSION TAG	UNP P67071
M	-3	GLY	-	EXPRESSION TAG	UNP P67071
M	-2	MET	-	EXPRESSION TAG	UNP P67071
M	-1	ALA	-	EXPRESSION TAG	UNP P67071
M	0	SER	-	EXPRESSION TAG	UNP P67071

- Molecule 2 is a protein called Uracil-DNA glycosylase inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	82	Total	C	N	O	S	0	0	0
			639	402	98	136	3			
2	D	82	Total	C	N	O	S	0	0	0
			647	406	99	139	3			
2	F	82	Total	C	N	O	S	0	0	0
			635	399	98	135	3			
2	H	82	Total	C	N	O	S	0	0	0
			628	394	98	133	3			
2	J	82	Total	C	N	O	S	0	0	0
			618	388	97	131	2			
2	L	82	Total	C	N	O	S	0	0	0
			613	387	96	127	3			
2	N	82	Total	C	N	O	S	0	0	0
			595	371	95	127	2			

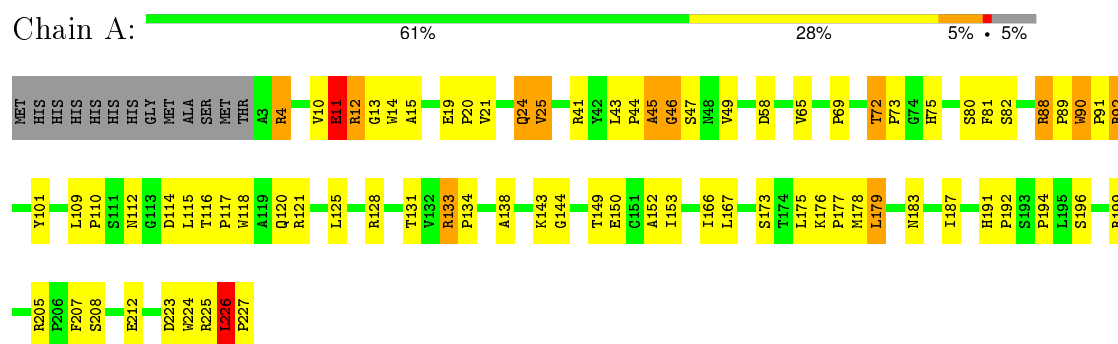
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total 69	O 69	0	0
3	B	23	Total 23	O 23	0	0
3	C	50	Total 50	O 50	0	0
3	D	46	Total 46	O 46	0	0
3	E	52	Total 52	O 52	0	0
3	F	16	Total 16	O 16	0	0
3	G	42	Total 42	O 42	0	0
3	H	25	Total 25	O 25	0	0
3	I	41	Total 41	O 41	0	0
3	J	20	Total 20	O 20	0	0
3	K	57	Total 57	O 57	0	0
3	L	20	Total 20	O 20	0	0
3	M	42	Total 42	O 42	0	0
3	N	16	Total 16	O 16	0	0

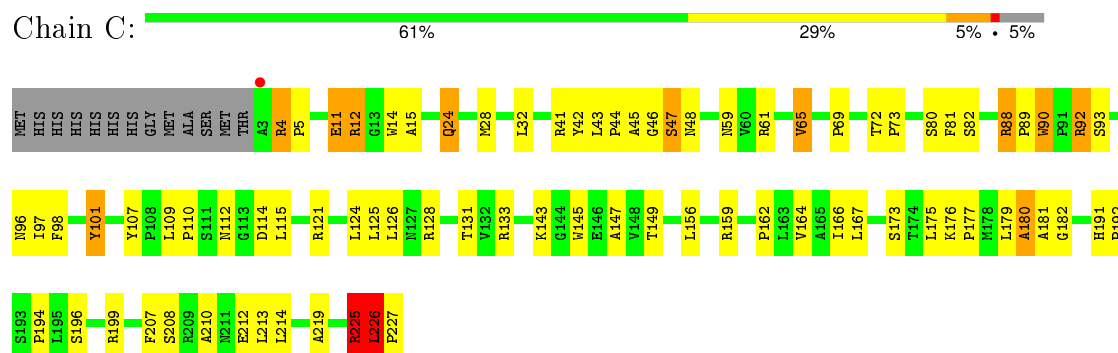
3 Residue-property plots

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.

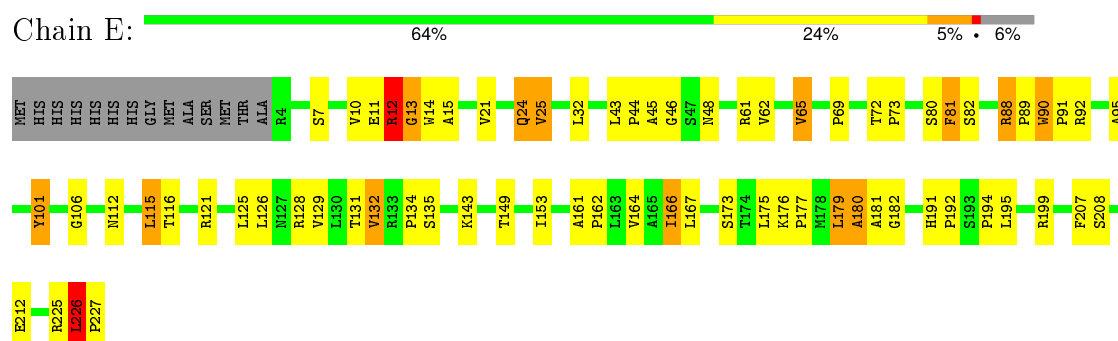
• Molecule 1: Uracil-DNA glycosylase



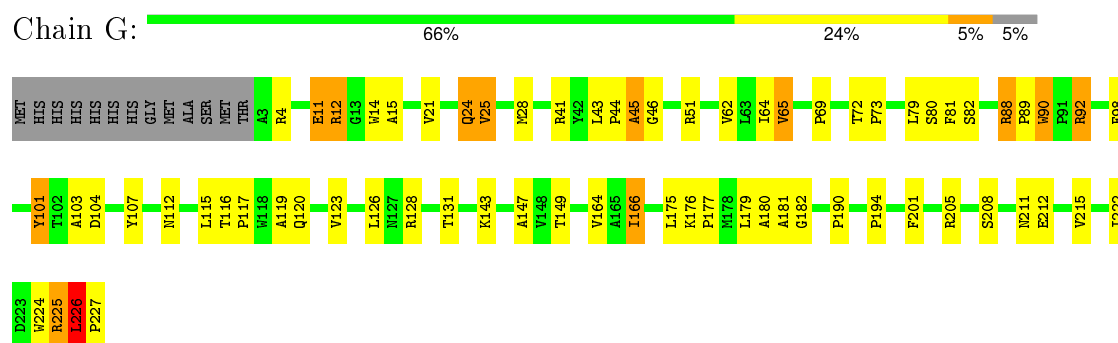
• Molecule 1: Uracil-DNA glycosylase



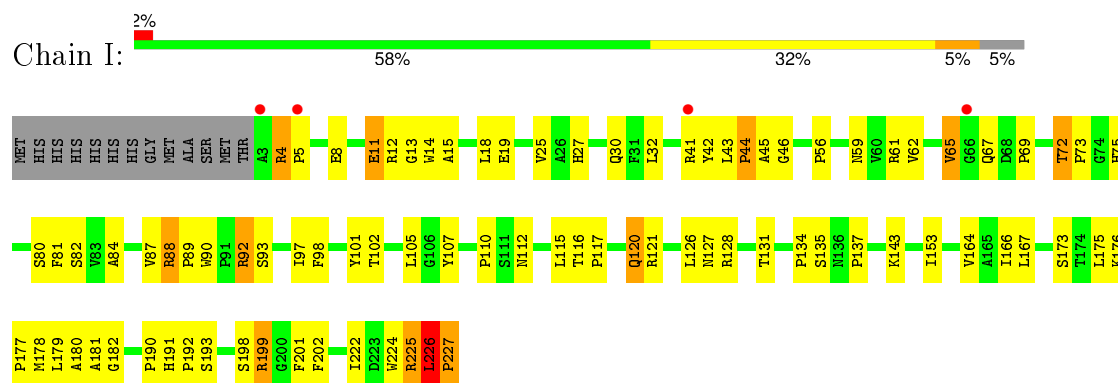
• Molecule 1: Uracil-DNA glycosylase



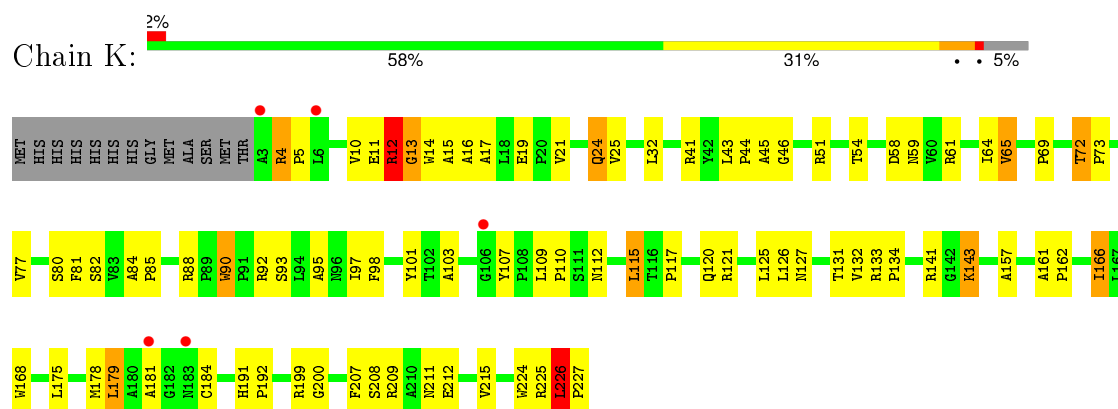
- Molecule 1: Uracil-DNA glycosylase



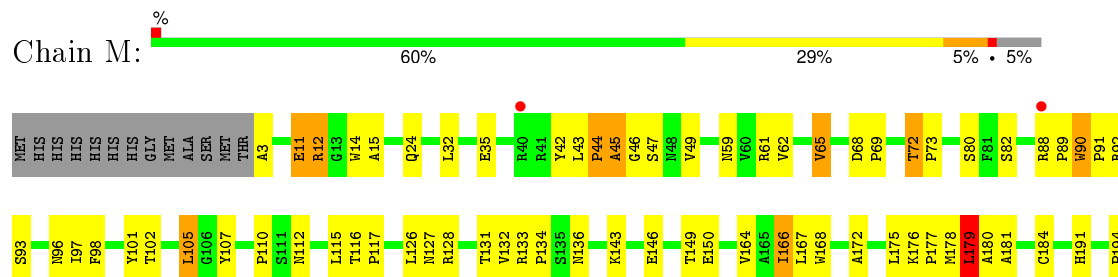
- Molecule 1: Uracil-DNA glycosylase



- Molecule 1: Uracil-DNA glycosylase



- Molecule 1: Uracil-DNA glycosylase





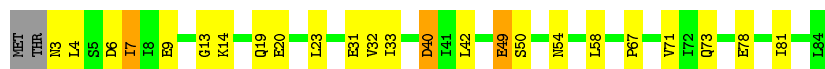
- Molecule 2: Uracil-DNA glycosylase inhibitor

Chain B: 71% 21% 5%



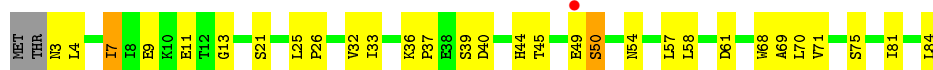
- Molecule 2: Uracil-DNA glycosylase inhibitor

Chain D: 69% 25%



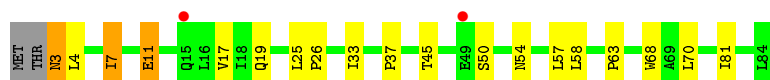
- Molecule 2: Uracil-DNA glycosylase inhibitor

Chain F: 62% 33%



- Molecule 2: Uracil-DNA glycosylase inhibitor

Chain H: 75% 19%



- Molecule 2: Uracil-DNA glycosylase inhibitor

Chain J: 76% 20%



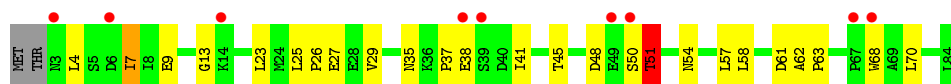
- Molecule 2: Uracil-DNA glycosylase inhibitor

Chain L: 74% 21%



- Molecule 2: Uracil-DNA glycosylase inhibitor

Chain N: 68% 27%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	201.14Å 64.27Å 203.68Å 90.00° 109.72° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 29.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (30.00-3.10) 97.2 (29.96-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.276 0.217 , 0.258	Depositor DCC
R_{free} test set	2228 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 43788 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16840	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.61	0/1766	0.74	0/2416
1	C	0.68	2/1760 (0.1%)	0.77	2/2409 (0.1%)
1	E	0.59	0/1755	0.74	0/2402
1	G	0.61	0/1758	0.71	1/2406 (0.0%)
1	I	0.68	3/1756 (0.2%)	0.72	0/2404
1	K	0.67	2/1756 (0.1%)	0.70	3/2404 (0.1%)
1	M	0.66	2/1752 (0.1%)	0.72	2/2399 (0.1%)
2	B	0.61	0/647	0.66	1/877 (0.1%)
2	D	0.71	2/655 (0.3%)	0.77	1/887 (0.1%)
2	F	0.65	0/643	0.61	0/873
2	H	0.66	0/635	0.63	0/864
2	J	0.79	2/626 (0.3%)	0.65	1/853 (0.1%)
2	L	0.61	1/621 (0.2%)	0.65	1/845 (0.1%)
2	N	1.04	6/602 (1.0%)	0.70	0/823
All	All	0.67	20/16732 (0.1%)	0.71	12/22862 (0.1%)

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	E	0	1
1	K	0	1
All	All	0	2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	27	GLU	CD-OE2	10.89	1.37	1.25
2	N	27	GLU	CD-OE1	9.87	1.36	1.25
1	I	8	GLU	CD-OE1	8.42	1.34	1.25
2	J	49	GLU	CA-CB	-8.13	1.36	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	88	ARG	CZ-NH2	8.07	1.43	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	K	133	ARG	NE-CZ-NH1	-7.19	116.71	120.30
1	K	133	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	M	179	LEU	CA-CB-CG	5.83	128.72	115.30
1	G	179	LEU	CA-CB-CG	5.82	128.70	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	10	VAL	Peptide
1	K	10	VAL	Peptide

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	1715	0	1707	88	0
1	C	1709	0	1696	70	0
1	E	1704	0	1691	67	0
1	G	1707	0	1697	65	0
1	I	1705	0	1692	73	0
1	K	1705	0	1690	76	0
1	M	1701	0	1686	76	0
2	B	639	0	630	18	0
2	D	647	0	640	23	0
2	F	635	0	621	18	0
2	H	628	0	606	14	0
2	J	618	0	588	10	0
2	L	613	0	590	9	0
2	N	595	0	549	11	0
3	A	69	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	23	0	0	0	0
3	C	50	0	0	0	0
3	D	46	0	0	0	0
3	E	52	0	0	2	0
3	F	16	0	0	1	0
3	G	42	0	0	0	0
3	H	25	0	0	0	0
3	I	41	0	0	0	0
3	J	20	0	0	0	0
3	K	57	0	0	1	0
3	L	20	0	0	1	0
3	M	42	0	0	1	0
3	N	16	0	0	0	0
All	All	16840	0	16083	582	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 18.

The worst 5 of 582 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:G:44:PRO:HG2	1:G:131:THR:HA	1.25	1.13
1:C:44:PRO:HG2	1:C:131:THR:HA	1.27	1.11
1:K:44:PRO:HG2	1:K:131:THR:HA	1.13	1.09
1:A:44:PRO:HG2	1:A:131:THR:HA	1.13	1.07
1:I:44:PRO:HG2	1:I:131:THR:HA	1.32	1.06

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	223/238 (94%)	195 (87%)	20 (9%)	8 (4%)	4	24
1	C	223/238 (94%)	189 (85%)	26 (12%)	8 (4%)	4	24
1	E	222/238 (93%)	187 (84%)	24 (11%)	11 (5%)	3	16
1	G	223/238 (94%)	194 (87%)	22 (10%)	7 (3%)	5	27
1	I	223/238 (94%)	193 (86%)	21 (9%)	9 (4%)	4	21
1	K	223/238 (94%)	190 (85%)	26 (12%)	7 (3%)	5	27
1	M	223/238 (94%)	185 (83%)	30 (14%)	8 (4%)	4	24
2	B	80/84 (95%)	68 (85%)	9 (11%)	3 (4%)	4	22
2	D	80/84 (95%)	70 (88%)	8 (10%)	2 (2%)	7	32
2	F	80/84 (95%)	68 (85%)	10 (12%)	2 (2%)	7	32
2	H	80/84 (95%)	69 (86%)	9 (11%)	2 (2%)	7	32
2	J	80/84 (95%)	69 (86%)	9 (11%)	2 (2%)	7	32
2	L	80/84 (95%)	71 (89%)	7 (9%)	2 (2%)	7	32
2	N	80/84 (95%)	73 (91%)	4 (5%)	3 (4%)	4	22
All	All	2120/2254 (94%)	1821 (86%)	225 (11%)	74 (4%)	4	24

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	61	ASP
1	C	180	ALA
1	C	181	ALA
1	E	180	ALA
1	E	181	ALA

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	175/186 (94%)	160 (91%)	15 (9%)	13	45
1	C	174/186 (94%)	157 (90%)	17 (10%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	174/186 (94%)	160 (92%)	14 (8%)	15	48
1	G	173/186 (93%)	159 (92%)	14 (8%)	15	47
1	I	173/186 (93%)	160 (92%)	13 (8%)	17	51
1	K	173/186 (93%)	158 (91%)	15 (9%)	13	44
1	M	172/186 (92%)	156 (91%)	16 (9%)	11	39
2	B	74/78 (95%)	70 (95%)	4 (5%)	27	64
2	D	76/78 (97%)	75 (99%)	1 (1%)	76	91
2	F	73/78 (94%)	69 (94%)	4 (6%)	27	63
2	H	71/78 (91%)	67 (94%)	4 (6%)	26	62
2	J	68/78 (87%)	67 (98%)	1 (2%)	72	90
2	L	67/78 (86%)	64 (96%)	3 (4%)	34	70
2	N	63/78 (81%)	60 (95%)	3 (5%)	31	69
All	All	1706/1848 (92%)	1582 (93%)	124 (7%)	17	52

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	12	ARG
2	H	3	ASN
1	M	143	LYS
1	G	24	GLN
1	G	90	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	120	GLN
2	H	3	ASN
1	M	59	ASN
2	F	44	HIS
1	G	59	ASN

5.3.3 RNA ⓘ

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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	225/238 (94%)	-0.23	0 100 100	32, 46, 70, 130	0
1	C	225/238 (94%)	-0.24	1 (0%) 93 85	27, 43, 77, 127	0
1	E	224/238 (94%)	-0.25	0 100 100	32, 44, 72, 127	0
1	G	225/238 (94%)	-0.17	0 100 100	31, 48, 73, 133	0
1	I	225/238 (94%)	-0.11	4 (1%) 71 50	34, 51, 78, 132	0
1	K	225/238 (94%)	-0.11	5 (2%) 65 42	36, 56, 84, 140	0
1	M	225/238 (94%)	0.01	2 (0%) 85 72	40, 63, 89, 139	0
2	B	82/84 (97%)	-0.06	0 100 100	40, 57, 91, 110	0
2	D	82/84 (97%)	-0.14	0 100 100	34, 52, 80, 109	0
2	F	82/84 (97%)	-0.08	1 (1%) 81 64	38, 56, 87, 106	0
2	H	82/84 (97%)	0.16	2 (2%) 62 39	56, 75, 100, 111	0
2	J	82/84 (97%)	0.73	13 (15%) 3 1	71, 95, 128, 142	0
2	L	82/84 (97%)	0.05	0 100 100	62, 82, 116, 149	0
2	N	82/84 (97%)	0.66	9 (10%) 7 2	82, 103, 125, 151	0
All	All	2148/2254 (95%)	-0.06	37 (1%) 73 52	27, 54, 102, 151	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	39	SER	5.4
1	I	3	ALA	5.0
1	K	3	ALA	3.8
2	N	49	GLU	3.4
2	J	36	LYS	3.2

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 carbohydrates 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.