



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 12:18 PM EST

PDB ID : 1FLZ  
Title : URACIL DNA GLYCOSYLASE WITH UAAP  
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Deposited on : 2000-08-15  
Resolution : 2.30 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

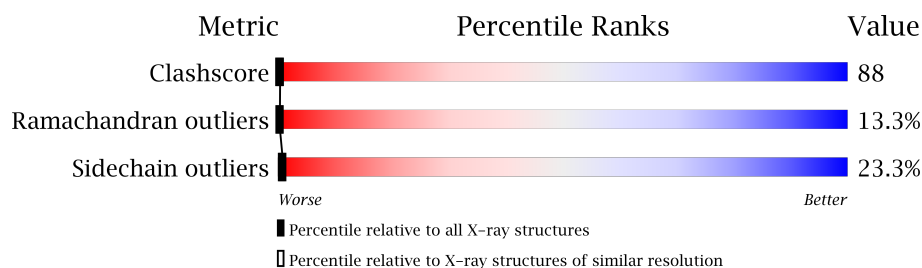
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	228	

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	URA	A	230	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1940 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.

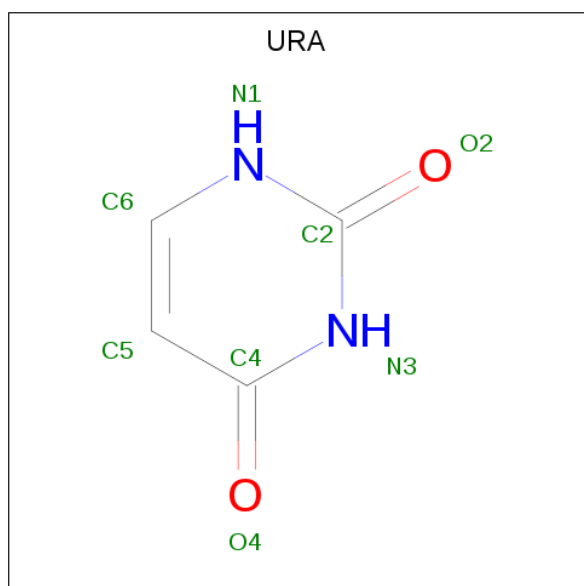
- Molecule 1 is a protein called URACIL-DNA GLYCOSYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	228	1810	1160	324	323	3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	HIS	TYR	ENGINEERED	UNP P12295
A	213	HIS	ARG	ENGINEERED MUTATION	UNP P12295

- Molecule 2 is URACIL (three-letter code: URA) (formula: C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	8	4	2	2	0	0

- Molecule 3 is water.

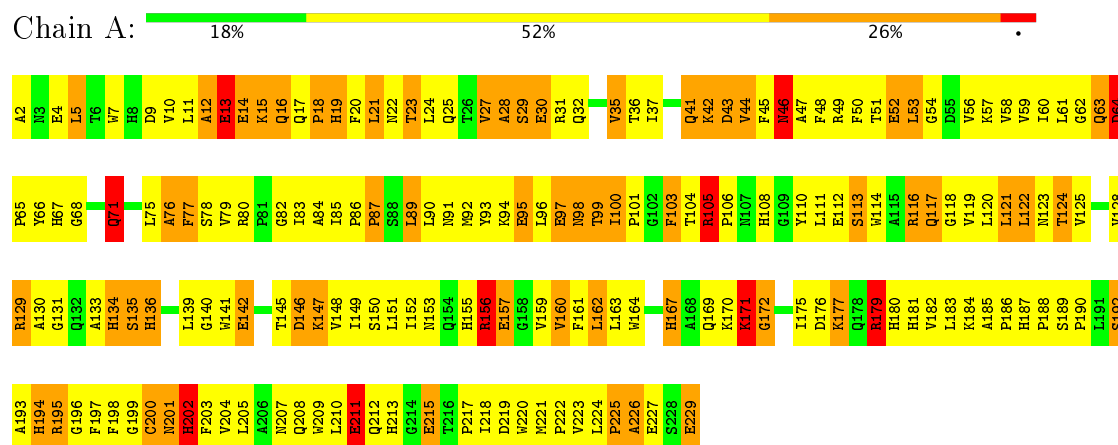
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total 122	O 122	0	0

### 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 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 ( $\text{RSRZ} > 2$ ). 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.

Note EDS was not executed.

#### • Molecule 1: URACIL-DNA GLYCOSYLASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.21Å 78.21Å 80.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (36.00-2.30)	Depositor
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1940	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: URA

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	0.78	11/1867 (0.6%)	1.23	14/2545 (0.6%)

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	A	3	0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	GLU	CD-OE2	6.38	1.32	1.25
1	A	142	GLU	CD-OE2	6.26	1.32	1.25
1	A	112	GLU	CD-OE2	5.96	1.32	1.25
1	A	4	GLU	CD-OE2	5.92	1.32	1.25
1	A	229	GLU	CD-OE2	5.74	1.31	1.25
1	A	52	GLU	CD-OE2	5.53	1.31	1.25
1	A	211	GLU	CD-OE2	5.50	1.31	1.25
1	A	215	GLU	CD-OE2	5.49	1.31	1.25
1	A	13	GLU	CD-OE2	5.48	1.31	1.25
1	A	95	GLU	CD-OE2	5.40	1.31	1.25
1	A	227	GLU	CD-OE2	5.14	1.31	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	GLU	N-CA-CB	8.89	126.60	110.60
1	A	64	ASP	CB-CG-OD2	-7.35	111.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	LEU	CB-CA-C	6.58	122.70	110.20
1	A	179	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	43	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	105	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	43	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	9	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	176	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	120	LEU	N-CA-CB	5.16	120.72	110.40
1	A	176	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	156	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	146	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	A	219	ASP	CB-CG-OD1	5.03	122.82	118.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	14	GLU	CA
1	A	120	LEU	CA
1	A	227	GLU	CA

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	1810	0	1762	315	0
2	A	8	0	3	4	0
3	A	122	0	0	19	0
All	All	1940	0	1765	315	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 88.

All (315) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PRO:HB3	1:A:190:PRO:HG2	1.35	1.09
1:A:63:GLN:HA	1:A:124:THR:H	1.29	0.94
1:A:161:PHE:HB3	1:A:163:LEU:HD21	1.50	0.94
1:A:96:LEU:HD21	1:A:203:PHE:CD2	2.03	0.93
1:A:147:LYS:HD2	1:A:151:LEU:HG	1.51	0.90
1:A:116:ARG:HH11	1:A:116:ARG:HG2	1.35	0.89
1:A:14:GLU:CB	1:A:17:GLN:HG3	2.04	0.87
1:A:63:GLN:NE2	1:A:167:HIS:ND1	2.22	0.87
1:A:129:ARG:HG2	1:A:129:ARG:HH11	1.37	0.86
1:A:122:LEU:HG	1:A:123:ASN:H	1.39	0.86
1:A:63:GLN:HB2	1:A:124:THR:HG23	1.56	0.85
1:A:164:TRP:CD1	1:A:185:ALA:HB3	2.11	0.85
1:A:10:VAL:HB	1:A:151:LEU:HD13	1.55	0.85
1:A:67:HIS:HB2	1:A:131:GLY:H	1.42	0.85
1:A:108:HIS:CD2	1:A:224:LEU:HD21	2.12	0.84
1:A:164:TRP:HE1	1:A:202:HIS:CD2	1.94	0.84
1:A:162:LEU:HD13	1:A:202:HIS:HB3	1.59	0.83
1:A:61:LEU:CD1	1:A:122:LEU:HD23	2.08	0.83
1:A:103:PHE:HE2	1:A:105:ARG:HA	1.46	0.81
1:A:162:LEU:CD1	1:A:202:HIS:HB3	2.11	0.80
1:A:159:VAL:H	1:A:180:HIS:HD2	1.30	0.80
1:A:50:PHE:HB3	1:A:116:ARG:HH12	1.45	0.80
1:A:142:GLU:HB3	1:A:171:LYS:HD3	1.63	0.79
1:A:14:GLU:HB3	1:A:17:GLN:HG3	1.64	0.79
1:A:99:THR:HG21	1:A:201:ASN:HD21	1.46	0.79
1:A:187:HIS:CG	1:A:188:PRO:HD2	2.18	0.79
1:A:172:GLY:O	1:A:175:ILE:HD12	1.84	0.78
1:A:67:HIS:ND1	1:A:131:GLY:HA2	1.98	0.78
1:A:108:HIS:CE1	1:A:224:LEU:HG	2.19	0.77
1:A:188:PRO:O	1:A:193:ALA:HB2	1.83	0.77
1:A:7:TRP:HA	1:A:10:VAL:CG2	2.13	0.77
1:A:10:VAL:HB	1:A:151:LEU:CD1	2.15	0.77
1:A:89:LEU:HD23	1:A:92:MET:HB2	1.66	0.76
1:A:68:GLY:C	1:A:71:GLN:HG3	2.06	0.76
1:A:203:PHE:HB2	3:A:331:HOH:O	1.86	0.76
1:A:61:LEU:HD13	1:A:122:LEU:HD23	1.66	0.75
1:A:108:HIS:CG	1:A:224:LEU:HD11	2.21	0.75
1:A:100:ILE:HG23	1:A:101:PRO:HD2	1.69	0.74
1:A:50:PHE:HB3	1:A:116:ARG:NH1	2.01	0.74
1:A:147:LYS:CD	1:A:151:LEU:HG	2.17	0.73
1:A:207:ASN:ND2	1:A:217:PRO:HB2	2.03	0.73
1:A:175:ILE:O	1:A:177:LYS:HD2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:PRO:O	1:A:197:PHE:HB2	1.88	0.72
1:A:50:PHE:HD2	1:A:116:ARG:HH22	1.38	0.72
1:A:146:ASP:N	1:A:171:LYS:HZ3	1.89	0.71
1:A:106:PRO:HG3	1:A:222:PRO:HG2	1.71	0.71
1:A:57:LYS:HG2	3:A:353:HOH:O	1.90	0.71
1:A:122:LEU:HG	1:A:123:ASN:N	2.05	0.71
1:A:96:LEU:HD11	1:A:220:TRP:HB3	1.74	0.70
1:A:159:VAL:HG12	1:A:161:PHE:CE1	2.27	0.70
1:A:159:VAL:N	1:A:180:HIS:HD2	1.88	0.70
1:A:64:ASP:OD1	1:A:128:VAL:HB	1.90	0.70
1:A:159:VAL:H	1:A:180:HIS:CD2	2.10	0.70
1:A:113:SER:HB2	3:A:368:HOH:O	1.90	0.70
1:A:13:GLU:O	1:A:17:GLN:HG2	1.91	0.70
1:A:63:GLN:O	1:A:125:VAL:N	2.22	0.70
1:A:87:PRO:HB3	1:A:190:PRO:CG	2.19	0.70
1:A:96:LEU:CD1	1:A:220:TRP:HB3	2.22	0.70
1:A:90:LEU:O	1:A:93:TYR:HB2	1.92	0.70
1:A:160:VAL:CG1	1:A:181:HIS:HB3	2.22	0.69
1:A:108:HIS:CB	1:A:224:LEU:HD11	2.22	0.69
1:A:113:SER:O	1:A:117:GLN:HG3	1.93	0.69
1:A:12:ALA:O	1:A:13:GLU:C	2.31	0.69
1:A:157:GLU:OE1	1:A:179:ARG:HD2	1.92	0.69
1:A:200:CYS:HB2	1:A:202:HIS:CE1	2.27	0.69
1:A:7:TRP:HA	1:A:10:VAL:HG23	1.73	0.69
1:A:96:LEU:HD21	1:A:203:PHE:CG	2.28	0.68
1:A:100:ILE:CG2	1:A:101:PRO:HD2	2.23	0.68
1:A:31:ARG:HH11	1:A:37:ILE:HB	1.60	0.67
1:A:85:ILE:HG23	1:A:89:LEU:HB3	1.75	0.67
1:A:162:LEU:CD2	1:A:183:LEU:HD12	2.25	0.66
1:A:30:GLU:OE2	1:A:129:ARG:NH2	2.29	0.66
1:A:87:PRO:CB	1:A:190:PRO:HG2	2.22	0.66
1:A:63:GLN:HG3	1:A:63:GLN:O	1.95	0.66
1:A:18:PRO:O	1:A:20:PHE:N	2.29	0.66
1:A:2:ALA:HB2	3:A:329:HOH:O	1.96	0.66
1:A:77:PHE:N	2:A:230:URA:O4	2.29	0.65
1:A:68:GLY:CA	1:A:71:GLN:HG3	2.25	0.65
1:A:86:PRO:HB3	3:A:372:HOH:O	1.96	0.65
1:A:196:GLY:O	1:A:197:PHE:C	2.33	0.65
1:A:46:ASN:O	1:A:49:ARG:HB2	1.97	0.65
1:A:67:HIS:HB2	1:A:131:GLY:N	2.12	0.65
1:A:210:LEU:CD2	1:A:215:GLU:HB3	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:NZ	1:A:171:LYS:HB3	2.11	0.64
1:A:86:PRO:CB	1:A:87:PRO:HD2	2.26	0.64
1:A:147:LYS:HD2	1:A:151:LEU:CG	2.26	0.64
1:A:50:PHE:CB	1:A:116:ARG:HH12	2.11	0.64
1:A:164:TRP:HE1	1:A:202:HIS:HD2	1.43	0.64
1:A:105:ARG:NH1	3:A:403:HOH:O	2.30	0.64
1:A:133:ALA:O	1:A:135:SER:N	2.30	0.64
1:A:116:ARG:NH1	1:A:116:ARG:HG2	2.10	0.64
1:A:159:VAL:HB	1:A:180:HIS:CD2	2.34	0.63
1:A:21:LEU:O	1:A:25:GLN:HG3	1.98	0.63
1:A:27:VAL:O	1:A:28:ALA:C	2.36	0.63
1:A:83:ILE:HD12	1:A:83:ILE:N	2.14	0.63
1:A:209:TRP:O	1:A:213:HIS:ND1	2.30	0.63
1:A:50:PHE:HD1	1:A:75:LEU:HD21	1.63	0.63
1:A:12:ALA:O	1:A:15:LYS:N	2.32	0.63
1:A:108:HIS:HB3	1:A:224:LEU:HD11	1.79	0.63
1:A:46:ASN:HA	1:A:49:ARG:HE	1.64	0.62
1:A:103:PHE:CE2	1:A:105:ARG:HA	2.30	0.62
1:A:153:ASN:ND2	1:A:175:ILE:HA	2.14	0.62
1:A:29:SER:O	1:A:32:GLN:N	2.32	0.62
1:A:210:LEU:HA	1:A:215:GLU:HB2	1.82	0.62
1:A:108:HIS:CG	1:A:224:LEU:HD21	2.34	0.62
1:A:31:ARG:NH1	1:A:37:ILE:HB	2.15	0.62
1:A:82:GLY:C	1:A:83:ILE:HD12	2.20	0.61
1:A:156:ARG:N	3:A:382:HOH:O	2.27	0.61
1:A:96:LEU:HD21	1:A:203:PHE:CE2	2.35	0.61
1:A:210:LEU:CA	1:A:215:GLU:HB2	2.31	0.61
1:A:63:GLN:HA	1:A:124:THR:N	2.11	0.61
1:A:20:PHE:O	1:A:23:THR:N	2.33	0.60
1:A:192:SER:HA	1:A:195:ARG:HD2	1.83	0.60
1:A:95:GLU:OE1	1:A:199:GLY:N	2.34	0.60
1:A:41:GLN:HA	1:A:44:VAL:HG23	1.82	0.60
1:A:76:ALA:HB3	1:A:121:LEU:C	2.22	0.60
1:A:63:GLN:CB	1:A:124:THR:HG23	2.28	0.60
1:A:18:PRO:O	1:A:19:HIS:C	2.40	0.60
1:A:220:TRP:O	1:A:222:PRO:HD3	2.01	0.60
1:A:84:ALA:O	1:A:86:PRO:HD3	2.01	0.60
1:A:91:ASN:ND2	3:A:309:HOH:O	2.29	0.59
1:A:223:VAL:O	1:A:225:PRO:HD3	2.02	0.59
1:A:203:PHE:HD2	1:A:220:TRP:CD2	2.21	0.59
1:A:7:TRP:CZ3	1:A:148:VAL:HG13	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:O	1:A:147:LYS:HD3	2.03	0.59
1:A:23:THR:O	1:A:27:VAL:HG23	2.03	0.59
1:A:66:TYR:CD1	2:A:230:URA:H6	2.21	0.58
1:A:85:ILE:CG2	1:A:89:LEU:HB3	2.32	0.58
1:A:125:VAL:HA	1:A:141:TRP:HB3	1.85	0.58
1:A:146:ASP:HA	1:A:171:LYS:NZ	2.18	0.58
1:A:76:ALA:HA	1:A:123:ASN:HD21	1.69	0.58
1:A:162:LEU:HD21	1:A:183:LEU:HD12	1.86	0.57
1:A:160:VAL:HG12	1:A:181:HIS:HB3	1.87	0.57
1:A:218:ILE:HG21	1:A:220:TRP:CZ3	2.39	0.57
1:A:202:HIS:N	1:A:202:HIS:ND1	2.51	0.57
1:A:156:ARG:O	1:A:180:HIS:NE2	2.29	0.57
1:A:211:GLU:HA	1:A:211:GLU:OE2	2.03	0.57
1:A:181:HIS:CD2	1:A:182:VAL:H	2.23	0.56
1:A:29:SER:O	1:A:32:GLN:HB3	2.05	0.56
1:A:149:ILE:O	1:A:152:ILE:HB	2.06	0.56
1:A:160:VAL:HG13	1:A:181:HIS:HB3	1.87	0.56
1:A:170:LYS:O	1:A:172:GLY:N	2.31	0.56
1:A:45:PHE:O	1:A:47:ALA:N	2.38	0.55
1:A:108:HIS:ND1	1:A:224:LEU:HG	2.21	0.55
1:A:146:ASP:OD1	1:A:171:LYS:HD2	2.06	0.55
1:A:187:HIS:ND1	1:A:189:SER:HB3	2.23	0.54
1:A:224:LEU:HD12	3:A:379:HOH:O	2.07	0.54
1:A:63:GLN:NE2	1:A:124:THR:OG1	2.38	0.54
1:A:23:THR:OG1	1:A:140:GLY:N	2.37	0.54
1:A:96:LEU:O	1:A:103:PHE:HB3	2.08	0.54
1:A:103:PHE:HE1	1:A:220:TRP:O	1.91	0.54
1:A:68:GLY:HA3	1:A:71:GLN:OE1	2.08	0.54
1:A:146:ASP:OD1	1:A:171:LYS:NZ	2.30	0.54
1:A:129:ARG:NE	3:A:330:HOH:O	2.30	0.54
1:A:13:GLU:HG2	1:A:17:GLN:NE2	2.21	0.54
1:A:129:ARG:NH1	1:A:129:ARG:HG2	2.13	0.53
1:A:48:PHE:CE1	1:A:148:VAL:HG11	2.43	0.53
1:A:58:VAL:HG13	1:A:160:VAL:HG23	1.91	0.53
1:A:134:HIS:O	1:A:136:HIS:N	2.41	0.53
1:A:223:VAL:C	1:A:225:PRO:HD3	2.28	0.53
1:A:24:LEU:O	1:A:27:VAL:HB	2.09	0.53
1:A:89:LEU:HA	1:A:92:MET:HG3	1.90	0.53
1:A:207:ASN:CG	1:A:218:ILE:H	2.13	0.53
1:A:210:LEU:O	1:A:215:GLU:HB2	2.08	0.52
1:A:27:VAL:O	1:A:29:SER:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLN:HB2	1:A:124:THR:CG2	2.33	0.52
1:A:108:HIS:ND1	1:A:224:LEU:HD11	2.24	0.52
1:A:155:HIS:O	1:A:156:ARG:O	2.28	0.52
1:A:169:GLN:HG2	1:A:184:LYS:HG2	1.92	0.52
1:A:210:LEU:HD22	1:A:215:GLU:HB3	1.91	0.52
1:A:210:LEU:HD23	1:A:215:GLU:CB	2.40	0.52
1:A:128:VAL:HG22	1:A:129:ARG:N	2.24	0.52
1:A:125:VAL:O	1:A:125:VAL:HG12	2.10	0.51
1:A:79:VAL:O	1:A:110:TYR:HD1	1.93	0.51
1:A:43:ASP:O	1:A:46:ASN:HB2	2.10	0.51
1:A:7:TRP:N	1:A:52:GLU:OE1	2.28	0.51
1:A:146:ASP:CA	1:A:171:LYS:HZ3	2.23	0.51
1:A:14:GLU:HB2	1:A:17:GLN:HG3	1.88	0.51
1:A:75:LEU:HB2	1:A:78:SER:HB3	1.93	0.51
1:A:92:MET:HE1	1:A:164:TRP:HZ3	1.76	0.50
1:A:146:ASP:CG	1:A:171:LYS:HD2	2.32	0.50
1:A:66:TYR:CD1	2:A:230:URA:C6	2.99	0.50
1:A:2:ALA:N	3:A:339:HOH:O	2.43	0.50
1:A:36:THR:O	1:A:129:ARG:O	2.30	0.50
1:A:92:MET:CE	1:A:164:TRP:HZ3	2.25	0.50
1:A:218:ILE:HG21	1:A:220:TRP:CH2	2.46	0.50
1:A:98:ASN:OD1	1:A:98:ASN:N	2.45	0.50
1:A:63:GLN:O	1:A:125:VAL:HB	2.12	0.50
1:A:203:PHE:CD2	1:A:220:TRP:CD2	3.00	0.50
1:A:48:PHE:HE1	1:A:148:VAL:HG11	1.76	0.50
1:A:75:LEU:O	1:A:77:PHE:N	2.45	0.50
1:A:171:LYS:HZ1	1:A:171:LYS:HB3	1.76	0.49
1:A:99:THR:HG21	1:A:201:ASN:ND2	2.22	0.49
1:A:162:LEU:HD13	1:A:202:HIS:CB	2.36	0.49
1:A:96:LEU:HD13	1:A:220:TRP:HB3	1.93	0.49
1:A:104:THR:O	1:A:105:ARG:O	2.29	0.49
1:A:210:LEU:HD23	1:A:215:GLU:HB3	1.93	0.49
1:A:116:ARG:HG3	3:A:406:HOH:O	2.11	0.49
1:A:76:ALA:HA	2:A:230:URA:O4	2.13	0.49
1:A:145:THR:OG1	1:A:171:LYS:HE2	2.13	0.48
1:A:187:HIS:CD2	1:A:188:PRO:HD2	2.48	0.48
1:A:68:GLY:HA3	1:A:71:GLN:HG3	1.95	0.48
1:A:207:ASN:ND2	1:A:218:ILE:H	2.12	0.48
1:A:104:THR:O	1:A:105:ARG:C	2.50	0.48
1:A:142:GLU:O	1:A:171:LYS:HE2	2.14	0.48
1:A:67:HIS:CE1	1:A:131:GLY:HA2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LYS:HG3	1:A:42:LYS:H	1.38	0.47
1:A:63:GLN:HA	1:A:124:THR:HG23	1.96	0.47
1:A:153:ASN:HD21	1:A:175:ILE:HA	1.79	0.47
1:A:89:LEU:HD11	1:A:111:LEU:HD21	1.96	0.47
1:A:122:LEU:CG	1:A:123:ASN:N	2.76	0.47
1:A:148:VAL:O	1:A:152:ILE:HG13	2.15	0.47
1:A:24:LEU:O	1:A:28:ALA:N	2.41	0.47
1:A:11:LEU:HA	1:A:11:LEU:HD23	1.71	0.47
1:A:210:LEU:HB3	1:A:215:GLU:O	2.15	0.47
1:A:210:LEU:O	1:A:215:GLU:N	2.48	0.47
1:A:48:PHE:HE1	1:A:148:VAL:CG1	2.28	0.47
1:A:65:PRO:HD3	1:A:125:VAL:O	2.14	0.46
1:A:161:PHE:HE1	1:A:180:HIS:HB3	1.79	0.46
1:A:22:ASN:HB3	3:A:399:HOH:O	2.15	0.46
1:A:27:VAL:HG12	3:A:360:HOH:O	2.15	0.46
1:A:45:PHE:O	1:A:46:ASN:C	2.54	0.46
1:A:5:LEU:O	1:A:53:LEU:HD23	2.15	0.46
1:A:63:GLN:N	1:A:123:ASN:OD1	2.48	0.46
1:A:149:ILE:O	1:A:150:SER:C	2.53	0.46
1:A:103:PHE:CD2	1:A:104:THR:N	2.83	0.46
1:A:129:ARG:HB2	1:A:135:SER:OG	2.16	0.46
1:A:76:ALA:O	1:A:77:PHE:HD1	1.99	0.46
1:A:149:ILE:O	1:A:152:ILE:N	2.48	0.46
1:A:146:ASP:CA	1:A:171:LYS:NZ	2.78	0.46
1:A:194:HIS:ND1	1:A:194:HIS:N	2.64	0.46
1:A:18:PRO:O	1:A:21:LEU:N	2.49	0.46
1:A:63:GLN:CA	1:A:124:THR:HG23	2.46	0.45
1:A:50:PHE:HD2	1:A:116:ARG:NH2	2.07	0.45
1:A:68:GLY:O	1:A:71:GLN:HG3	2.16	0.45
1:A:185:ALA:HB2	1:A:202:HIS:NE2	2.31	0.45
1:A:30:GLU:OE1	1:A:129:ARG:NH1	2.49	0.45
1:A:83:ILE:CG2	1:A:84:ALA:N	2.79	0.45
1:A:95:GLU:C	1:A:97:GLU:H	2.20	0.45
1:A:159:VAL:CG1	1:A:161:PHE:CZ	3.00	0.45
1:A:164:TRP:HA	1:A:185:ALA:O	2.16	0.45
1:A:128:VAL:CG2	1:A:129:ARG:N	2.79	0.45
1:A:108:HIS:ND1	1:A:224:LEU:CD1	2.80	0.45
1:A:76:ALA:HA	1:A:123:ASN:ND2	2.32	0.45
1:A:181:HIS:CD2	1:A:182:VAL:N	2.85	0.45
1:A:12:ALA:O	1:A:15:LYS:HB2	2.17	0.44
1:A:68:GLY:HA3	1:A:71:GLN:CD	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:PHE:HB3	1:A:163:LEU:CD2	2.35	0.44
1:A:79:VAL:HG23	1:A:80:ARG:O	2.17	0.44
1:A:92:MET:HE2	1:A:164:TRP:CZ3	2.52	0.44
1:A:116:ARG:NH1	1:A:116:ARG:CG	2.80	0.44
1:A:92:MET:CE	1:A:164:TRP:CZ3	3.01	0.44
1:A:94:LYS:HD2	1:A:198:PHE:CZ	2.53	0.44
1:A:204:VAL:HG23	3:A:331:HOH:O	2.17	0.44
1:A:201:ASN:HB3	1:A:205:LEU:HD12	2.00	0.44
1:A:108:HIS:ND1	1:A:224:LEU:CG	2.80	0.44
1:A:150:SER:OG	1:A:151:LEU:N	2.51	0.44
1:A:199:GLY:C	1:A:200:CYS:O	2.55	0.44
1:A:164:TRP:NE1	1:A:185:ALA:HB3	2.30	0.44
1:A:30:GLU:CD	1:A:129:ARG:HH12	2.20	0.44
1:A:37:ILE:HD13	1:A:129:ARG:HA	1.98	0.44
1:A:114:TRP:O	1:A:119:VAL:HG23	2.17	0.43
1:A:59:VAL:HG12	1:A:59:VAL:O	2.16	0.43
1:A:159:VAL:CG1	1:A:161:PHE:CE1	2.99	0.43
1:A:75:LEU:O	1:A:76:ALA:C	2.56	0.43
1:A:83:ILE:N	1:A:83:ILE:CD1	2.80	0.43
1:A:167:HIS:NE2	3:A:384:HOH:O	2.30	0.43
1:A:63:GLN:OE1	1:A:167:HIS:CG	2.72	0.43
1:A:199:GLY:O	1:A:200:CYS:O	2.35	0.43
1:A:93:TYR:O	1:A:94:LYS:C	2.55	0.43
1:A:42:LYS:HA	3:A:311:HOH:O	2.19	0.43
1:A:134:HIS:C	1:A:136:HIS:H	2.22	0.43
1:A:169:GLN:NE2	1:A:184:LYS:HB3	2.34	0.43
1:A:35:VAL:HA	3:A:316:HOH:O	2.18	0.43
1:A:11:LEU:O	1:A:12:ALA:C	2.57	0.43
1:A:146:ASP:HA	1:A:171:LYS:HZ3	1.83	0.43
1:A:14:GLU:OE2	1:A:147:LYS:HG2	2.18	0.43
1:A:187:HIS:ND1	1:A:188:PRO:HD2	2.34	0.43
1:A:19:HIS:CG	1:A:20:PHE:N	2.86	0.43
1:A:62:GLY:O	1:A:124:THR:HG23	2.18	0.43
1:A:207:ASN:ND2	1:A:217:PRO:CB	2.79	0.43
1:A:54:GLY:C	1:A:56:VAL:H	2.22	0.43
1:A:161:PHE:O	1:A:163:LEU:HG	2.19	0.42
1:A:24:LEU:HD23	1:A:24:LEU:N	2.34	0.42
1:A:42:LYS:HE2	1:A:42:LYS:HB2	1.53	0.42
1:A:83:ILE:HA	3:A:401:HOH:O	2.18	0.42
1:A:64:ASP:HA	1:A:125:VAL:O	2.19	0.42
1:A:93:TYR:HA	1:A:96:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:VAL:HB	1:A:180:HIS:HD2	1.83	0.42
1:A:181:HIS:C	1:A:182:VAL:HG23	2.40	0.42
1:A:193:ALA:HA	1:A:197:PHE:HB3	2.02	0.42
1:A:225:PRO:HB2	1:A:226:ALA:H	1.64	0.42
1:A:129:ARG:NH1	1:A:129:ARG:CG	2.80	0.41
1:A:79:VAL:O	1:A:110:TYR:HA	2.20	0.41
1:A:162:LEU:HD13	1:A:164:TRP:CZ2	2.55	0.41
1:A:13:GLU:O	1:A:16:GLN:N	2.54	0.41
1:A:164:TRP:NE1	1:A:202:HIS:HD2	2.13	0.41
1:A:86:PRO:O	1:A:87:PRO:C	2.59	0.41
1:A:60:ILE:HD12	1:A:121:LEU:CD2	2.50	0.41
1:A:89:LEU:O	1:A:90:LEU:C	2.57	0.41
1:A:210:LEU:HD23	1:A:215:GLU:HG3	2.02	0.41
1:A:103:PHE:HE2	1:A:105:ARG:CA	2.22	0.41
1:A:30:GLU:O	1:A:35:VAL:HB	2.21	0.41
1:A:87:PRO:HA	1:A:90:LEU:HD12	2.03	0.41
1:A:96:LEU:HA	1:A:96:LEU:HD23	1.75	0.41
1:A:5:LEU:HD22	1:A:5:LEU:HA	1.81	0.40
1:A:181:HIS:HB2	1:A:209:TRP:CE3	2.56	0.40
1:A:29:SER:O	1:A:30:GLU:C	2.59	0.40
1:A:76:ALA:HB2	1:A:122:LEU:C	2.41	0.40
1:A:104:THR:C	1:A:105:ARG:O	2.59	0.40
1:A:207:ASN:HD21	1:A:218:ILE:N	2.19	0.40
1:A:52:GLU:O	1:A:56:VAL:HG23	2.21	0.40
1:A:7:TRP:HA	1:A:10:VAL:HG22	2.00	0.40
1:A:83:ILE:HG22	1:A:84:ALA:N	2.36	0.40
1:A:68:GLY:HA3	1:A:71:GLN:CG	2.51	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	226/228 (99%)	152 (67%)	44 (20%)	30 (13%)	0 0

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ALA
1	A	18	PRO
1	A	19	HIS
1	A	29	SER
1	A	46	ASN
1	A	76	ALA
1	A	87	PRO
1	A	121	LEU
1	A	129	ARG
1	A	135	SER
1	A	156	ARG
1	A	171	LYS
1	A	226	ALA
1	A	27	VAL
1	A	35	VAL
1	A	130	ALA
1	A	200	CYS
1	A	13	GLU
1	A	16	GLN
1	A	71	GLN
1	A	134	HIS
1	A	172	GLY
1	A	194	HIS
1	A	225	PRO
1	A	28	ALA
1	A	118	GLY
1	A	202	HIS
1	A	77	PHE
1	A	44	VAL
1	A	105	ARG

### 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	193/193 (100%)	148 (77%)	45 (23%)	<b>1</b> <b>1</b>

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	14	GLU
1	A	15	LYS
1	A	21	LEU
1	A	23	THR
1	A	30	GLU
1	A	41	GLN
1	A	42	LYS
1	A	46	ASN
1	A	51	THR
1	A	53	LEU
1	A	63	GLN
1	A	64	ASP
1	A	71	GLN
1	A	89	LEU
1	A	97	GLU
1	A	98	ASN
1	A	99	THR
1	A	100	ILE
1	A	103	PHE
1	A	105	ARG
1	A	113	SER
1	A	116	ARG
1	A	117	GLN
1	A	122	LEU
1	A	124	THR
1	A	136	HIS
1	A	139	LEU
1	A	147	LYS
1	A	156	ARG
1	A	160	VAL
1	A	162	LEU
1	A	167	HIS
1	A	171	LYS
1	A	177	LYS
1	A	179	ARG

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Mol	Chain	Res	Type
1	A	192	SER
1	A	195	ARG
1	A	201	ASN
1	A	202	HIS
1	A	208	GLN
1	A	211	GLU
1	A	212	GLN
1	A	221	MET
1	A	229	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	HIS
1	A	194	HIS
1	A	201	ASN
1	A	212	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	URA	A	230	-	6,8,8	1.69	2 (33%)	5,10,10	12.70	4 (80%)

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	URA	A	230	-	-	0/0/0/0	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	230	URA	C5-C6	-2.10	1.34	1.38
2	A	230	URA	C4-N3	3.13	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	230	URA	N1-C2-N3	-19.17	114.62	128.40
2	A	230	URA	C5-C4-N3	-3.54	114.68	123.12
2	A	230	URA	C6-N1-C2	13.75	121.05	114.41
2	A	230	URA	C4-N3-C2	15.40	127.36	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	230	URA	4	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.