wwPDB X-ray Structure Validation Summary Report (i)

Sep 12, 2023 – 03:23 AM EDT

PDB ID	:	4LZB
Title	:	Uracil binding pocket in Vaccinia virus uracil DNA glycosylase
Authors	:	Schormann, N.; Chattopadhyay, D.
Deposited on	:	2013-07-31
Resolution	:	2.03 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

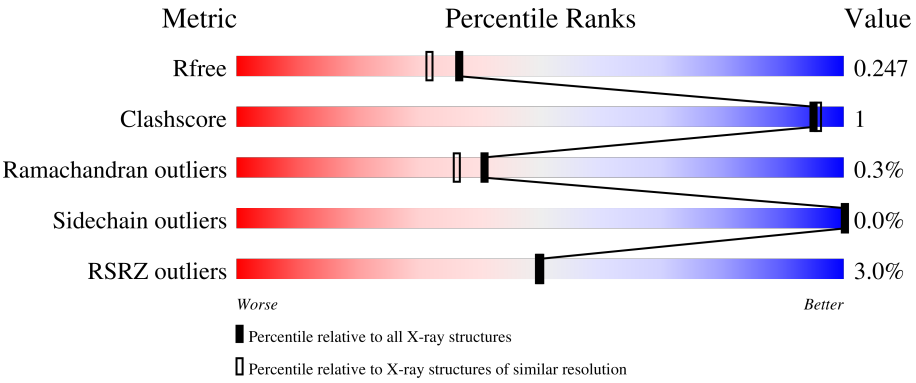
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 <=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	87% · 8%
1	B	238	89% · 8%
1	C	238	90% · 8%
1	D	238	89% · 8%
1	E	238	85% 5% 9%

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Mol	Chain	Length	Quality of chain
1	F	238	89% 8%
1	G	238	2% 88% 8%
1	H	238	2% 89% 10%
1	I	238	3% 86% 10%
1	J	238	5% 88% 9%
1	K	238	11% 88% 9%
1	L	238	5% 88% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	B	302	-	-	X	-
6	URA	B	312	-	X	-	-
6	URA	C	303	-	X	-	-
6	URA	D	305	-	X	-	-
6	URA	E	307	-	X	-	-
6	URA	F	305	-	X	-	-
6	URA	G	306	-	X	-	-
6	URA	H	304	-	X	-	-
6	URA	I	303	-	X	-	-
6	URA	K	303	-	X	-	-
6	URA	L	302	-	X	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 23231 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	218	Total	C	N	O	S	0	3	0
			1796	1161	299	330	6			
1	B	219	Total	C	N	O	S	0	5	0
			1812	1170	303	333	6			
1	C	218	Total	C	N	O	S	0	0	0
			1770	1147	294	323	6			
1	D	219	Total	C	N	O	S	0	6	0
			1827	1178	308	335	6			
1	E	216	Total	C	N	O	S	0	3	0
			1774	1149	295	324	6			
1	F	218	Total	C	N	O	S	0	5	0
			1808	1167	303	332	6			
1	G	219	Total	C	N	O	S	0	2	0
			1792	1159	299	328	6			
1	H	215	Total	C	N	O	S	0	1	0
			1748	1135	287	320	6			
1	I	214	Total	C	N	O	S	0	2	0
			1746	1134	287	319	6			
1	J	217	Total	C	N	O	S	0	3	0
			1780	1152	294	328	6			
1	K	217	Total	C	N	O	S	0	4	0
			1787	1156	296	329	6			
1	L	214	Total	C	N	O	S	0	2	0
			1750	1136	286	322	6			

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q91UM2
A	-18	GLY	-	expression tag	UNP Q91UM2
A	-17	SER	-	expression tag	UNP Q91UM2
A	-16	SER	-	expression tag	UNP Q91UM2
A	-15	HIS	-	expression tag	UNP Q91UM2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP Q91UM2
A	-13	HIS	-	expression tag	UNP Q91UM2
A	-12	HIS	-	expression tag	UNP Q91UM2
A	-11	HIS	-	expression tag	UNP Q91UM2
A	-10	HIS	-	expression tag	UNP Q91UM2
A	-9	SER	-	expression tag	UNP Q91UM2
A	-8	SER	-	expression tag	UNP Q91UM2
A	-7	GLY	-	expression tag	UNP Q91UM2
A	-6	LEU	-	expression tag	UNP Q91UM2
A	-5	VAL	-	expression tag	UNP Q91UM2
A	-4	PRO	-	expression tag	UNP Q91UM2
A	-3	ARG	-	expression tag	UNP Q91UM2
A	-2	GLY	-	expression tag	UNP Q91UM2
A	-1	SER	-	expression tag	UNP Q91UM2
A	0	HIS	-	expression tag	UNP Q91UM2
A	17	ASN	ASP	engineered mutation	UNP Q91UM2
B	-19	MET	-	expression tag	UNP Q91UM2
B	-18	GLY	-	expression tag	UNP Q91UM2
B	-17	SER	-	expression tag	UNP Q91UM2
B	-16	SER	-	expression tag	UNP Q91UM2
B	-15	HIS	-	expression tag	UNP Q91UM2
B	-14	HIS	-	expression tag	UNP Q91UM2
B	-13	HIS	-	expression tag	UNP Q91UM2
B	-12	HIS	-	expression tag	UNP Q91UM2
B	-11	HIS	-	expression tag	UNP Q91UM2
B	-10	HIS	-	expression tag	UNP Q91UM2
B	-9	SER	-	expression tag	UNP Q91UM2
B	-8	SER	-	expression tag	UNP Q91UM2
B	-7	GLY	-	expression tag	UNP Q91UM2
B	-6	LEU	-	expression tag	UNP Q91UM2
B	-5	VAL	-	expression tag	UNP Q91UM2
B	-4	PRO	-	expression tag	UNP Q91UM2
B	-3	ARG	-	expression tag	UNP Q91UM2
B	-2	GLY	-	expression tag	UNP Q91UM2
B	-1	SER	-	expression tag	UNP Q91UM2
B	0	HIS	-	expression tag	UNP Q91UM2
B	17	ASN	ASP	engineered mutation	UNP Q91UM2
C	-19	MET	-	expression tag	UNP Q91UM2
C	-18	GLY	-	expression tag	UNP Q91UM2
C	-17	SER	-	expression tag	UNP Q91UM2
C	-16	SER	-	expression tag	UNP Q91UM2
C	-15	HIS	-	expression tag	UNP Q91UM2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	expression tag	UNP Q91UM2
C	-13	HIS	-	expression tag	UNP Q91UM2
C	-12	HIS	-	expression tag	UNP Q91UM2
C	-11	HIS	-	expression tag	UNP Q91UM2
C	-10	HIS	-	expression tag	UNP Q91UM2
C	-9	SER	-	expression tag	UNP Q91UM2
C	-8	SER	-	expression tag	UNP Q91UM2
C	-7	GLY	-	expression tag	UNP Q91UM2
C	-6	LEU	-	expression tag	UNP Q91UM2
C	-5	VAL	-	expression tag	UNP Q91UM2
C	-4	PRO	-	expression tag	UNP Q91UM2
C	-3	ARG	-	expression tag	UNP Q91UM2
C	-2	GLY	-	expression tag	UNP Q91UM2
C	-1	SER	-	expression tag	UNP Q91UM2
C	0	HIS	-	expression tag	UNP Q91UM2
C	17	ASN	ASP	engineered mutation	UNP Q91UM2
D	-19	MET	-	expression tag	UNP Q91UM2
D	-18	GLY	-	expression tag	UNP Q91UM2
D	-17	SER	-	expression tag	UNP Q91UM2
D	-16	SER	-	expression tag	UNP Q91UM2
D	-15	HIS	-	expression tag	UNP Q91UM2
D	-14	HIS	-	expression tag	UNP Q91UM2
D	-13	HIS	-	expression tag	UNP Q91UM2
D	-12	HIS	-	expression tag	UNP Q91UM2
D	-11	HIS	-	expression tag	UNP Q91UM2
D	-10	HIS	-	expression tag	UNP Q91UM2
D	-9	SER	-	expression tag	UNP Q91UM2
D	-8	SER	-	expression tag	UNP Q91UM2
D	-7	GLY	-	expression tag	UNP Q91UM2
D	-6	LEU	-	expression tag	UNP Q91UM2
D	-5	VAL	-	expression tag	UNP Q91UM2
D	-4	PRO	-	expression tag	UNP Q91UM2
D	-3	ARG	-	expression tag	UNP Q91UM2
D	-2	GLY	-	expression tag	UNP Q91UM2
D	-1	SER	-	expression tag	UNP Q91UM2
D	0	HIS	-	expression tag	UNP Q91UM2
D	17	ASN	ASP	engineered mutation	UNP Q91UM2
E	-19	MET	-	expression tag	UNP Q91UM2
E	-18	GLY	-	expression tag	UNP Q91UM2
E	-17	SER	-	expression tag	UNP Q91UM2
E	-16	SER	-	expression tag	UNP Q91UM2
E	-15	HIS	-	expression tag	UNP Q91UM2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-14	HIS	-	expression tag	UNP Q91UM2
E	-13	HIS	-	expression tag	UNP Q91UM2
E	-12	HIS	-	expression tag	UNP Q91UM2
E	-11	HIS	-	expression tag	UNP Q91UM2
E	-10	HIS	-	expression tag	UNP Q91UM2
E	-9	SER	-	expression tag	UNP Q91UM2
E	-8	SER	-	expression tag	UNP Q91UM2
E	-7	GLY	-	expression tag	UNP Q91UM2
E	-6	LEU	-	expression tag	UNP Q91UM2
E	-5	VAL	-	expression tag	UNP Q91UM2
E	-4	PRO	-	expression tag	UNP Q91UM2
E	-3	ARG	-	expression tag	UNP Q91UM2
E	-2	GLY	-	expression tag	UNP Q91UM2
E	-1	SER	-	expression tag	UNP Q91UM2
E	0	HIS	-	expression tag	UNP Q91UM2
E	17	ASN	ASP	engineered mutation	UNP Q91UM2
F	-19	MET	-	expression tag	UNP Q91UM2
F	-18	GLY	-	expression tag	UNP Q91UM2
F	-17	SER	-	expression tag	UNP Q91UM2
F	-16	SER	-	expression tag	UNP Q91UM2
F	-15	HIS	-	expression tag	UNP Q91UM2
F	-14	HIS	-	expression tag	UNP Q91UM2
F	-13	HIS	-	expression tag	UNP Q91UM2
F	-12	HIS	-	expression tag	UNP Q91UM2
F	-11	HIS	-	expression tag	UNP Q91UM2
F	-10	HIS	-	expression tag	UNP Q91UM2
F	-9	SER	-	expression tag	UNP Q91UM2
F	-8	SER	-	expression tag	UNP Q91UM2
F	-7	GLY	-	expression tag	UNP Q91UM2
F	-6	LEU	-	expression tag	UNP Q91UM2
F	-5	VAL	-	expression tag	UNP Q91UM2
F	-4	PRO	-	expression tag	UNP Q91UM2
F	-3	ARG	-	expression tag	UNP Q91UM2
F	-2	GLY	-	expression tag	UNP Q91UM2
F	-1	SER	-	expression tag	UNP Q91UM2
F	0	HIS	-	expression tag	UNP Q91UM2
F	17	ASN	ASP	engineered mutation	UNP Q91UM2
G	-19	MET	-	expression tag	UNP Q91UM2
G	-18	GLY	-	expression tag	UNP Q91UM2
G	-17	SER	-	expression tag	UNP Q91UM2
G	-16	SER	-	expression tag	UNP Q91UM2
G	-15	HIS	-	expression tag	UNP Q91UM2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	HIS	-	expression tag	UNP Q91UM2
G	-13	HIS	-	expression tag	UNP Q91UM2
G	-12	HIS	-	expression tag	UNP Q91UM2
G	-11	HIS	-	expression tag	UNP Q91UM2
G	-10	HIS	-	expression tag	UNP Q91UM2
G	-9	SER	-	expression tag	UNP Q91UM2
G	-8	SER	-	expression tag	UNP Q91UM2
G	-7	GLY	-	expression tag	UNP Q91UM2
G	-6	LEU	-	expression tag	UNP Q91UM2
G	-5	VAL	-	expression tag	UNP Q91UM2
G	-4	PRO	-	expression tag	UNP Q91UM2
G	-3	ARG	-	expression tag	UNP Q91UM2
G	-2	GLY	-	expression tag	UNP Q91UM2
G	-1	SER	-	expression tag	UNP Q91UM2
G	0	HIS	-	expression tag	UNP Q91UM2
G	17	ASN	ASP	engineered mutation	UNP Q91UM2
H	-19	MET	-	expression tag	UNP Q91UM2
H	-18	GLY	-	expression tag	UNP Q91UM2
H	-17	SER	-	expression tag	UNP Q91UM2
H	-16	SER	-	expression tag	UNP Q91UM2
H	-15	HIS	-	expression tag	UNP Q91UM2
H	-14	HIS	-	expression tag	UNP Q91UM2
H	-13	HIS	-	expression tag	UNP Q91UM2
H	-12	HIS	-	expression tag	UNP Q91UM2
H	-11	HIS	-	expression tag	UNP Q91UM2
H	-10	HIS	-	expression tag	UNP Q91UM2
H	-9	SER	-	expression tag	UNP Q91UM2
H	-8	SER	-	expression tag	UNP Q91UM2
H	-7	GLY	-	expression tag	UNP Q91UM2
H	-6	LEU	-	expression tag	UNP Q91UM2
H	-5	VAL	-	expression tag	UNP Q91UM2
H	-4	PRO	-	expression tag	UNP Q91UM2
H	-3	ARG	-	expression tag	UNP Q91UM2
H	-2	GLY	-	expression tag	UNP Q91UM2
H	-1	SER	-	expression tag	UNP Q91UM2
H	0	HIS	-	expression tag	UNP Q91UM2
H	17	ASN	ASP	engineered mutation	UNP Q91UM2
I	-19	MET	-	expression tag	UNP Q91UM2
I	-18	GLY	-	expression tag	UNP Q91UM2
I	-17	SER	-	expression tag	UNP Q91UM2
I	-16	SER	-	expression tag	UNP Q91UM2
I	-15	HIS	-	expression tag	UNP Q91UM2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-14	HIS	-	expression tag	UNP Q91UM2
I	-13	HIS	-	expression tag	UNP Q91UM2
I	-12	HIS	-	expression tag	UNP Q91UM2
I	-11	HIS	-	expression tag	UNP Q91UM2
I	-10	HIS	-	expression tag	UNP Q91UM2
I	-9	SER	-	expression tag	UNP Q91UM2
I	-8	SER	-	expression tag	UNP Q91UM2
I	-7	GLY	-	expression tag	UNP Q91UM2
I	-6	LEU	-	expression tag	UNP Q91UM2
I	-5	VAL	-	expression tag	UNP Q91UM2
I	-4	PRO	-	expression tag	UNP Q91UM2
I	-3	ARG	-	expression tag	UNP Q91UM2
I	-2	GLY	-	expression tag	UNP Q91UM2
I	-1	SER	-	expression tag	UNP Q91UM2
I	0	HIS	-	expression tag	UNP Q91UM2
I	17	ASN	ASP	engineered mutation	UNP Q91UM2
J	-19	MET	-	expression tag	UNP Q91UM2
J	-18	GLY	-	expression tag	UNP Q91UM2
J	-17	SER	-	expression tag	UNP Q91UM2
J	-16	SER	-	expression tag	UNP Q91UM2
J	-15	HIS	-	expression tag	UNP Q91UM2
J	-14	HIS	-	expression tag	UNP Q91UM2
J	-13	HIS	-	expression tag	UNP Q91UM2
J	-12	HIS	-	expression tag	UNP Q91UM2
J	-11	HIS	-	expression tag	UNP Q91UM2
J	-10	HIS	-	expression tag	UNP Q91UM2
J	-9	SER	-	expression tag	UNP Q91UM2
J	-8	SER	-	expression tag	UNP Q91UM2
J	-7	GLY	-	expression tag	UNP Q91UM2
J	-6	LEU	-	expression tag	UNP Q91UM2
J	-5	VAL	-	expression tag	UNP Q91UM2
J	-4	PRO	-	expression tag	UNP Q91UM2
J	-3	ARG	-	expression tag	UNP Q91UM2
J	-2	GLY	-	expression tag	UNP Q91UM2
J	-1	SER	-	expression tag	UNP Q91UM2
J	0	HIS	-	expression tag	UNP Q91UM2
J	17	ASN	ASP	engineered mutation	UNP Q91UM2
K	-19	MET	-	expression tag	UNP Q91UM2
K	-18	GLY	-	expression tag	UNP Q91UM2
K	-17	SER	-	expression tag	UNP Q91UM2
K	-16	SER	-	expression tag	UNP Q91UM2
K	-15	HIS	-	expression tag	UNP Q91UM2

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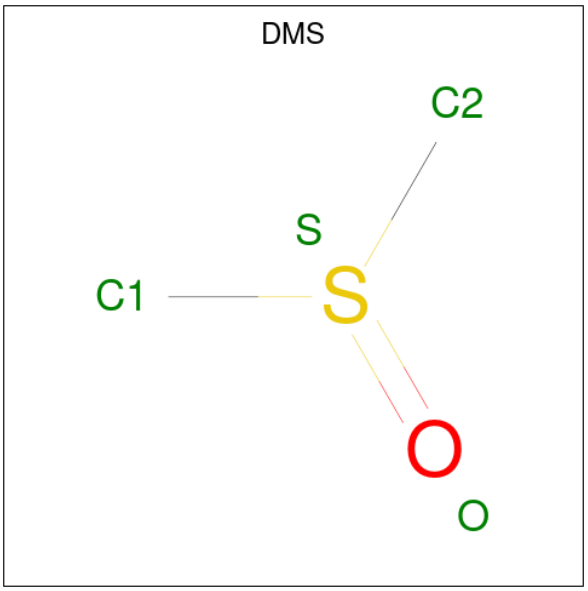
Chain	Residue	Modelled	Actual	Comment	Reference
K	-14	HIS	-	expression tag	UNP Q91UM2
K	-13	HIS	-	expression tag	UNP Q91UM2
K	-12	HIS	-	expression tag	UNP Q91UM2
K	-11	HIS	-	expression tag	UNP Q91UM2
K	-10	HIS	-	expression tag	UNP Q91UM2
K	-9	SER	-	expression tag	UNP Q91UM2
K	-8	SER	-	expression tag	UNP Q91UM2
K	-7	GLY	-	expression tag	UNP Q91UM2
K	-6	LEU	-	expression tag	UNP Q91UM2
K	-5	VAL	-	expression tag	UNP Q91UM2
K	-4	PRO	-	expression tag	UNP Q91UM2
K	-3	ARG	-	expression tag	UNP Q91UM2
K	-2	GLY	-	expression tag	UNP Q91UM2
K	-1	SER	-	expression tag	UNP Q91UM2
K	0	HIS	-	expression tag	UNP Q91UM2
K	17	ASN	ASP	engineered mutation	UNP Q91UM2
L	-19	MET	-	expression tag	UNP Q91UM2
L	-18	GLY	-	expression tag	UNP Q91UM2
L	-17	SER	-	expression tag	UNP Q91UM2
L	-16	SER	-	expression tag	UNP Q91UM2
L	-15	HIS	-	expression tag	UNP Q91UM2
L	-14	HIS	-	expression tag	UNP Q91UM2
L	-13	HIS	-	expression tag	UNP Q91UM2
L	-12	HIS	-	expression tag	UNP Q91UM2
L	-11	HIS	-	expression tag	UNP Q91UM2
L	-10	HIS	-	expression tag	UNP Q91UM2
L	-9	SER	-	expression tag	UNP Q91UM2
L	-8	SER	-	expression tag	UNP Q91UM2
L	-7	GLY	-	expression tag	UNP Q91UM2
L	-6	LEU	-	expression tag	UNP Q91UM2
L	-5	VAL	-	expression tag	UNP Q91UM2
L	-4	PRO	-	expression tag	UNP Q91UM2
L	-3	ARG	-	expression tag	UNP Q91UM2
L	-2	GLY	-	expression tag	UNP Q91UM2
L	-1	SER	-	expression tag	UNP Q91UM2
L	0	HIS	-	expression tag	UNP Q91UM2
L	17	ASN	ASP	engineered mutation	UNP Q91UM2

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O S 4 2 1 1	0	0
2	B	1	Total C O S 4 2 1 1	0	0
2	B	1	Total C O S 4 2 1 1	0	0
2	B	1	Total C O S 4 2 1 1	0	0
2	E	1	Total C O S 4 2 1 1	0	0
2	F	1	Total C O S 4 2 1 1	0	0
2	G	1	Total C O S 4 2 1 1	0	0
2	H	1	Total C O S 4 2 1 1	0	0
2	H	1	Total C O S 4 2 1 1	0	0
2	J	1	Total C O S 4 2 1 1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0
3	B	2	Total K 2 2	0	0

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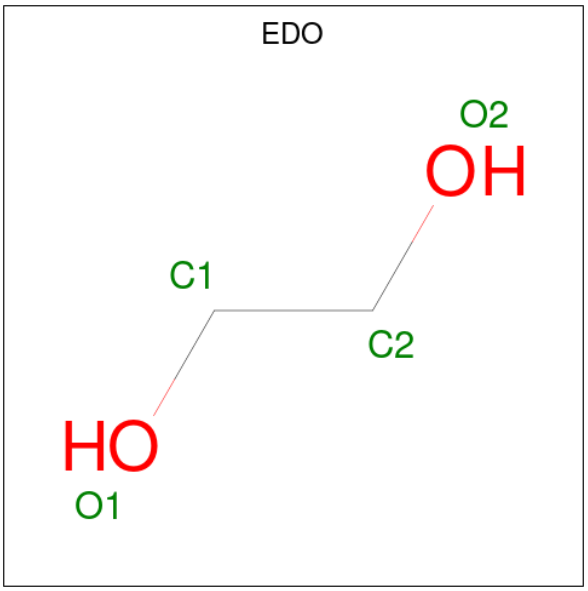
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total K 1 1	0	0
3	D	1	Total K 1 1	0	0
3	E	2	Total K 2 2	0	0
3	F	1	Total K 1 1	0	0
3	G	1	Total K 1 1	0	0
3	J	1	Total K 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0
4	B	3	Total Cl 3 3	0	0
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	E	2	Total Cl 2 2	0	0
4	F	1	Total Cl 1 1	0	0
4	G	2	Total Cl 2 2	0	0
4	H	1	Total Cl 1 1	0	0
4	K	1	Total Cl 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		

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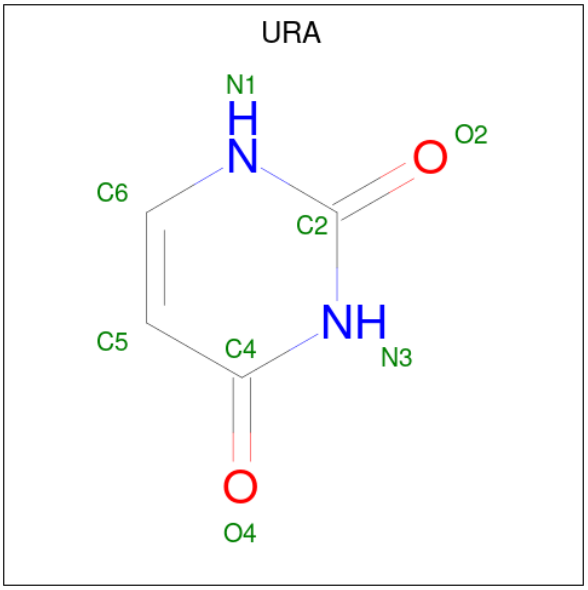
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	1	Total C O 4 2 2	0	0
5	L	1	Total C O 4 2 2	0	0

- Molecule 6 is URACIL (three-letter code: URA) (formula: $C_4H_4N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 8 4 2 2	0	0
6	B	1	Total C N O 8 4 2 2	0	0
6	C	1	Total C N O 8 4 2 2	0	0
6	D	1	Total C N O 8 4 2 2	0	0
6	E	1	Total C N O 8 4 2 2	0	0
6	F	1	Total C N O 8 4 2 2	0	0
6	G	1	Total C N O 8 4 2 2	0	0
6	H	1	Total C N O 8 4 2 2	0	0
6	I	1	Total C N O 8 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total C N O 8 4 2 2	0	0
6	K	1	Total C N O 8 4 2 2	0	0
6	L	1	Total C N O 8 4 2 2	0	0

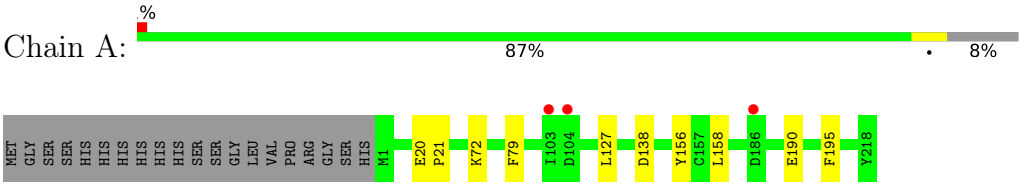
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	233	Total O 233 233	0	0
7	B	200	Total O 200 200	0	0
7	C	94	Total O 94 94	0	0
7	D	96	Total O 96 96	0	0
7	E	178	Total O 178 178	0	0
7	F	186	Total O 186 186	0	0
7	G	143	Total O 143 143	0	0
7	H	133	Total O 133 133	0	0
7	I	100	Total O 100 100	0	0
7	J	108	Total O 108 108	0	0
7	K	68	Total O 68 68	0	0
7	L	78	Total O 78 78	0	0

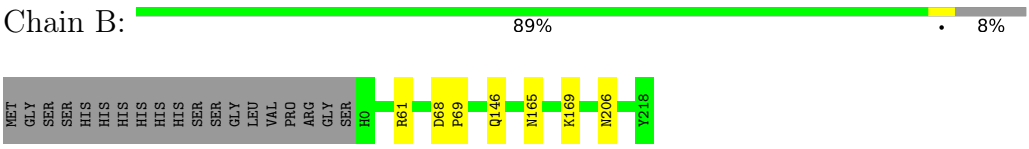
3 Residue-property plots (i)

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.

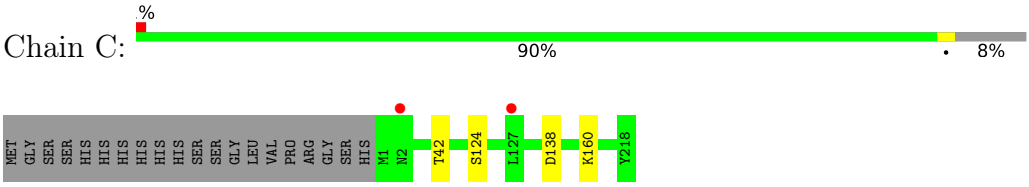
• Molecule 1: Uracil-DNA glycosylase



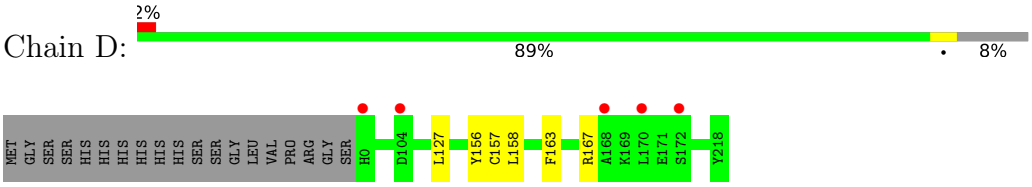
• Molecule 1: Uracil-DNA glycosylase



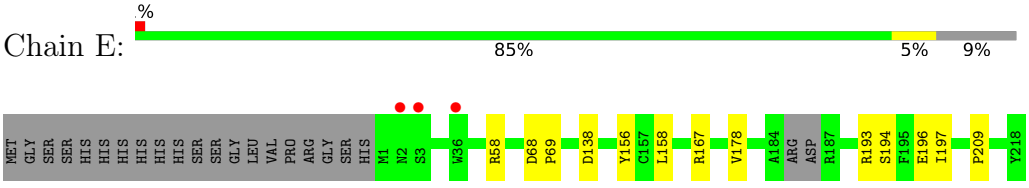
• Molecule 1: Uracil-DNA glycosylase



• Molecule 1: Uracil-DNA glycosylase

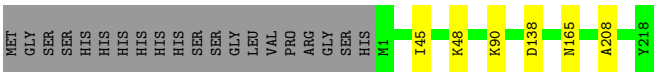


• Molecule 1: Uracil-DNA glycosylase



• Molecule 1: Uracil-DNA glycosylase

Chain F:

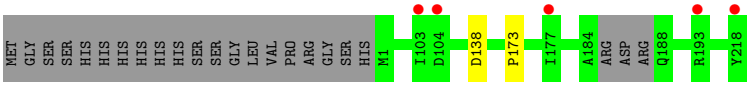


• Molecule 1: Uracil-DNA glycosylase

Chain G:

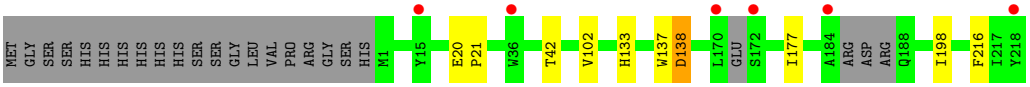
• Molecule 1: Uracil-DNA glycosylase

Chain H:



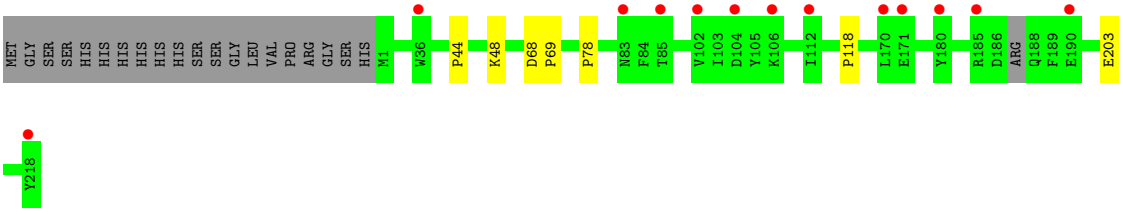
• Molecule 1: Uracil-DNA glycosylase

Chain I:



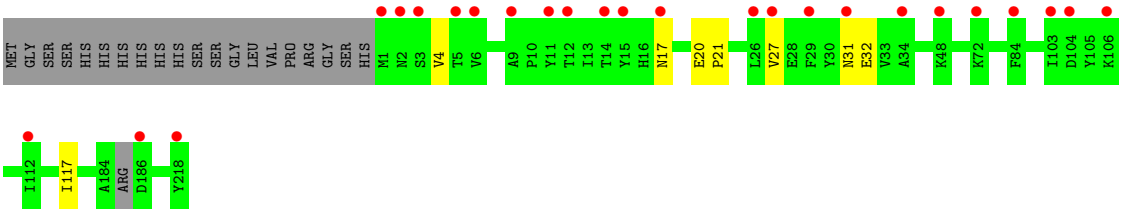
• Molecule 1: Uracil-DNA glycosylase

Chain J:



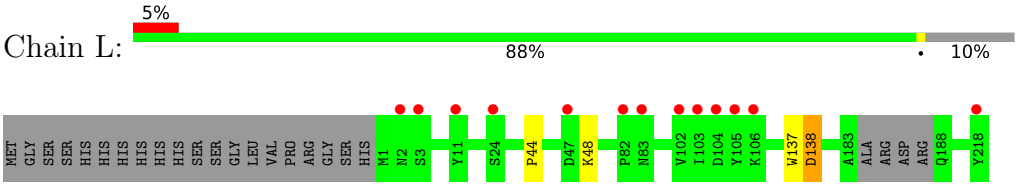
• Molecule 1: Uracil-DNA glycosylase

Chain K:



• Molecule 1: Uracil-DNA glycosylase

Chain L:


5%
88%
10%
MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS M1 N2 S3 Y11 S24 P44 D47 K48 P82 N83 V102 I103 D104 Y105 K106 W137 D138 A183 ALA ARG ASP ARG Q188 Y218

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.47Å 114.05Å 302.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.64 – 2.03 49.64 – 2.03	Depositor EDS
% Data completeness (in resolution range)	94.9 (49.64-2.03) 94.9 (49.64-2.03)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.213 , 0.246 0.217 , 0.247	Depositor DCC
R_{free} test set	10025 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23231	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: URA, K, DMS, CL, EDO

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	0.36	0/1845	0.55	0/2509
1	B	0.34	0/1861	0.55	0/2530
1	C	0.29	0/1819	0.48	0/2474
1	D	0.30	0/1876	0.50	0/2550
1	E	0.34	0/1822	0.55	0/2476
1	F	0.33	0/1857	0.53	0/2525
1	G	0.31	0/1842	0.52	0/2505
1	H	0.31	0/1796	0.49	0/2443
1	I	0.31	0/1793	0.50	0/2437
1	J	0.30	0/1828	0.50	0/2486
1	K	0.28	0/1838	0.47	0/2500
1	L	0.30	0/1798	0.49	0/2447
All	All	0.32	0/21975	0.51	0/29882

There are no bond length outliers.

There are no bond angle outliers.

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	1796	0	1785	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1812	0	1800	8	0
1	C	1770	0	1768	2	0
1	D	1827	0	1815	3	0
1	E	1774	0	1770	10	0
1	F	1808	0	1799	4	0
1	G	1792	0	1783	6	0
1	H	1748	0	1742	1	0
1	I	1746	0	1741	5	0
1	J	1780	0	1769	4	0
1	K	1787	0	1777	6	0
1	L	1750	0	1743	2	0
2	A	4	0	6	0	0
2	B	12	0	18	7	0
2	E	4	0	6	0	0
2	F	4	0	6	0	0
2	G	4	0	6	0	0
2	H	8	0	12	0	0
2	J	4	0	6	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	J	1	0	0	0	0
4	A	2	0	0	0	0
4	B	3	0	0	1	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
5	A	12	0	18	0	0
5	B	12	0	18	0	0
5	D	8	0	12	0	0
5	E	4	0	6	0	0
5	F	4	0	6	0	0
5	G	8	0	12	0	0
5	I	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	4	0	6	0	0
5	L	4	0	6	0	0
6	A	8	0	3	0	0
6	B	8	0	3	0	0
6	C	8	0	3	0	0
6	D	8	0	3	0	0
6	E	8	0	3	0	0
6	F	8	0	3	0	0
6	G	8	0	3	0	0
6	H	8	0	3	0	0
6	I	8	0	3	0	0
6	J	8	0	3	0	0
6	K	8	0	3	0	0
6	L	8	0	3	0	0
7	A	233	0	0	1	0
7	B	200	0	0	3	0
7	C	94	0	0	1	0
7	D	96	0	0	0	0
7	E	178	0	0	0	0
7	F	186	0	0	1	0
7	G	143	0	0	0	0
7	H	133	0	0	0	0
7	I	100	0	0	0	0
7	J	108	0	0	0	0
7	K	68	0	0	0	0
7	L	78	0	0	0	0
All	All	23231	0	21484	53	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 1.

The worst 5 of 53 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:B:169:LYS:HE3	2:B:303:DMS:H21	1.74	0.70
1:A:195:PHE:O	7:A:544:HOH:O	2.10	0.69
1:A:190:GLU:OE1	1:E:58:ARG:NH1	2.30	0.63
1:B:146:GLN:NE2	7:B:458:HOH:O	2.28	0.58
1:K:17[B]:ASN:OD1	1:K:17[B]:ASN:O	2.25	0.54

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	219/238 (92%)	216 (99%)	2 (1%)	1 (0%)	29	22
1	B	222/238 (93%)	217 (98%)	5 (2%)	0	100	100
1	C	216/238 (91%)	210 (97%)	5 (2%)	1 (0%)	29	22
1	D	223/238 (94%)	217 (97%)	5 (2%)	1 (0%)	34	28
1	E	215/238 (90%)	210 (98%)	4 (2%)	1 (0%)	29	22
1	F	221/238 (93%)	216 (98%)	4 (2%)	1 (0%)	29	22
1	G	219/238 (92%)	214 (98%)	5 (2%)	0	100	100
1	H	212/238 (89%)	207 (98%)	4 (2%)	1 (0%)	29	22
1	I	210/238 (88%)	200 (95%)	9 (4%)	1 (0%)	29	22
1	J	216/238 (91%)	207 (96%)	9 (4%)	0	100	100
1	K	217/238 (91%)	211 (97%)	6 (3%)	0	100	100
1	L	212/238 (89%)	207 (98%)	4 (2%)	1 (0%)	29	22
All	All	2602/2856 (91%)	2532 (97%)	62 (2%)	8 (0%)	41	36

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	138	ASP
1	H	138	ASP
1	I	138	ASP
1	L	138	ASP
1	A	138	ASP

5.3.2 Protein sidechains (i)

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	202/216 (94%)	202 (100%)	0	100	100
1	B	204/216 (94%)	204 (100%)	0	100	100
1	C	199/216 (92%)	199 (100%)	0	100	100
1	D	205/216 (95%)	205 (100%)	0	100	100
1	E	200/216 (93%)	200 (100%)	0	100	100
1	F	204/216 (94%)	204 (100%)	0	100	100
1	G	202/216 (94%)	201 (100%)	1 (0%)	88	91
1	H	197/216 (91%)	197 (100%)	0	100	100
1	I	197/216 (91%)	197 (100%)	0	100	100
1	J	201/216 (93%)	201 (100%)	0	100	100
1	K	202/216 (94%)	202 (100%)	0	100	100
1	L	198/216 (92%)	198 (100%)	0	100	100
All	All	2411/2592 (93%)	2410 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	35	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 62 ligands modelled in this entry, 24 are monoatomic - leaving 38 for Mogul analysis.

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	$\#\|Z\| > 2$
6	URA	E	307	-	8,8,8	1.77	3 (37%)	9,10,10	3.07	6 (66%)
5	EDO	F	304	-	3,3,3	0.46	0	2,2,2	0.25	0
5	EDO	A	306	-	3,3,3	0.42	0	2,2,2	0.23	0
5	EDO	D	303	-	3,3,3	0.38	0	2,2,2	0.42	0
5	EDO	I	302	-	3,3,3	0.45	0	2,2,2	0.25	0
6	URA	F	305	-	8,8,8	1.65	3 (37%)	9,10,10	3.21	6 (66%)
2	DMS	E	301	-	3,3,3	0.51	0	3,3,3	0.68	0
6	URA	B	312	-	8,8,8	1.76	3 (37%)	9,10,10	3.33	6 (66%)
5	EDO	B	309	3	3,3,3	0.46	0	2,2,2	0.07	0
6	URA	K	303	-	8,8,8	1.59	3 (37%)	9,10,10	3.50	6 (66%)
5	EDO	G	304	-	3,3,3	0.18	0	2,2,2	1.25	0
5	EDO	A	305	-	3,3,3	0.27	0	2,2,2	0.96	0
5	EDO	B	310	-	3,3,3	0.43	0	2,2,2	0.32	0
2	DMS	G	302	-	3,3,3	0.53	0	3,3,3	0.59	0
5	EDO	D	304	-	3,3,3	0.46	0	2,2,2	0.46	0
6	URA	C	303	-	8,8,8	1.70	2 (25%)	9,10,10	3.09	6 (66%)
5	EDO	A	307	-	3,3,3	0.41	0	2,2,2	0.32	0
6	URA	G	306	-	8,8,8	1.71	2 (25%)	9,10,10	3.17	6 (66%)
6	URA	H	304	-	8,8,8	1.63	3 (37%)	9,10,10	3.27	6 (66%)
6	URA	I	303	-	8,8,8	1.81	2 (25%)	9,10,10	3.18	6 (66%)
5	EDO	K	302	-	3,3,3	0.44	0	2,2,2	0.38	0
2	DMS	H	303	-	3,3,3	0.57	0	3,3,3	0.44	0
2	DMS	J	302	-	3,3,3	0.56	0	3,3,3	0.54	0
5	EDO	L	301	-	3,3,3	0.44	0	2,2,2	0.40	0
2	DMS	B	301	-	3,3,3	0.50	0	3,3,3	0.53	0
6	URA	J	301	-	8,8,8	1.73	2 (25%)	9,10,10	2.72	5 (55%)
2	DMS	F	301	-	3,3,3	0.58	0	3,3,3	0.64	0
6	URA	L	302	-	8,8,8	1.78	4 (50%)	9,10,10	2.84	5 (55%)
5	EDO	E	306	-	3,3,3	0.27	0	2,2,2	1.33	0
2	DMS	A	301	-	3,3,3	0.54	0	3,3,3	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	DMS	B	303	-	3,3,3	0.71	0	3,3,3	0.49	0
5	EDO	I	301	-	3,3,3	0.43	0	2,2,2	0.33	0
2	DMS	H	302	-	3,3,3	0.50	0	3,3,3	0.56	0
5	EDO	G	307	-	3,3,3	0.23	0	2,2,2	0.49	0
6	URA	A	308	-	8,8,8	1.54	2 (25%)	9,10,10	3.19	5 (55%)
5	EDO	B	311	-	3,3,3	0.29	0	2,2,2	1.62	0
2	DMS	B	302	-	3,3,3	0.64	0	3,3,3	0.47	0
6	URA	D	305	-	8,8,8	1.76	4 (50%)	9,10,10	3.00	6 (66%)

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
6	URA	E	307	-	-	-	0/1/1/1
5	EDO	F	304	-	-	1/1/1/1	-
5	EDO	A	306	-	-	1/1/1/1	-
5	EDO	D	303	-	-	1/1/1/1	-
5	EDO	I	302	-	-	1/1/1/1	-
6	URA	F	305	-	-	-	0/1/1/1
6	URA	B	312	-	-	-	0/1/1/1
5	EDO	B	309	3	-	1/1/1/1	-
6	URA	K	303	-	-	-	0/1/1/1
5	EDO	G	304	-	-	1/1/1/1	-
5	EDO	A	305	-	-	0/1/1/1	-
5	EDO	B	310	-	-	1/1/1/1	-
5	EDO	D	304	-	-	1/1/1/1	-
6	URA	C	303	-	-	-	0/1/1/1
5	EDO	A	307	-	-	0/1/1/1	-
6	URA	G	306	-	-	-	0/1/1/1
6	URA	H	304	-	-	-	0/1/1/1
6	URA	I	303	-	-	-	0/1/1/1
5	EDO	K	302	-	-	0/1/1/1	-
5	EDO	L	301	-	-	1/1/1/1	-
6	URA	J	301	-	-	-	0/1/1/1
6	URA	L	302	-	-	-	0/1/1/1
5	EDO	E	306	-	-	1/1/1/1	-
5	EDO	I	301	-	-	0/1/1/1	-
5	EDO	G	307	-	-	0/1/1/1	-
6	URA	A	308	-	-	-	0/1/1/1
5	EDO	B	311	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	URA	D	305	-	-	-	0/1/1/1

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	312	URA	C4-N3	-3.03	1.33	1.38
6	I	303	URA	C4-N3	-2.81	1.33	1.38
6	D	305	URA	C4-N3	-2.73	1.33	1.38
6	L	302	URA	C4-N3	-2.69	1.33	1.38
6	G	306	URA	C4-N3	-2.60	1.33	1.38

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	K	303	URA	C4-N3-C2	-5.57	120.18	125.70
6	B	312	URA	N1-C2-N3	5.55	121.41	115.13
6	G	306	URA	C4-N3-C2	-5.37	120.37	125.70
6	I	303	URA	N1-C2-N3	5.29	121.12	115.13
6	K	303	URA	N1-C2-N3	5.29	121.12	115.13

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	311	EDO	O1-C1-C2-O2
5	E	306	EDO	O1-C1-C2-O2
5	B	310	EDO	O1-C1-C2-O2
5	F	304	EDO	O1-C1-C2-O2
5	I	302	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	303	DMS	3	0
2	B	302	DMS	4	0

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, 95^{th} 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	218/238 (91%)	0.20	3 (1%) 75 74	13, 22, 35, 59	0
1	B	219/238 (92%)	0.27	0 100 100	14, 21, 34, 53	0
1	C	218/238 (91%)	0.35	2 (0%) 84 83	25, 35, 49, 71	0
1	D	219/238 (92%)	0.36	5 (2%) 60 59	21, 31, 52, 68	0
1	E	216/238 (90%)	0.24	3 (1%) 75 74	14, 24, 40, 48	0
1	F	218/238 (91%)	0.19	0 100 100	14, 25, 36, 51	0
1	G	219/238 (92%)	0.19	4 (1%) 68 67	18, 28, 46, 66	0
1	H	215/238 (90%)	0.26	5 (2%) 60 59	21, 32, 50, 61	0
1	I	214/238 (89%)	0.46	6 (2%) 53 52	24, 34, 50, 58	0
1	J	217/238 (91%)	0.50	13 (5%) 21 21	22, 36, 57, 72	0
1	K	217/238 (91%)	0.77	25 (11%) 4 4	25, 42, 58, 73	0
1	L	214/238 (89%)	0.63	13 (6%) 21 20	24, 40, 57, 64	0
All	All	2604/2856 (91%)	0.37	79 (3%) 50 50	13, 31, 51, 73	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	103	ILE	7.2
1	H	103	ILE	4.4
1	I	218	TYR	4.0
1	K	3	SER	4.0
1	J	104	ASP	3.9

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	D	304	4/4	0.68	0.28	39,41,41,41	0
5	EDO	D	303	4/4	0.76	0.22	47,48,49,50	0
5	EDO	A	307	4/4	0.81	0.22	41,41,41,41	0
5	EDO	G	307	4/4	0.81	0.19	50,50,50,51	0
5	EDO	B	310	4/4	0.83	0.19	47,47,47,48	0
2	DMS	B	302	4/4	0.84	0.21	30,32,32,34	0
5	EDO	L	301	4/4	0.84	0.23	42,43,43,45	0
5	EDO	B	309	4/4	0.86	0.23	23,24,25,26	0
5	EDO	A	305	4/4	0.87	0.21	51,51,51,52	0
5	EDO	A	306	4/4	0.87	0.21	48,49,49,50	0
5	EDO	K	302	4/4	0.87	0.15	41,41,42,42	0
2	DMS	A	301	4/4	0.87	0.16	65,65,66,67	0
5	EDO	I	301	4/4	0.89	0.14	48,48,49,49	0
3	K	D	301	1/1	0.90	0.09	51,51,51,51	0
5	EDO	F	304	4/4	0.90	0.15	44,45,46,48	0
2	DMS	G	302	4/4	0.91	0.18	49,49,51,51	0
2	DMS	H	303	4/4	0.91	0.16	57,57,59,60	0
5	EDO	I	302	4/4	0.91	0.19	44,44,44,45	0
5	EDO	E	306	4/4	0.91	0.19	50,51,52,52	0
2	DMS	J	302	4/4	0.91	0.19	58,59,59,61	0
6	URA	H	304	8/8	0.91	0.16	25,27,29,30	0
2	DMS	B	303	4/4	0.93	0.22	39,39,39,42	0
5	EDO	G	304	4/4	0.93	0.12	52,52,53,53	0
2	DMS	H	302	4/4	0.93	0.17	46,46,46,46	0
5	EDO	B	311	4/4	0.93	0.10	61,61,62,63	0
6	URA	A	308	8/8	0.94	0.12	22,24,25,25	0
6	URA	I	303	8/8	0.94	0.14	33,33,34,35	0
6	URA	L	302	8/8	0.94	0.13	28,29,30,30	0
6	URA	B	312	8/8	0.95	0.12	19,20,20,21	0
6	URA	C	303	8/8	0.95	0.12	28,29,30,30	0
6	URA	D	305	8/8	0.95	0.10	28,29,29,30	0
4	CL	H	301	1/1	0.95	0.16	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	K	B	305	1/1	0.95	0.08	38,38,38,38	0
6	URA	J	301	8/8	0.95	0.14	29,30,31,31	0
2	DMS	B	301	4/4	0.95	0.12	30,30,31,31	0
6	URA	E	307	8/8	0.96	0.09	20,21,21,22	0
6	URA	F	305	8/8	0.96	0.11	19,22,23,23	0
6	URA	G	306	8/8	0.96	0.11	18,18,18,18	0
2	DMS	F	301	4/4	0.96	0.14	37,37,38,39	0
3	K	E	303	1/1	0.96	0.10	40,40,40,40	0
4	CL	D	302	1/1	0.96	0.08	39,39,39,39	0
6	URA	K	303	8/8	0.96	0.12	30,32,33,33	0
3	K	C	301	1/1	0.96	0.07	42,42,42,42	0
3	K	J	303	1/1	0.97	0.07	43,43,43,43	0
3	K	A	302	1/1	0.97	0.10	42,42,42,42	0
4	CL	G	301	1/1	0.97	0.08	36,36,36,36	0
3	K	G	303	1/1	0.97	0.08	34,34,34,34	0
2	DMS	E	301	4/4	0.98	0.15	38,39,40,40	0
4	CL	E	304	1/1	0.98	0.10	29,29,29,29	0
4	CL	E	305	1/1	0.98	0.09	38,38,38,38	0
3	K	F	302	1/1	0.98	0.11	41,41,41,41	0
4	CL	G	305	1/1	0.98	0.07	37,37,37,37	0
4	CL	B	308	1/1	0.98	0.07	36,36,36,36	0
4	CL	K	301	1/1	0.98	0.09	39,39,39,39	0
4	CL	A	304	1/1	0.99	0.17	36,36,36,36	0
4	CL	B	306	1/1	0.99	0.14	15,15,15,15	0
4	CL	B	307	1/1	0.99	0.08	25,25,25,25	0
4	CL	F	303	1/1	0.99	0.09	26,26,26,26	0
4	CL	A	303	1/1	0.99	0.11	30,30,30,30	0
4	CL	C	302	1/1	0.99	0.10	39,39,39,39	0
3	K	B	304	1/1	1.00	0.09	16,16,16,16	0
3	K	E	302	1/1	1.00	0.08	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.