



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:41 PM GMT

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 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
<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

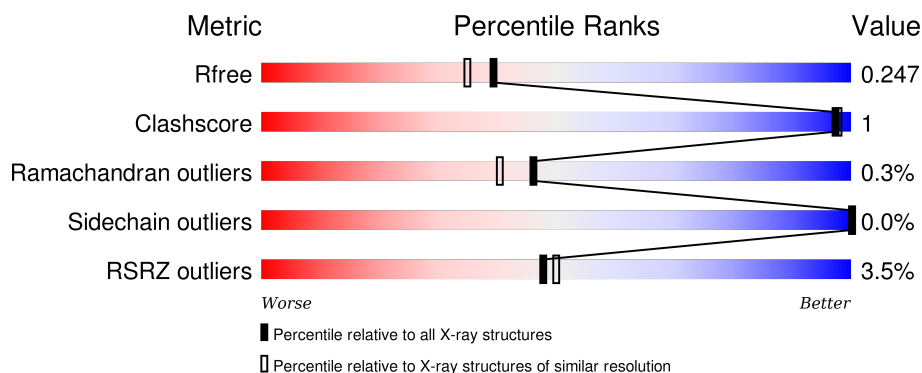
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (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 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	<div> <div>87%</div> <div>8%</div> </div>
1	B	238	<div> <div>89%</div> <div>8%</div> </div>
1	C	238	<div> <div>2%</div> <div>90%</div> <div>8%</div> </div>
1	D	238	<div> <div>4%</div> <div>89%</div> <div>8%</div> </div>
1	E	238	<div> <div>85%</div> <div>5%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	238	
1	G	238	
1	H	238	
1	I	238	
1	J	238	
1	K	238	
1	L	238	

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	X
2	DMS	B	303	-	-	-	X
5	EDO	B	309	-	-	-	X
5	EDO	L	301	-	-	-	X

2 Entry composition

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
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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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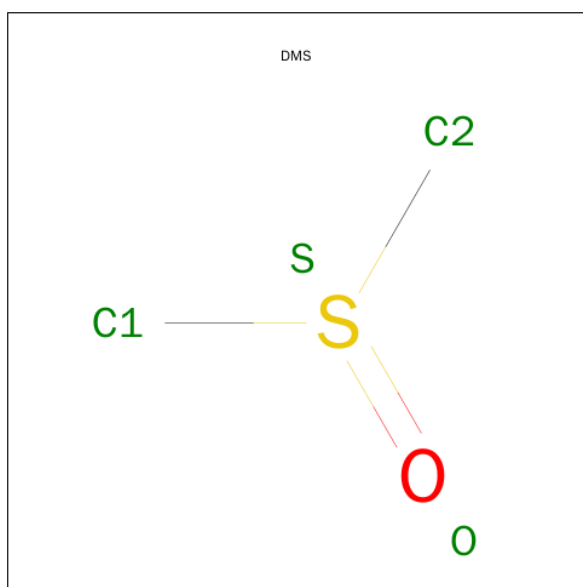
Chain	Residue	Modelled	Actual	Comment	Reference
I	-14	HIS	-	EXPRESSION TAG	UNP Q91UM2
I	-13	HIS	-	EXPRESSION TAG	UNP Q91UM2
I	-12	HIS	-	EXPRESSION TAG	UNP Q91UM2
I	-11	HIS	-	EXPRESSION TAG	UNP Q91UM2
I	-10	HIS	-	EXPRESSION TAG	UNP Q91UM2
I	-9	SER	-	EXPRESSION TAG	UNP Q91UM2
I	-8	SER	-	EXPRESSION TAG	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: C₂H₆OS).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	K	0	0
			1	1		
3	J	1	Total	K	0	0
			1	1		

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



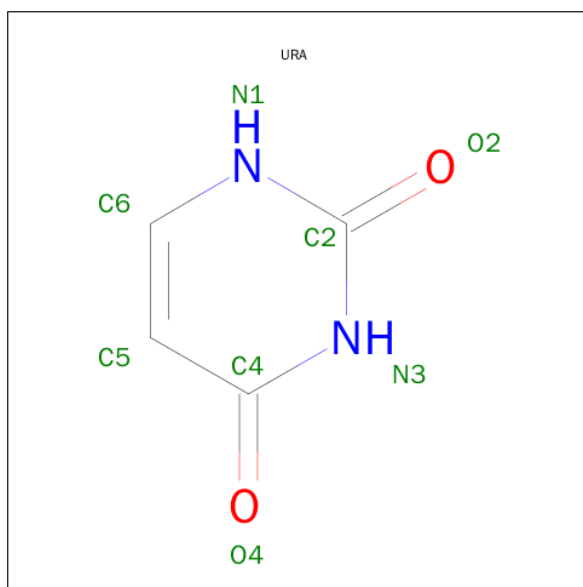
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total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

- 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	0	0
			8	4	2	2		
6	B	1	Total	C	N	O	0	0
			8	4	2	2		
6	C	1	Total	C	N	O	0	0
			8	4	2	2		
6	D	1	Total	C	N	O	0	0
			8	4	2	2		
6	E	1	Total	C	N	O	0	0
			8	4	2	2		
6	F	1	Total	C	N	O	0	0
			8	4	2	2		
6	H	1	Total	C	N	O	0	0
			8	4	2	2		
6	J	1	Total	C	N	O	0	0
			8	4	2	2		
6	G	1	Total	C	N	O	0	0
			8	4	2	2		

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

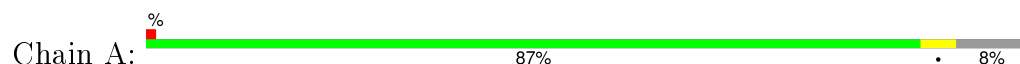
- Molecule 7 is water.

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

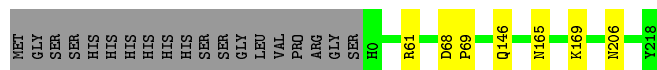
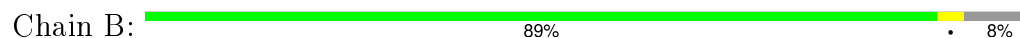
3 Residue-property plots [i](#)

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.

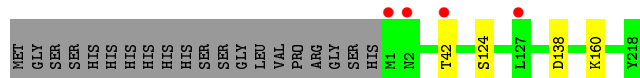
- Molecule 1: Uracil-DNA glycosylase



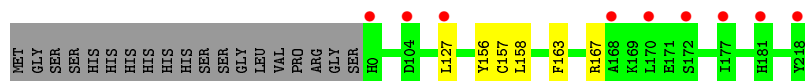
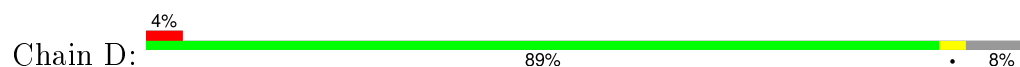
- Molecule 1: Uracil-DNA glycosylase



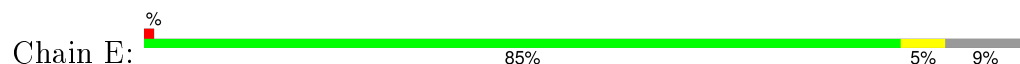
- Molecule 1: Uracil-DNA glycosylase



- Molecule 1: Uracil-DNA glycosylase

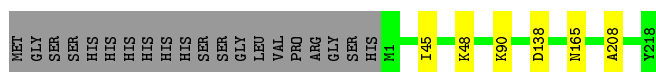


- Molecule 1: Uracil-DNA glycosylase

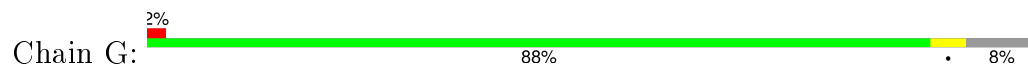


- Molecule 1: Uracil-DNA glycosylase

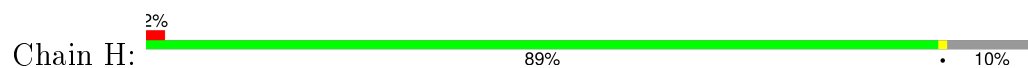




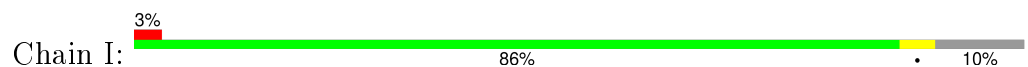
- Molecule 1: Uracil-DNA glycosylase



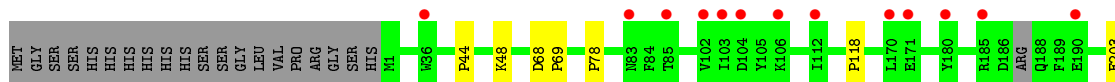
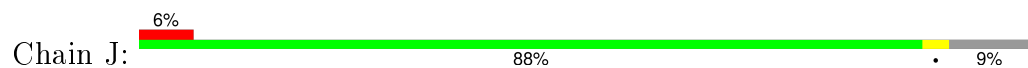
- Molecule 1: Uracil-DNA glycosylase



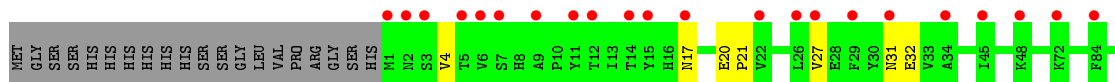
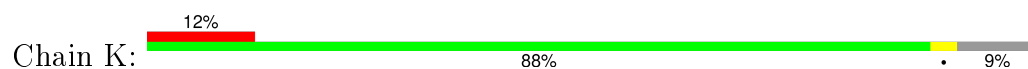
- Molecule 1: Uracil-DNA glycosylase



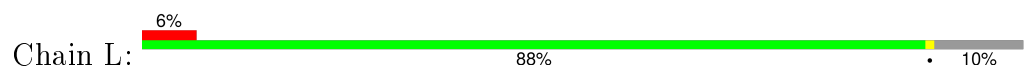
- Molecule 1: Uracil-DNA glycosylase

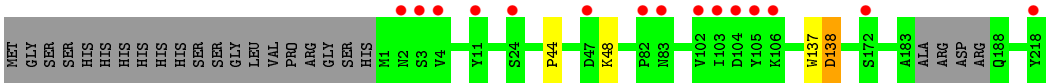


- Molecule 1: Uracil-DNA glycosylase



- Molecule 1: Uracil-DNA glycosylase





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	10022 reflections (5.32%)	DCC
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 , 43.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 198460 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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

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.

All (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:O	1:K:17[B]:ASN:OD1	2.25	0.54
1:G:193:ARG:NH2	1:J:203:GLU:OE2	2.41	0.53
1:B:165[A]:ASN:ND2	7:B:557:HOH:O	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ASN:OD1	7:B:454:HOH:O	2.19	0.52
1:G:180:TYR:CZ	1:G:188:GLN:HG2	2.45	0.51
1:A:79:PHE:CZ	1:A:158:LEU:HD12	2.46	0.51
1:F:45:ILE:HD11	1:F:48:LYS:HG2	1.93	0.51
1:K:31[A]:ASN:C	1:K:31[A]:ASN:OD1	2.48	0.50
1:K:4:VAL:HG11	1:K:27:VAL:HG21	1.94	0.49
2:B:302:DMS:C2	1:E:178:VAL:H	2.26	0.49
1:D:156:TYR:CZ	1:D:158:LEU:HD21	2.48	0.48
1:A:20:GLU:HB3	1:A:21:PRO:HD3	1.94	0.48
1:E:209:PRO:HG2	1:F:208:ALA:HB2	1.93	0.48
1:G:158:LEU:HD22	1:G:182:PRO:HD3	1.95	0.48
1:B:169:LYS:HE3	2:B:303:DMS:C2	2.41	0.48
1:E:193[B]:ARG:HD2	1:E:196:GLU:OE1	2.14	0.47
1:A:72:LYS:HD2	1:A:127:LEU:HD11	1.97	0.47
1:L:44:PRO:HB2	1:L:48:LYS:HB2	1.97	0.46
2:B:302:DMS:H21	1:E:178:VAL:H	1.82	0.45
1:I:102:VAL:CG1	1:I:216:PHE:CE2	3.00	0.45
1:A:156:TYR:CZ	1:A:158:LEU:HD21	2.52	0.45
2:B:302:DMS:H23	1:E:167:ARG:HH22	1.81	0.45
1:B:169:LYS:CE	2:B:303:DMS:H21	2.44	0.45
1:C:42:THR:CG2	1:C:124:SER:HB2	2.46	0.44
1:K:31[A]:ASN:OD1	1:K:32:GLU:N	2.52	0.43
1:I:177:ILE:HD11	1:I:198:ILE:HG13	2.01	0.43
1:J:68:ASP:HB2	1:J:69:PRO:CD	2.50	0.42
1:G:180:TYR:CE1	1:G:188:GLN:HG2	2.55	0.42
1:F:90:LYS:NZ	7:F:572:HOH:O	2.52	0.42
1:E:68:ASP:HB2	1:E:69:PRO:CD	2.50	0.42
1:I:137:TRP:O	1:I:138:ASP:C	2.58	0.42
1:E:156:TYR:CZ	1:E:158:LEU:HD21	2.55	0.41
1:G:61:ARG:NE	1:G:208:ALA:O	2.51	0.41
1:F:165[B]:ASN:N	1:F:165[B]:ASN:OD1	2.53	0.41
1:K:117:ILE:O	1:K:117:ILE:HG23	2.20	0.41
1:I:42:THR:HG22	1:I:133:HIS:HE1	1.85	0.41
1:G:19:TRP:O	1:G:22:VAL:HG22	2.19	0.41
1:B:68:ASP:HB2	1:B:69:PRO:CD	2.51	0.41
1:B:61:ARG:HD3	4:B:308:CL:CL	2.58	0.41
1:C:160:LYS:NZ	7:C:440:HOH:O	2.46	0.40
1:I:20:GLU:HB3	1:I:21:PRO:HD3	2.03	0.40
1:D:167:ARG:CZ	1:H:173:PRO:HA	2.51	0.40
1:J:78:PRO:HB2	1:J:118:PRO:HB2	2.03	0.40
1:J:44:PRO:HB2	1:J:48:LYS:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:20:GLU:HB3	1:K:21:PRO:HD3	2.03	0.40
2:B:302:DMS:C2	1:E:167:ARG:HH22	2.34	0.40
1:E:194:SER:O	1:E:197:ILE:HG22	2.21	0.40
1:D:157:CYS:HB3	1:D:163:PHE:CD2	2.56	0.40
1:L:137:TRP:O	1:L:138:ASP:C	2.60	0.40

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%)	34	26
1	B	222/238 (93%)	217 (98%)	5 (2%)	0	100	100
1	C	216/238 (91%)	210 (97%)	5 (2%)	1 (0%)	34	26
1	D	223/238 (94%)	217 (97%)	5 (2%)	1 (0%)	39	32
1	E	215/238 (90%)	210 (98%)	4 (2%)	1 (0%)	34	26
1	F	221/238 (93%)	216 (98%)	4 (2%)	1 (0%)	34	26
1	G	219/238 (92%)	214 (98%)	5 (2%)	0	100	100
1	H	212/238 (89%)	207 (98%)	4 (2%)	1 (0%)	34	26
1	I	210/238 (88%)	200 (95%)	9 (4%)	1 (0%)	34	26
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%)	34	26
All	All	2602/2856 (91%)	2532 (97%)	62 (2%)	8 (0%)	46	40

All (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
1	C	138	ASP
1	E	138	ASP
1	D	127	LEU

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	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%)	92	94
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

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	$\# Z > 2$
2	DMS	A	301	-	3,3,3	0.50	0	3,3,3	0.52	0
5	EDO	A	305	-	3,3,3	0.26	0	2,2,2	1.05	0
5	EDO	A	306	-	3,3,3	0.44	0	2,2,2	0.32	0
5	EDO	A	307	-	3,3,3	0.43	0	2,2,2	0.37	0
6	URA	A	308	-	4,8,8	0.50	0	6,10,10	8.46	4 (66%)
2	DMS	B	301	-	3,3,3	0.47	0	3,3,3	0.48	0
2	DMS	B	302	-	3,3,3	0.60	0	3,3,3	0.43	0
2	DMS	B	303	-	3,3,3	0.67	0	3,3,3	0.46	0
5	EDO	B	309	3	3,3,3	0.47	0	2,2,2	0.12	0
5	EDO	B	310	-	3,3,3	0.44	0	2,2,2	0.41	0
5	EDO	B	311	-	3,3,3	0.28	0	2,2,2	1.72	0
6	URA	B	312	-	4,8,8	0.27	0	6,10,10	7.25	4 (66%)
6	URA	C	303	-	4,8,8	0.32	0	6,10,10	8.23	4 (66%)
5	EDO	D	303	-	3,3,3	0.39	0	2,2,2	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	D	304	-	3,3,3	0.47	0	2,2,2	0.51	0
6	URA	D	305	-	4,8,8	0.26	0	6,10,10	7.84	4 (66%)
2	DMS	E	301	-	3,3,3	0.48	0	3,3,3	0.61	0
5	EDO	E	306	-	3,3,3	0.26	0	2,2,2	1.42	0
6	URA	E	307	-	4,8,8	0.23	0	6,10,10	8.01	4 (66%)
2	DMS	F	301	-	3,3,3	0.54	0	3,3,3	0.59	0
5	EDO	F	304	-	3,3,3	0.47	0	2,2,2	0.34	0
6	URA	F	305	-	4,8,8	0.52	0	6,10,10	7.75	4 (66%)
2	DMS	G	302	-	3,3,3	0.49	0	3,3,3	0.54	0
5	EDO	G	304	-	3,3,3	0.20	0	2,2,2	1.34	0
6	URA	G	306	-	4,8,8	0.25	0	6,10,10	8.01	4 (66%)
5	EDO	G	307	-	3,3,3	0.24	0	2,2,2	0.57	0
2	DMS	H	302	-	3,3,3	0.46	0	3,3,3	0.52	0
2	DMS	H	303	-	3,3,3	0.54	0	3,3,3	0.40	0
6	URA	H	304	-	4,8,8	0.36	0	6,10,10	7.94	4 (66%)
5	EDO	I	301	-	3,3,3	0.45	0	2,2,2	0.42	0
5	EDO	I	302	-	3,3,3	0.46	0	2,2,2	0.34	0
6	URA	I	303	-	4,8,8	0.33	0	6,10,10	7.67	4 (66%)
6	URA	J	301	-	4,8,8	0.38	0	6,10,10	8.48	4 (66%)
2	DMS	J	302	-	3,3,3	0.52	0	3,3,3	0.51	0
5	EDO	K	302	-	3,3,3	0.45	0	2,2,2	0.46	0
6	URA	K	303	-	4,8,8	0.45	0	6,10,10	7.53	4 (66%)
5	EDO	L	301	-	3,3,3	0.45	0	2,2,2	0.48	0
6	URA	L	302	-	4,8,8	0.22	0	6,10,10	8.31	4 (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
2	DMS	A	301	-	-	0/0/0/0	0/0/0/0
5	EDO	A	305	-	-	0/1/1/1	0/0/0/0
5	EDO	A	306	-	-	0/1/1/1	0/0/0/0
5	EDO	A	307	-	-	0/1/1/1	0/0/0/0
6	URA	A	308	-	-	0/0/0/0	0/1/1/1
2	DMS	B	301	-	-	0/0/0/0	0/0/0/0
2	DMS	B	302	-	-	0/0/0/0	0/0/0/0
2	DMS	B	303	-	-	0/0/0/0	0/0/0/0
5	EDO	B	309	3	-	0/1/1/1	0/0/0/0
5	EDO	B	310	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	311	-	-	0/1/1/1	0/0/0/0
6	URA	B	312	-	-	0/0/0/0	0/1/1/1
6	URA	C	303	-	-	0/0/0/0	0/1/1/1
5	EDO	D	303	-	-	0/1/1/1	0/0/0/0
5	EDO	D	304	-	-	0/1/1/1	0/0/0/0
6	URA	D	305	-	-	0/0/0/0	0/1/1/1
2	DMS	E	301	-	-	0/0/0/0	0/0/0/0
5	EDO	E	306	-	-	0/1/1/1	0/0/0/0
6	URA	E	307	-	-	0/0/0/0	0/1/1/1
2	DMS	F	301	-	-	0/0/0/0	0/0/0/0
5	EDO	F	304	-	-	0/1/1/1	0/0/0/0
6	URA	F	305	-	-	0/0/0/0	0/1/1/1
2	DMS	G	302	-	-	0/0/0/0	0/0/0/0
5	EDO	G	304	-	-	0/1/1/1	0/0/0/0
6	URA	G	306	-	-	0/0/0/0	0/1/1/1
5	EDO	G	307	-	-	0/1/1/1	0/0/0/0
2	DMS	H	302	-	-	0/0/0/0	0/0/0/0
2	DMS	H	303	-	-	0/0/0/0	0/0/0/0
6	URA	H	304	-	-	0/0/0/0	0/1/1/1
5	EDO	I	301	-	-	0/1/1/1	0/0/0/0
5	EDO	I	302	-	-	0/1/1/1	0/0/0/0
6	URA	I	303	-	-	0/0/0/0	0/1/1/1
6	URA	J	301	-	-	0/0/0/0	0/1/1/1
2	DMS	J	302	-	-	0/0/0/0	0/0/0/0
5	EDO	K	302	-	-	0/1/1/1	0/0/0/0
6	URA	K	303	-	-	0/0/0/0	0/1/1/1
5	EDO	L	301	-	-	0/1/1/1	0/0/0/0
6	URA	L	302	-	-	0/0/0/0	0/1/1/1

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	301	URA	N1-C2-N3	-13.09	119.98	128.33
6	A	308	URA	N1-C2-N3	-13.06	120.00	128.33
6	L	302	URA	N1-C2-N3	-12.91	120.10	128.33
6	C	303	URA	N1-C2-N3	-12.45	120.39	128.33
6	E	307	URA	N1-C2-N3	-12.31	120.48	128.33
6	H	304	URA	N1-C2-N3	-12.22	120.54	128.33
6	G	306	URA	N1-C2-N3	-12.21	120.54	128.33
6	D	305	URA	N1-C2-N3	-12.07	120.64	128.33
6	F	305	URA	N1-C2-N3	-11.84	120.78	128.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	303	URA	N1-C2-N3	-11.31	121.12	128.33
6	I	303	URA	N1-C2-N3	-11.30	121.12	128.33
6	B	312	URA	N1-C2-N3	-10.84	121.41	128.33
6	B	312	URA	C5-C6-N1	-4.16	119.15	123.90
6	C	303	URA	C5-C6-N1	-4.06	119.26	123.90
6	I	303	URA	C5-C6-N1	-4.00	119.34	123.90
6	F	305	URA	C5-C6-N1	-3.98	119.36	123.90
6	E	307	URA	C5-C6-N1	-3.94	119.41	123.90
6	G	306	URA	C5-C6-N1	-3.93	119.41	123.90
6	K	303	URA	C5-C6-N1	-3.93	119.42	123.90
6	A	308	URA	C5-C6-N1	-3.92	119.43	123.90
6	H	304	URA	C5-C6-N1	-3.91	119.44	123.90
6	L	302	URA	C5-C6-N1	-3.87	119.49	123.90
6	J	301	URA	C5-C6-N1	-3.79	119.57	123.90
6	D	305	URA	C5-C6-N1	-3.66	119.72	123.90
6	K	303	URA	C4-N3-C2	6.09	120.18	114.14
6	G	306	URA	C4-N3-C2	6.29	120.37	114.14
6	A	308	URA	C4-N3-C2	6.38	120.46	114.14
6	H	304	URA	C4-N3-C2	6.39	120.47	114.14
6	I	303	URA	C4-N3-C2	6.48	120.56	114.14
6	B	312	URA	C4-N3-C2	6.62	120.70	114.14
6	C	303	URA	C4-N3-C2	6.69	120.77	114.14
6	F	305	URA	C4-N3-C2	6.76	120.83	114.14
6	E	307	URA	C4-N3-C2	6.85	120.93	114.14
6	D	305	URA	C4-N3-C2	7.01	121.08	114.14
6	L	302	URA	C4-N3-C2	7.15	121.22	114.14
6	J	301	URA	C4-N3-C2	7.25	121.32	114.14
6	B	312	URA	C6-N1-C2	11.56	120.09	114.40
6	F	305	URA	C6-N1-C2	12.50	120.55	114.40
6	K	303	URA	C6-N1-C2	12.53	120.56	114.40
6	D	305	URA	C6-N1-C2	12.60	120.60	114.40
6	I	303	URA	C6-N1-C2	12.84	120.72	114.40
6	E	307	URA	C6-N1-C2	12.98	120.78	114.40
6	H	304	URA	C6-N1-C2	13.08	120.84	114.40
6	G	306	URA	C6-N1-C2	13.39	120.99	114.40
6	L	302	URA	C6-N1-C2	13.41	121.00	114.40
6	C	303	URA	C6-N1-C2	13.72	121.15	114.40
6	J	301	URA	C6-N1-C2	13.81	121.20	114.40
6	A	308	URA	C6-N1-C2	14.17	121.37	114.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	302	DMS	4	0
2	B	303	DMS	3	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, 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	218/238 (91%)	0.26	3 (1%) 78 79	13, 22, 35, 59	0
1	B	219/238 (92%)	0.33	0 100 100	14, 21, 34, 53	0
1	C	218/238 (91%)	0.41	4 (1%) 71 72	25, 35, 49, 71	0
1	D	219/238 (92%)	0.42	9 (4%) 41 43	21, 31, 52, 68	0
1	E	216/238 (90%)	0.31	3 (1%) 78 79	14, 24, 40, 48	0
1	F	218/238 (91%)	0.24	0 100 100	14, 25, 36, 51	0
1	G	219/238 (92%)	0.25	4 (1%) 71 72	18, 28, 46, 66	0
1	H	215/238 (90%)	0.32	5 (2%) 64 65	21, 32, 50, 61	0
1	I	214/238 (89%)	0.53	6 (2%) 56 58	25, 34, 50, 58	0
1	J	217/238 (91%)	0.57	14 (6%) 22 23	22, 36, 57, 72	0
1	K	217/238 (91%)	0.85	28 (12%) 5 5	25, 42, 58, 73	0
1	L	214/238 (89%)	0.71	15 (7%) 19 21	24, 40, 57, 64	0
All	All	2604/2856 (91%)	0.43	91 (3%) 48 50	13, 31, 51, 73	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	103	ILE	7.6
1	H	103	ILE	4.6
1	K	3	SER	4.2
1	J	104	ASP	4.2
1	I	218	TYR	4.1
1	J	218	TYR	4.1
1	K	12	THR	3.7
1	K	15	TYR	3.6
1	J	185	ARG	3.5
1	J	83[A]	ASN	3.5
1	K	48	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	184	ALA	3.4
1	K	9	ALA	3.3
1	K	2	ASN	3.3
1	K	27	VAL	3.2
1	L	106	LYS	3.1
1	L	218	TYR	3.1
1	K	6	VAL	3.1
1	K	14	THR	3.0
1	H	193	ARG	2.9
1	K	31[A]	ASN	2.9
1	K	103	ILE	2.9
1	G	0	HIS	2.9
1	K	34	ALA	2.8
1	K	26	LEU	2.8
1	E	36	TRP	2.8
1	D	0	HIS	2.8
1	I	172	SER	2.8
1	J	112	ILE	2.8
1	L	82	PRO	2.7
1	K	5	THR	2.7
1	L	2	ASN	2.7
1	K	106	LYS	2.7
1	L	105	TYR	2.7
1	L	104	ASP	2.7
1	J	102	VAL	2.6
1	G	186	ASP	2.6
1	D	172	SER	2.6
1	K	84	PHE	2.6
1	I	36	TRP	2.6
1	J	190	GLU	2.5
1	J	180	TYR	2.5
1	J	170	LEU	2.5
1	J	36	TRP	2.5
1	L	3	SER	2.5
1	L	102	VAL	2.5
1	G	171	GLU	2.5
1	I	170	LEU	2.5
1	H	177	ILE	2.5
1	K	17[A]	ASN	2.4
1	H	218	TYR	2.4
1	L	11	TYR	2.4
1	D	170	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	168	ALA	2.4
1	C	127	LEU	2.4
1	E	2	ASN	2.4
1	A	103	ILE	2.4
1	G	1	MET	2.4
1	J	171	GLU	2.4
1	K	218	TYR	2.4
1	C	2	ASN	2.4
1	K	186	ASP	2.3
1	J	85	THR	2.3
1	H	104	ASP	2.3
1	K	29	PHE	2.3
1	A	104	ASP	2.3
1	L	47	ASP	2.3
1	K	1	MET	2.2
1	L	83	ASN	2.2
1	K	112	ILE	2.2
1	E	3	SER	2.2
1	J	106	LYS	2.2
1	D	104	ASP	2.2
1	K	104	ASP	2.2
1	A	186	ASP	2.2
1	K	11	TYR	2.2
1	L	24	SER	2.1
1	L	4	VAL	2.1
1	K	72	LYS	2.1
1	I	15	TYR	2.1
1	J	103	ILE	2.1
1	D	127	LEU	2.1
1	D	218	TYR	2.1
1	L	172[A]	SER	2.1
1	K	45	ILE	2.1
1	C	1	MET	2.1
1	K	7	SER	2.1
1	K	22	VAL	2.1
1	C	42	THR	2.0
1	D	181	HIS	2.0
1	D	177	ILE	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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
5	EDO	B	309	4/4	0.85	0.23	3.06	23,24,25,26	0
2	DMS	B	303	4/4	0.93	0.22	2.77	39,39,39,42	0
2	DMS	B	302	4/4	0.84	0.21	2.15	30,32,32,34	0
5	EDO	L	301	4/4	0.84	0.23	2.09	42,43,43,45	0
2	DMS	G	302	4/4	0.91	0.18	1.91	49,49,51,51	0
5	EDO	D	304	4/4	0.68	0.28	1.75	39,41,41,41	0
2	DMS	J	302	4/4	0.91	0.19	1.59	58,59,59,61	0
5	EDO	A	307	4/4	0.80	0.22	1.35	41,41,41,41	0
6	URA	H	304	8/8	0.91	0.16	1.23	25,27,29,30	0
5	EDO	I	302	4/4	0.91	0.19	1.01	44,44,44,45	0
5	EDO	A	306	4/4	0.87	0.21	0.98	48,49,49,50	0
5	EDO	G	307	4/4	0.81	0.20	0.87	50,50,50,51	0
2	DMS	E	301	4/4	0.98	0.15	0.72	38,39,40,40	0
4	CL	H	301	1/1	0.95	0.16	0.57	39,39,39,39	0
2	DMS	H	302	4/4	0.93	0.17	0.57	46,46,46,46	0
6	URA	J	301	8/8	0.96	0.14	0.47	29,30,31,31	0
2	DMS	H	303	4/4	0.92	0.16	0.39	57,57,59,60	0
2	DMS	F	301	4/4	0.96	0.14	0.24	37,37,38,39	0
6	URA	I	303	8/8	0.94	0.14	0.23	33,33,34,35	0
5	EDO	K	302	4/4	0.88	0.15	0.10	41,41,42,42	0
6	URA	L	302	8/8	0.94	0.13	0.03	28,29,30,30	0
6	URA	A	308	8/8	0.94	0.12	-0.36	22,24,25,25	0
6	URA	B	312	8/8	0.95	0.12	-0.61	19,20,20,21	0
6	URA	F	305	8/8	0.96	0.11	-0.63	19,22,23,23	0
3	K	A	302	1/1	0.96	0.11	-0.77	42,42,42,42	0
6	URA	G	306	8/8	0.96	0.11	-0.81	18,18,18,18	0
6	URA	K	303	8/8	0.96	0.12	-0.85	30,32,33,33	0
6	URA	D	305	8/8	0.96	0.10	-0.89	28,29,29,30	0
3	K	F	302	1/1	0.98	0.11	-0.98	41,41,41,41	0
4	CL	B	306	1/1	0.99	0.14	-1.14	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	URA	C	303	8/8	0.95	0.12	-1.18	28,29,30,30	0
4	CL	D	302	1/1	0.96	0.08	-1.28	39,39,39,39	0
6	URA	E	307	8/8	0.96	0.09	-1.29	20,21,21,22	0
5	EDO	B	311	4/4	0.93	0.10	-1.48	61,61,62,63	0
4	CL	C	302	1/1	0.99	0.10	-1.79	39,39,39,39	0
3	K	D	301	1/1	0.90	0.09	-1.80	51,51,51,51	0
3	K	G	303	1/1	0.97	0.08	-1.86	34,34,34,34	0
4	CL	A	303	1/1	0.99	0.11	-1.99	30,30,30,30	0
3	K	B	305	1/1	0.95	0.08	-2.01	38,38,38,38	0
4	CL	F	303	1/1	0.99	0.09	-2.07	26,26,26,26	0
3	K	E	303	1/1	0.95	0.09	-2.12	40,40,40,40	0
4	CL	K	301	1/1	0.98	0.09	-2.12	39,39,39,39	0
2	DMS	B	301	4/4	0.95	0.12	-2.86	30,30,31,31	0
3	K	B	304	1/1	1.00	0.09	-2.97	16,16,16,16	0
4	CL	G	305	1/1	0.98	0.07	-3.11	37,37,37,37	0
3	K	E	302	1/1	1.00	0.08	-3.53	19,19,19,19	0
3	K	C	301	1/1	0.96	0.07	-3.81	42,42,42,42	0
4	CL	E	304	1/1	0.98	0.09	-3.92	29,29,29,29	0
3	K	J	303	1/1	0.97	0.07	-4.36	43,43,43,43	0
4	CL	B	307	1/1	0.99	0.08	-6.27	25,25,25,25	0
4	CL	B	308	1/1	0.98	0.08	-6.35	36,36,36,36	0
5	EDO	I	301	4/4	0.90	0.14	-	48,48,49,49	0
5	EDO	G	304	4/4	0.93	0.12	-	52,52,53,53	0
4	CL	E	305	1/1	0.98	0.09	-	38,38,38,38	0
2	DMS	A	301	4/4	0.87	0.15	-	65,65,66,67	0
4	CL	G	301	1/1	0.97	0.08	-	36,36,36,36	0
5	EDO	B	310	4/4	0.83	0.19	-	47,47,47,48	0
5	EDO	D	303	4/4	0.76	0.22	-	47,48,49,50	0
4	CL	A	304	1/1	0.99	0.17	-	36,36,36,36	0
5	EDO	A	305	4/4	0.87	0.21	-	51,51,51,52	0
5	EDO	E	306	4/4	0.90	0.19	-	50,51,52,52	0
5	EDO	F	304	4/4	0.90	0.15	-	44,45,46,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.