Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2023 – 02:16 AM EDT

PDB ID	:	4O8R
Title	:	Crystal structure of orotidine 5'-monophosphate decarboxylase from methanobacterium thermoautotrophicum complexed with 5,6-dihydrouridine 5'-monophosphate
Authors	:	Fedorov, A.A.; Fedorov, E.V.; Chan, K.K.; Gerlt, J.A.; Almo, S.C.
Deposited on	:	2013-12-29
Resolution	:	2.29 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

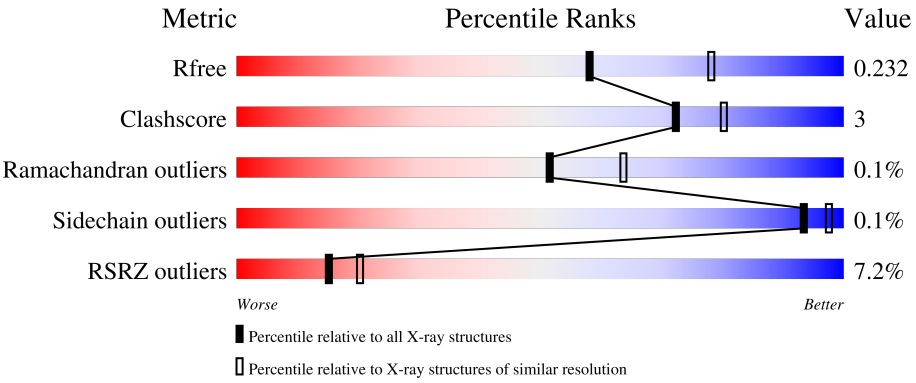
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 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	228	89% 7%
1	B	228	4% 92%
1	C	228	90% 8%
1	D	228	8% 85% 10% 5%

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Mol	Chain	Length	Quality of chain
1	E	228	4% 88% 7% 5%
1	F	228	9% 82% 12% 6%
1	G	228	6% 84% 10% 7%
1	H	228	3% 86% 8% 6%
1	I	228	11% 79% 8% 14%
1	J	228	3% 89% 7%
1	K	228	18% 82% 13% 5%
1	L	228	21% 84% 10% 7%
1	M	228	% 90% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21847 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 Orotidine 5'-phosphate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	2	0
			1693	1063	299	319	12			
1	B	219	Total	C	N	O	S	0	2	0
			1683	1058	295	318	12			
1	C	225	Total	C	N	O	S	0	1	0
			1726	1083	306	324	13			
1	D	216	Total	C	N	O	S	0	2	0
			1659	1044	292	311	12			
1	E	217	Total	C	N	O	S	0	1	0
			1657	1043	289	313	12			
1	F	215	Total	C	N	O	S	0	1	0
			1641	1033	287	309	12			
1	G	213	Total	C	N	O	S	0	1	0
			1624	1021	284	307	12			
1	H	215	Total	C	N	O	S	0	1	0
			1639	1032	286	309	12			
1	I	197	Total	C	N	O	S	0	0	0
			1505	951	262	282	10			
1	J	218	Total	C	N	O	S	0	0	0
			1653	1039	289	313	12			
1	K	216	Total	C	N	O	S	0	0	0
			1638	1029	287	311	11			
1	L	213	Total	C	N	O	S	0	0	0
			1613	1013	283	306	11			
1	M	218	Total	C	N	O	S	0	1	0
			1664	1048	290	314	12			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	PRO	ARG	engineered mutation	UNP O26232
B	101	PRO	ARG	engineered mutation	UNP O26232
C	101	PRO	ARG	engineered mutation	UNP O26232

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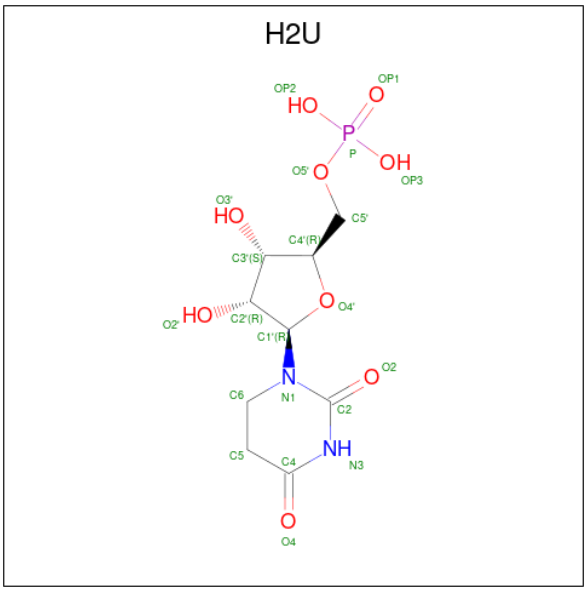
Chain	Residue	Modelled	Actual	Comment	Reference
D	101	PRO	ARG	engineered mutation	UNP O26232
E	101	PRO	ARG	engineered mutation	UNP O26232
F	101	PRO	ARG	engineered mutation	UNP O26232
G	101	PRO	ARG	engineered mutation	UNP O26232
H	101	PRO	ARG	engineered mutation	UNP O26232
I	101	PRO	ARG	engineered mutation	UNP O26232
J	101	PRO	ARG	engineered mutation	UNP O26232
K	101	PRO	ARG	engineered mutation	UNP O26232
L	101	PRO	ARG	engineered mutation	UNP O26232
M	101	PRO	ARG	engineered mutation	UNP O26232

- Molecule 2 is 5,6-DIHYDROURIDINE-5'-MONOPHOSPHATE (three-letter code: H2U) (formula: $C_9H_{15}N_2O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	B	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	C	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	D	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	E	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	F	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	H	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	J	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	K	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	L	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	M	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total	O	0	0
			36	36		
4	B	22	Total	O	0	0
			22	22		
4	C	34	Total	O	0	0
			34	34		
4	D	19	Total	O	0	0
			19	19		
4	E	7	Total	O	0	0
			7	7		
4	F	11	Total	O	0	0
			11	11		
4	G	6	Total	O	0	0
			6	6		
4	H	6	Total	O	0	0
			6	6		
4	I	11	Total	O	0	0
			11	11		
4	J	20	Total	O	0	0
			20	20		

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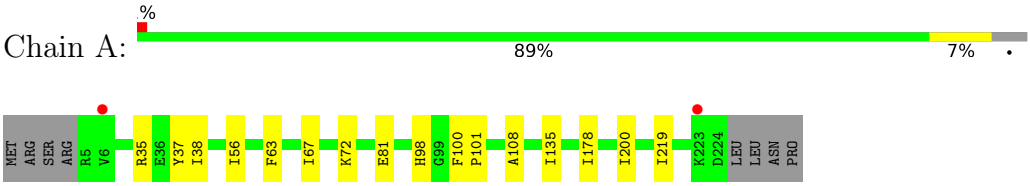
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	4	Total O 4 4	0	0
4	M	23	Total O 23 23	0	0

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.

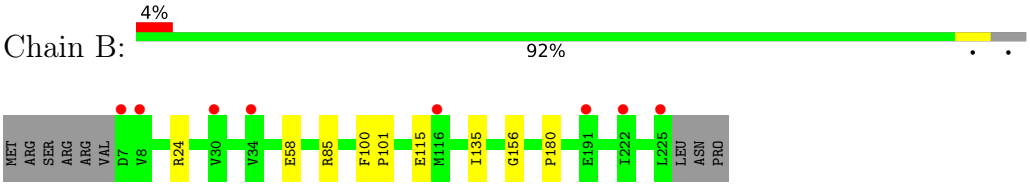
• Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain A:



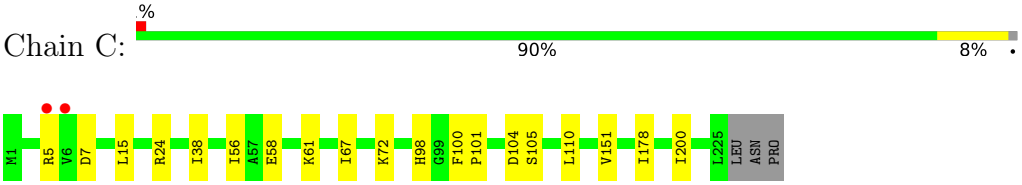
• Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain B:



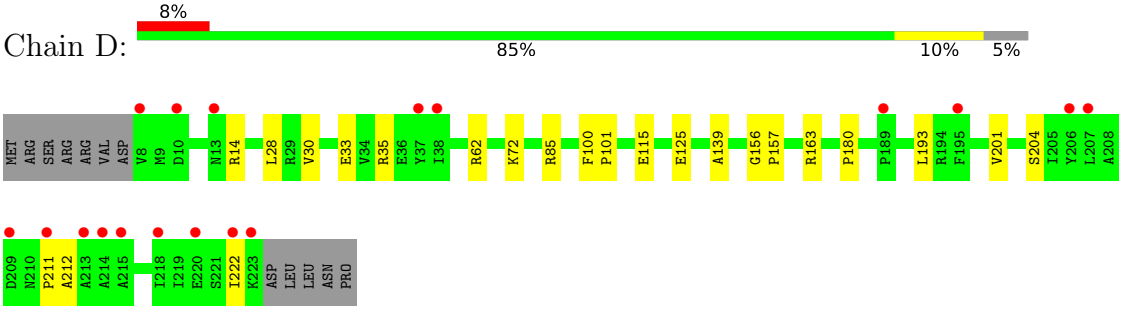
• Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain C:



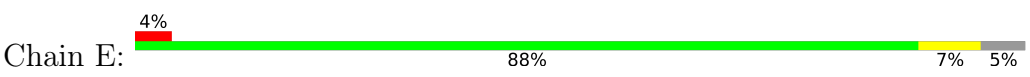
• Molecule 1: Orotidine 5'-phosphate decarboxylase

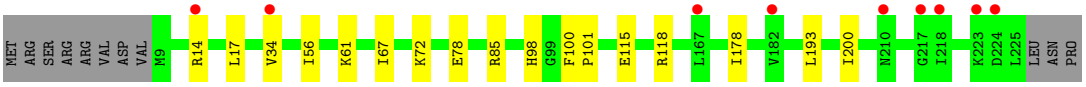
Chain D:



• Molecule 1: Orotidine 5'-phosphate decarboxylase

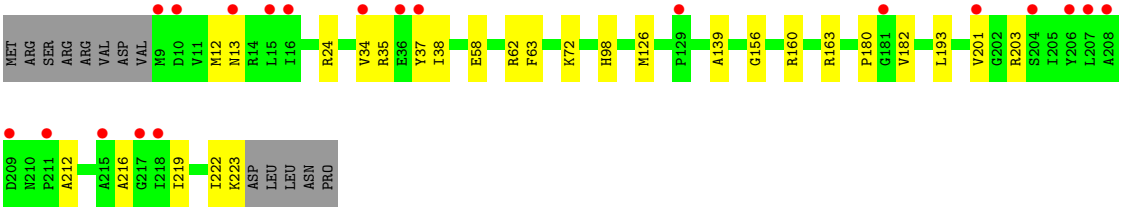
Chain E:





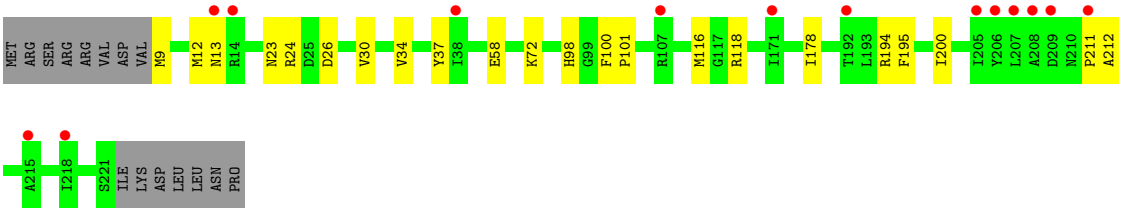
• Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain F:



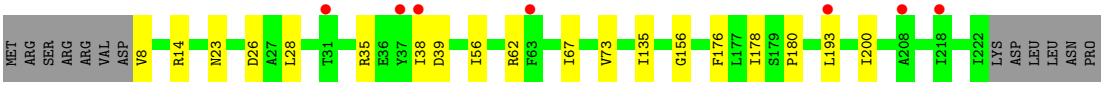
• Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain G:



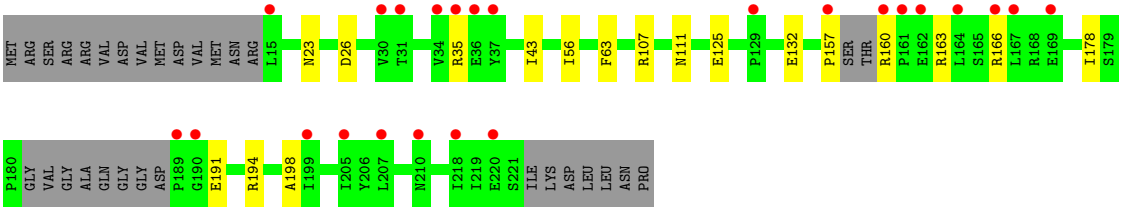
• Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain H:



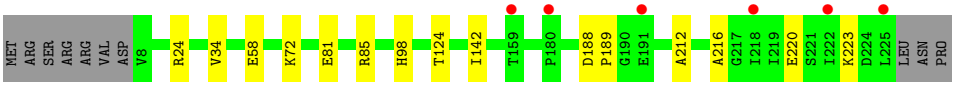
• Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain I:



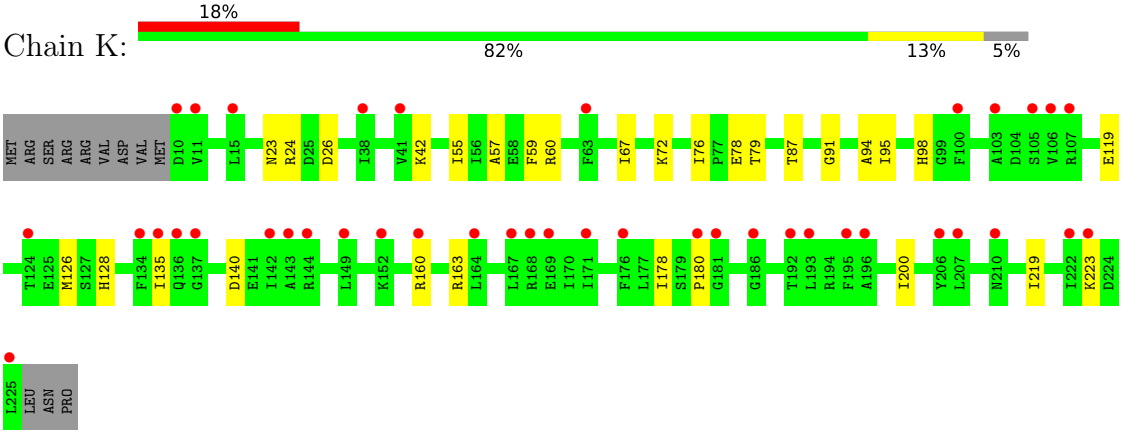
• Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain J:



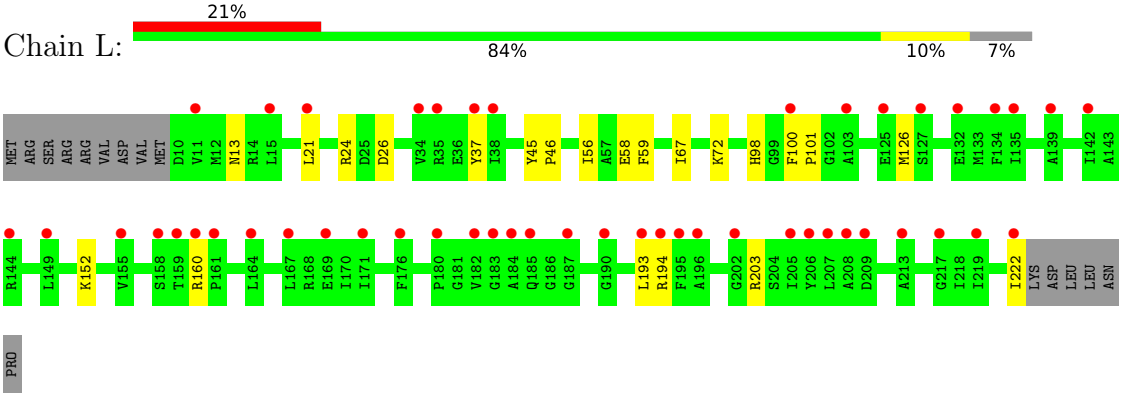
• Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain K:



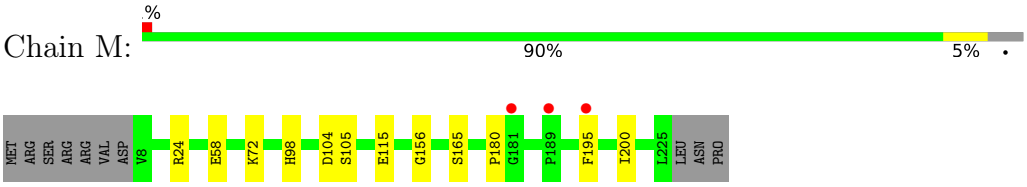
• Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain L:



• Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	147.90Å 101.80Å 192.84Å 90.00° 91.59° 90.00°	Depositor
Resolution (Å)	48.19 – 2.29 48.19 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.19-2.29) 99.4 (48.19-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.203 , 0.231 0.205 , 0.232	Depositor DCC
R_{free} test set	3840 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å^2)	46.3	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21847	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: H2U, 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	0.24	0/1717	0.43	0/2316
1	B	0.23	0/1707	0.41	0/2303
1	C	0.24	0/1750	0.43	0/2359
1	D	0.23	0/1683	0.41	0/2270
1	E	0.22	0/1681	0.39	0/2268
1	F	0.22	0/1665	0.40	0/2246
1	G	0.22	0/1648	0.39	0/2224
1	H	0.21	0/1663	0.39	0/2245
1	I	0.22	0/1526	0.39	0/2056
1	J	0.23	0/1676	0.40	0/2261
1	K	0.21	0/1661	0.38	0/2241
1	L	0.21	0/1636	0.37	0/2208
1	M	0.24	0/1688	0.42	0/2278
All	All	0.23	0/21701	0.40	0/29275

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	1693	0	1705	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1683	0	1691	6	0
1	C	1726	0	1747	10	0
1	D	1659	0	1671	15	0
1	E	1657	0	1669	10	0
1	F	1641	0	1654	17	0
1	G	1624	0	1630	15	0
1	H	1639	0	1650	11	0
1	I	1505	0	1520	10	0
1	J	1653	0	1669	8	0
1	K	1638	0	1651	21	0
1	L	1613	0	1623	15	0
1	M	1664	0	1678	9	0
2	A	21	0	13	0	0
2	B	21	0	13	0	0
2	C	21	0	13	0	0
2	D	21	0	13	2	0
2	E	21	0	13	0	0
2	F	21	0	13	0	0
2	G	21	0	13	0	0
2	H	21	0	13	0	0
2	J	21	0	13	0	0
2	K	21	0	13	0	0
2	L	21	0	13	2	0
2	M	21	0	13	3	0
3	A	1	0	0	0	0
4	A	36	0	0	0	0
4	B	22	0	0	0	0
4	C	34	0	0	0	0
4	D	19	0	0	0	0
4	E	7	0	0	0	0
4	F	11	0	0	0	0
4	G	6	0	0	0	0
4	H	6	0	0	0	0
4	I	11	0	0	0	0
4	J	20	0	0	0	0
4	K	4	0	0	1	0
4	M	23	0	0	0	0
All	All	21847	0	21714	147	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 3.

All (147) 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:K:140:ASP:OD1	1:K:163:ARG:NH2	2.30	0.64
1:C:5:ARG:HG3	1:C:7:ASP:H	1.62	0.64
1:K:126:MET:O	1:K:160:ARG:NH2	2.31	0.63
1:G:23:ASN:ND2	1:G:26:ASP:OD2	2.28	0.61
1:J:81:GLU:HG2	1:J:85:ARG:HH22	1.66	0.61
1:D:33:GLU:HB3	1:D:212:ALA:HB2	1.83	0.60
1:G:116:MET:HB3	1:G:118:ARG:HH11	1.65	0.60
1:L:21:LEU:HD13	1:L:26:ASP:HB3	1.82	0.60
1:L:72:LYS:HZ1	2:L:301:H2U:H62	1.66	0.60
1:H:35:ARG:NH1	1:H:38:ILE:O	2.38	0.57
1:B:85:ARG:NH1	1:B:115:GLU:OE2	2.35	0.57
1:I:23:ASN:HB3	1:I:26:ASP:HB2	1.87	0.57
1:I:107:ARG:NH1	1:I:111:ASN:OD1	2.38	0.57
1:K:55:ILE:O	1:K:59:PHE:HB2	2.05	0.56
1:M:180:PRO:HA	1:M:200:ILE:HB	1.87	0.56
1:F:35:ARG:HD3	1:F:63:PHE:HB3	1.87	0.56
1:F:35:ARG:NH1	1:F:38:ILE:O	2.38	0.56
1:F:12:MET:HG2	1:F:13:ASN:HD22	1.70	0.55
1:F:139:ALA:HB3	1:F:163:ARG:HH22	1.72	0.55
1:L:126:MET:O	1:L:160:ARG:NH1	2.40	0.54
1:K:178:ILE:HD12	1:K:200:ILE:HD11	1.89	0.54
1:F:35:ARG:NH1	1:F:35:ARG:O	2.39	0.53
1:D:35:ARG:O	1:D:35:ARG:NH1	2.38	0.53
1:K:59:PHE:HD2	1:K:67:ILE:HD11	1.74	0.53
1:G:101:PRO:HA	1:H:135:ILE:HD11	1.91	0.53
1:C:178:ILE:HD12	1:C:200:ILE:HD11	1.92	0.52
1:E:85:ARG:NH1	1:E:115:GLU:OE1	2.43	0.52
1:H:8:VAL:HG21	1:H:176:PHE:HB2	1.90	0.52
1:E:56:ILE:HG23	1:E:67:ILE:HG21	1.91	0.51
1:E:61:LYS:HG2	1:G:9:MET:HA	1.93	0.51
1:K:60:ARG:NH1	1:K:91:GLY:O	2.42	0.51
1:J:220:GLU:HA	1:J:223:LYS:HG3	1.93	0.51
1:A:81:GLU:HG3	1:A:108:ALA:HB1	1.91	0.51
1:J:124:THR:HG22	1:J:142:ILE:HG22	1.93	0.51
1:G:178:ILE:HD12	1:G:200:ILE:HD11	1.92	0.50
1:A:56:ILE:HG23	1:A:67:ILE:HG21	1.93	0.50
1:L:72:LYS:HB3	1:L:98:HIS:CD2	2.47	0.50
1:M:24:ARG:NH2	1:M:58:GLU:OE2	2.39	0.50
1:D:14:ARG:HE	1:D:193:LEU:HD13	1.76	0.50
1:C:56:ILE:HG23	1:C:67:ILE:HG21	1.94	0.49
1:D:125:GLU:HB3	1:D:157:PRO:HD3	1.93	0.49
1:I:35:ARG:NE	1:I:63:PHE:O	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:LEU:HD12	1:D:222:ILE:HG21	1.93	0.49
1:G:194:ARG:HH21	1:G:195:PHE:HZ	1.61	0.49
1:H:35:ARG:HH12	1:H:39:ASP:HA	1.77	0.49
1:M:72:LYS:NZ	2:M:301:H2U:H62	2.28	0.49
1:D:72:LYS:CE	2:D:301:H2U:H62	2.43	0.48
1:M:72:LYS:HB3	1:M:98:HIS:CD2	2.47	0.48
1:D:85:ARG:NH2	1:D:115:GLU:OE1	2.40	0.48
1:D:139:ALA:HB3	1:D:163:ARG:HH21	1.77	0.48
1:H:56:ILE:HG23	1:H:67:ILE:HG21	1.95	0.48
1:K:23:ASN:HB3	1:K:26:ASP:HB2	1.95	0.48
1:J:72:LYS:HB3	1:J:98:HIS:CD2	2.48	0.48
1:H:178:ILE:HD12	1:H:200:ILE:HD11	1.96	0.48
1:K:87:THR:HG21	1:K:95:ILE:HD12	1.96	0.48
1:L:193:LEU:HD21	1:L:222:ILE:HG23	1.94	0.48
1:E:118:ARG:CZ	1:G:118:ARG:HH21	2.27	0.48
1:K:135:ILE:HD11	1:L:101:PRO:HA	1.96	0.48
1:L:56:ILE:HG23	1:L:67:ILE:HG21	1.96	0.47
1:F:126:MET:O	1:F:160:ARG:NH1	2.48	0.47
1:G:34:VAL:HG12	1:G:212:ALA:HA	1.95	0.47
1:F:72:LYS:HB3	1:F:98:HIS:CD2	2.50	0.47
1:J:24:ARG:NH2	1:J:58:GLU:OE2	2.48	0.47
1:K:42:LYS:HD3	1:K:200:ILE:HD13	1.97	0.47
1:K:180:PRO:HA	1:K:200:ILE:HB	1.96	0.47
1:A:100[A]:PHE:CD2	1:B:135:ILE:HG12	2.51	0.46
1:I:178:ILE:HG22	1:I:198:ALA:HB3	1.98	0.46
1:A:72:LYS:HB3	1:A:98:HIS:CD2	2.50	0.46
1:E:14:ARG:HE	1:E:193:LEU:HD13	1.80	0.46
1:F:72:LYS:HE3	1:F:72:LYS:HB2	1.78	0.46
1:C:24:ARG:NH2	1:C:58:GLU:OE2	2.46	0.46
1:F:24:ARG:NH2	1:F:58:GLU:OE2	2.41	0.45
1:K:128:HIS:NE2	1:L:101:PRO:O	2.34	0.45
1:E:17:LEU:HD22	1:E:34:VAL:HG21	1.97	0.45
1:L:72:LYS:NZ	2:L:301:H2U:H62	2.30	0.45
1:G:13:ASN:ND2	1:G:37:TYR:O	2.46	0.45
1:G:100[A]:PHE:CG	1:G:101:PRO:HD3	2.52	0.45
1:I:163:ARG:HD2	1:I:166:ARG:HH21	1.82	0.45
1:J:34:VAL:HG12	1:J:212:ALA:HA	1.98	0.45
1:L:13:ASN:ND2	1:L:37:TYR:O	2.46	0.45
1:A:35:ARG:HD3	1:A:63:PHE:HB3	1.99	0.45
1:E:78:GLU:HG2	1:F:203:ARG:NH1	2.31	0.45
1:F:193:LEU:HD12	1:F:222:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:23:ASN:OD1	1:K:24:ARG:N	2.45	0.45
1:K:57:ALA:C	1:K:59:PHE:H	2.20	0.45
1:G:24:ARG:NH2	1:G:58:GLU:OE2	2.40	0.44
1:M:165:SER:HB2	1:M:195:PHE:CE1	2.52	0.44
1:C:15:LEU:HB3	1:C:38:ILE:HG22	1.99	0.44
1:J:188:ASP:HA	1:J:189:PRO:HD3	1.88	0.44
1:F:58:GLU:HG2	1:F:62:ARG:HD2	2.00	0.44
1:E:100[B]:PHE:CG	1:E:101:PRO:HD3	2.53	0.44
1:L:45:TYR:N	1:L:46:PRO:HD2	2.32	0.44
1:C:104:ASP:OD1	1:C:105:SER:N	2.50	0.44
1:D:100[A]:PHE:CG	1:D:101:PRO:HD3	2.53	0.44
1:I:160:ARG:HB2	1:I:163:ARG:HB2	1.98	0.44
1:K:78:GLU:HG2	1:L:203:ARG:HH12	1.83	0.44
1:K:42:LYS:NZ	4:K:404:HOH:O	2.38	0.44
1:M:180:PRO:HG3	2:M:301:H2U:H52	2.00	0.44
1:M:156:GLY:O	1:M:180:PRO:HD2	2.18	0.44
1:A:35:ARG:NH1	1:A:38:ILE:O	2.51	0.43
1:L:24:ARG:NH2	1:L:58:GLU:OE2	2.35	0.43
1:B:156:GLY:O	1:B:180:PRO:HD2	2.18	0.43
1:K:219:ILE:O	1:K:223:LYS:N	2.50	0.43
1:C:61:LYS:HB2	1:C:61:LYS:HE3	1.72	0.43
1:H:14:ARG:HE	1:H:193:LEU:HD22	1.83	0.43
1:M:72:LYS:HZ1	2:M:301:H2U:H62	1.82	0.43
1:A:135:ILE:HG12	1:B:100[B]:PHE:CD2	2.54	0.43
1:F:219:ILE:HG22	1:F:223:LYS:HD3	2.00	0.43
1:C:110:LEU:HD21	1:C:151:VAL:HG22	2.01	0.43
1:D:193:LEU:HD12	1:D:222:ILE:HD13	2.00	0.43
1:G:12:MET:HG2	1:G:13:ASN:ND2	2.34	0.42
1:I:125:GLU:HB3	1:I:157:PRO:HG3	2.01	0.42
1:F:34:VAL:HG12	1:F:212:ALA:HA	2.01	0.42
1:K:72:LYS:HG2	1:K:98:HIS:HD2	1.84	0.42
1:K:98:HIS:CE1	1:L:100:PHE:HE1	2.37	0.42
1:D:72:LYS:NZ	2:D:301:H2U:H62	2.35	0.42
1:I:157:PRO:HB2	1:I:160:ARG:HG2	2.01	0.42
1:G:100[A]:PHE:CD2	1:G:101:PRO:HD3	2.54	0.42
1:D:201:VAL:HG13	1:D:204:SER:HB3	2.01	0.42
1:E:72:LYS:HB3	1:E:98:HIS:CD2	2.54	0.42
1:G:30:VAL:HG13	1:G:211:PRO:HB3	2.02	0.42
1:G:72:LYS:HB3	1:G:98:HIS:CD2	2.55	0.42
1:H:28:LEU:HD13	1:H:62:ARG:NH1	2.35	0.42
1:I:191:GLU:HG2	1:I:194:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ARG:NH2	1:B:58:GLU:OE2	2.46	0.42
1:B:100[A]:PHE:CG	1:B:101:PRO:HD3	2.54	0.42
1:A:178:ILE:HD12	1:A:200:ILE:HD11	2.03	0.41
1:I:43:ILE:HD11	1:I:56:ILE:HG12	2.01	0.41
1:C:100[B]:PHE:CG	1:C:101:PRO:HD3	2.55	0.41
1:D:28:LEU:HD13	1:D:62:ARG:NH1	2.35	0.41
1:H:23:ASN:ND2	1:H:26:ASP:H	2.18	0.41
1:K:76:ILE:HG13	1:K:79:THR:H	1.85	0.41
1:L:152:LYS:HB3	1:L:152:LYS:HE2	1.85	0.41
1:A:100[B]:PHE:CG	1:A:101:PRO:HD3	2.55	0.41
1:A:37:TYR:HB3	1:A:219:ILE:CD1	2.51	0.41
1:C:72:LYS:HB3	1:C:98:HIS:CD2	2.56	0.41
1:M:104:ASP:OD1	1:M:105:SER:N	2.54	0.41
1:F:156:GLY:O	1:F:180:PRO:HD2	2.21	0.41
1:F:182:VAL:HB	1:F:201:VAL:HG22	2.02	0.41
1:J:216:ALA:O	1:J:220:GLU:HG2	2.21	0.41
1:K:94:ALA:HB2	1:K:119:GLU:HB2	2.03	0.41
1:F:37:TYR:CZ	1:F:216:ALA:HB2	2.55	0.41
1:D:30:VAL:HG13	1:D:211:PRO:HB3	2.03	0.40
1:D:156:GLY:O	1:D:180:PRO:HD2	2.21	0.40
1:E:178:ILE:HD12	1:E:200:ILE:HD11	2.04	0.40
1:H:14:ARG:HE	1:H:193:LEU:HD13	1.87	0.40
1:H:156:GLY:O	1:H:180:PRO:HD2	2.22	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	220/228 (96%)	215 (98%)	5 (2%)	0	100	100
1	B	219/228 (96%)	213 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	224/228 (98%)	217 (97%)	7 (3%)	0	100	100
1	D	216/228 (95%)	211 (98%)	5 (2%)	0	100	100
1	E	216/228 (95%)	208 (96%)	8 (4%)	0	100	100
1	F	214/228 (94%)	205 (96%)	9 (4%)	0	100	100
1	G	212/228 (93%)	206 (97%)	6 (3%)	0	100	100
1	H	214/228 (94%)	209 (98%)	4 (2%)	1 (0%)	29	35
1	I	191/228 (84%)	186 (97%)	5 (3%)	0	100	100
1	J	216/228 (95%)	209 (97%)	7 (3%)	0	100	100
1	K	214/228 (94%)	205 (96%)	9 (4%)	0	100	100
1	L	211/228 (92%)	201 (95%)	9 (4%)	1 (0%)	29	35
1	M	217/228 (95%)	211 (97%)	6 (3%)	0	100	100
All	All	2784/2964 (94%)	2696 (97%)	86 (3%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	194	ARG
1	H	73	VAL

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	176/182 (97%)	176 (100%)	0	100	100
1	B	175/182 (96%)	175 (100%)	0	100	100
1	C	180/182 (99%)	180 (100%)	0	100	100
1	D	172/182 (94%)	172 (100%)	0	100	100
1	E	172/182 (94%)	172 (100%)	0	100	100
1	F	170/182 (93%)	170 (100%)	0	100	100
1	G	168/182 (92%)	168 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	170/182 (93%)	170 (100%)	0	100 100
1	I	156/182 (86%)	155 (99%)	1 (1%)	86 94
1	J	172/182 (94%)	172 (100%)	0	100 100
1	K	170/182 (93%)	170 (100%)	0	100 100
1	L	167/182 (92%)	166 (99%)	1 (1%)	86 94
1	M	173/182 (95%)	172 (99%)	1 (1%)	86 94
All	All	2221/2366 (94%)	2218 (100%)	3 (0%)	93 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	132	GLU
1	L	59	PHE
1	M	115	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	98	HIS
1	M	98	HIS

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 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	H2U	D	301	-	22,22,22	0.67	0	28,33,33	1.76	4 (14%)
2	H2U	F	301	-	22,22,22	0.64	0	28,33,33	1.74	5 (17%)
2	H2U	L	301	-	22,22,22	0.67	0	28,33,33	1.75	4 (14%)
2	H2U	A	301	-	22,22,22	0.64	0	28,33,33	1.73	5 (17%)
2	H2U	J	301	-	22,22,22	0.64	0	28,33,33	1.74	4 (14%)
2	H2U	G	301	-	22,22,22	0.63	0	28,33,33	1.73	4 (14%)
2	H2U	K	301	-	22,22,22	0.61	0	28,33,33	1.71	5 (17%)
2	H2U	H	301	-	22,22,22	0.65	0	28,33,33	1.74	4 (14%)
2	H2U	B	301	-	22,22,22	0.66	0	28,33,33	1.73	5 (17%)
2	H2U	M	301	-	22,22,22	0.64	0	28,33,33	1.77	4 (14%)
2	H2U	E	301	-	22,22,22	0.66	0	28,33,33	1.74	4 (14%)
2	H2U	C	301	-	22,22,22	0.68	0	28,33,33	1.78	5 (17%)

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	H2U	D	301	-	-	5/10/39/39	0/2/2/2
2	H2U	F	301	-	-	3/10/39/39	0/2/2/2
2	H2U	L	301	-	-	5/10/39/39	0/2/2/2
2	H2U	A	301	-	-	6/10/39/39	0/2/2/2
2	H2U	J	301	-	-	8/10/39/39	0/2/2/2
2	H2U	G	301	-	-	5/10/39/39	0/2/2/2
2	H2U	K	301	-	-	3/10/39/39	0/2/2/2
2	H2U	H	301	-	-	4/10/39/39	0/2/2/2
2	H2U	B	301	-	-	3/10/39/39	0/2/2/2
2	H2U	M	301	-	-	8/10/39/39	0/2/2/2
2	H2U	E	301	-	-	3/10/39/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	H2U	C	301	-	-	6/10/39/39	0/2/2/2

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	H2U	C4-N3-C2	-5.80	120.98	125.79
2	L	301	H2U	C4-N3-C2	-5.77	121.01	125.79
2	M	301	H2U	C4-N3-C2	-5.73	121.03	125.79
2	H	301	H2U	C4-N3-C2	-5.66	121.09	125.79
2	E	301	H2U	C4-N3-C2	-5.57	121.17	125.79
2	J	301	H2U	C4-N3-C2	-5.57	121.17	125.79
2	B	301	H2U	C4-N3-C2	-5.54	121.20	125.79
2	G	301	H2U	C4-N3-C2	-5.53	121.20	125.79
2	F	301	H2U	C4-N3-C2	-5.41	121.31	125.79
2	C	301	H2U	N3-C2-N1	5.40	122.36	116.65
2	C	301	H2U	C4-N3-C2	-5.28	121.41	125.79
2	K	301	H2U	C4-N3-C2	-5.22	121.47	125.79
2	A	301	H2U	C4-N3-C2	-5.18	121.49	125.79
2	M	301	H2U	N3-C2-N1	5.18	122.13	116.65
2	L	301	H2U	N3-C2-N1	5.15	122.09	116.65
2	J	301	H2U	N3-C2-N1	5.13	122.08	116.65
2	D	301	H2U	N3-C2-N1	5.09	122.04	116.65
2	H	301	H2U	N3-C2-N1	5.08	122.03	116.65
2	F	301	H2U	N3-C2-N1	5.07	122.02	116.65
2	E	301	H2U	N3-C2-N1	4.98	121.92	116.65
2	K	301	H2U	N3-C2-N1	4.95	121.89	116.65
2	G	301	H2U	N3-C2-N1	4.94	121.88	116.65
2	B	301	H2U	N3-C2-N1	4.94	121.88	116.65
2	A	301	H2U	N3-C2-N1	4.85	121.79	116.65
2	M	301	H2U	O2-C2-N1	-3.42	118.81	123.11
2	E	301	H2U	O2-C2-N1	-3.41	118.83	123.11
2	C	301	H2U	O2-C2-N1	-3.40	118.83	123.11
2	G	301	H2U	O2-C2-N1	-3.40	118.83	123.11
2	K	301	H2U	O2-C2-N1	-3.34	118.91	123.11
2	F	301	H2U	O2-C2-N1	-3.33	118.92	123.11
2	J	301	H2U	O2-C2-N1	-3.31	118.95	123.11
2	H	301	H2U	O2-C2-N1	-3.28	118.99	123.11
2	B	301	H2U	O2-C2-N1	-3.23	119.05	123.11
2	D	301	H2U	O2-C2-N1	-3.21	119.08	123.11
2	A	301	H2U	C5-C4-N3	3.04	120.06	116.65
2	A	301	H2U	O2-C2-N1	-3.03	119.30	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	301	H2U	O2-C2-N1	-3.03	119.31	123.11
2	K	301	H2U	C5-C4-N3	2.47	119.42	116.65
2	A	301	H2U	OP2-P-OP1	2.36	119.91	110.68
2	D	301	H2U	OP2-P-OP1	2.24	119.44	110.68
2	J	301	H2U	OP2-P-OP1	2.18	119.21	110.68
2	M	301	H2U	OP2-P-OP1	2.17	119.19	110.68
2	F	301	H2U	OP2-P-OP1	2.17	119.17	110.68
2	G	301	H2U	OP2-P-OP1	2.17	119.16	110.68
2	B	301	H2U	C5-C4-N3	2.15	119.07	116.65
2	H	301	H2U	OP2-P-OP1	2.08	118.83	110.68
2	L	301	H2U	OP2-P-OP1	2.08	118.81	110.68
2	E	301	H2U	OP2-P-OP1	2.07	118.79	110.68
2	C	301	H2U	OP2-P-OP1	2.06	118.76	110.68
2	K	301	H2U	OP2-P-OP1	2.04	118.66	110.68
2	B	301	H2U	OP2-P-OP1	2.03	118.63	110.68
2	C	301	H2U	C5-C4-N3	2.03	118.92	116.65
2	F	301	H2U	C5-C4-N3	2.00	118.90	116.65

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	H2U	C5'-O5'-P-OP1
2	A	301	H2U	C5'-O5'-P-OP2
2	A	301	H2U	C5'-O5'-P-OP3
2	A	301	H2U	O4'-C1'-N1-C6
2	B	301	H2U	O4'-C1'-N1-C6
2	C	301	H2U	C5'-O5'-P-OP2
2	C	301	H2U	C5'-O5'-P-OP3
2	C	301	H2U	O4'-C1'-N1-C6
2	D	301	H2U	O4'-C1'-N1-C6
2	E	301	H2U	O4'-C1'-N1-C6
2	F	301	H2U	O4'-C1'-N1-C6
2	G	301	H2U	O4'-C4'-C5'-O5'
2	G	301	H2U	O4'-C1'-N1-C6
2	H	301	H2U	O4'-C1'-N1-C6
2	J	301	H2U	C5'-O5'-P-OP2
2	J	301	H2U	C5'-O5'-P-OP3
2	J	301	H2U	O4'-C1'-N1-C6
2	K	301	H2U	O4'-C1'-N1-C6
2	L	301	H2U	O4'-C1'-N1-C6
2	M	301	H2U	C5'-O5'-P-OP1

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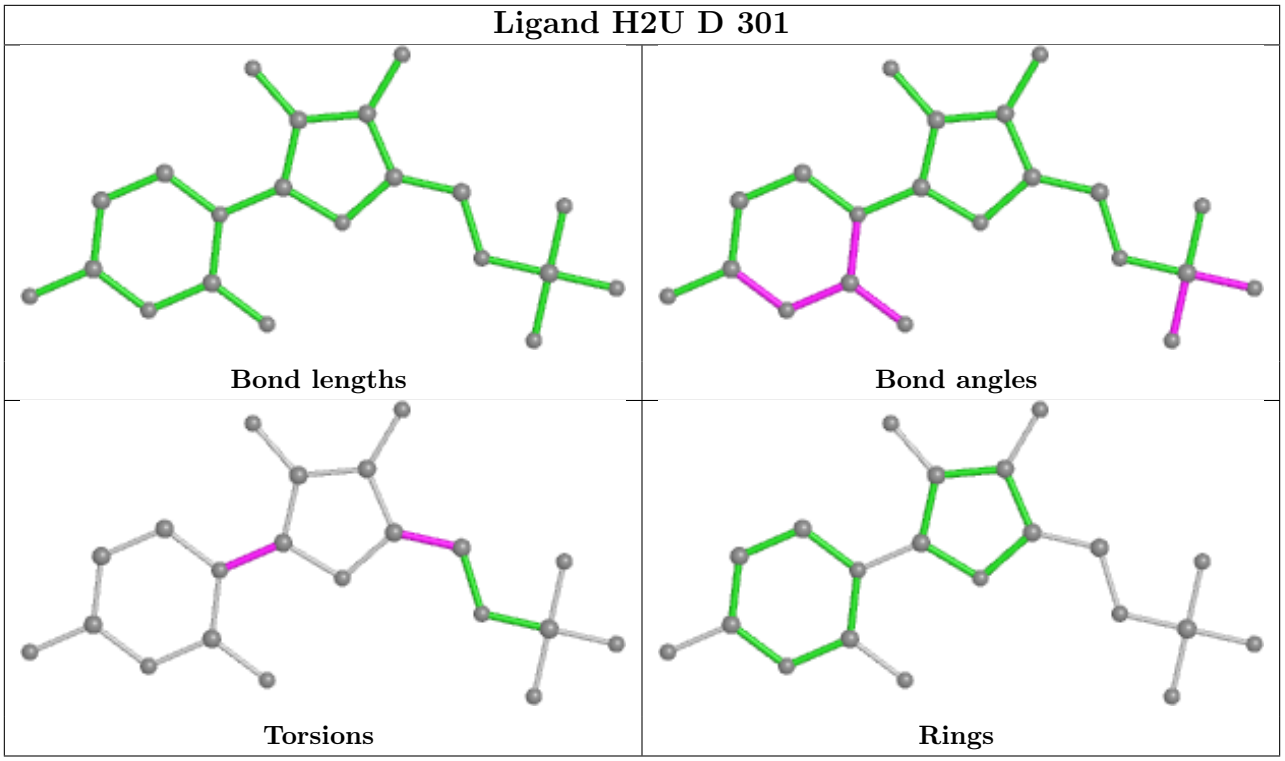
Mol	Chain	Res	Type	Atoms
2	M	301	H2U	C5'-O5'-P-OP2
2	M	301	H2U	C5'-O5'-P-OP3
2	M	301	H2U	O4'-C1'-N1-C6
2	J	301	H2U	O4'-C4'-C5'-O5'
2	J	301	H2U	C3'-C4'-C5'-O5'
2	M	301	H2U	O4'-C4'-C5'-O5'
2	M	301	H2U	C3'-C4'-C5'-O5'
2	E	301	H2U	O4'-C4'-C5'-O5'
2	E	301	H2U	O4'-C1'-N1-C2
2	A	301	H2U	O4'-C4'-C5'-O5'
2	F	301	H2U	O4'-C4'-C5'-O5'
2	A	301	H2U	O4'-C1'-N1-C2
2	K	301	H2U	O4'-C1'-N1-C2
2	B	301	H2U	O4'-C1'-N1-C2
2	C	301	H2U	O4'-C1'-N1-C2
2	F	301	H2U	O4'-C1'-N1-C2
2	G	301	H2U	O4'-C1'-N1-C2
2	K	301	H2U	O4'-C4'-C5'-O5'
2	D	301	H2U	C2'-C1'-N1-C6
2	D	301	H2U	O4'-C4'-C5'-O5'
2	L	301	H2U	C2'-C1'-N1-C6
2	H	301	H2U	O4'-C1'-N1-C2
2	J	301	H2U	O4'-C1'-N1-C2
2	G	301	H2U	C3'-C4'-C5'-O5'
2	M	301	H2U	O4'-C1'-N1-C2
2	L	301	H2U	C2'-C1'-N1-C2
2	C	301	H2U	C5'-O5'-P-OP1
2	J	301	H2U	C5'-O5'-P-OP1
2	J	301	H2U	C2'-C1'-N1-C2
2	M	301	H2U	C2'-C1'-N1-C2
2	H	301	H2U	O4'-C4'-C5'-O5'
2	L	301	H2U	O4'-C4'-C5'-O5'
2	D	301	H2U	O4'-C1'-N1-C2
2	D	301	H2U	C2'-C1'-N1-C2
2	L	301	H2U	O4'-C1'-N1-C2
2	B	301	H2U	O4'-C4'-C5'-O5'
2	C	301	H2U	O4'-C4'-C5'-O5'
2	G	301	H2U	C2'-C1'-N1-C2
2	H	301	H2U	C2'-C1'-N1-C2

There are no ring outliers.

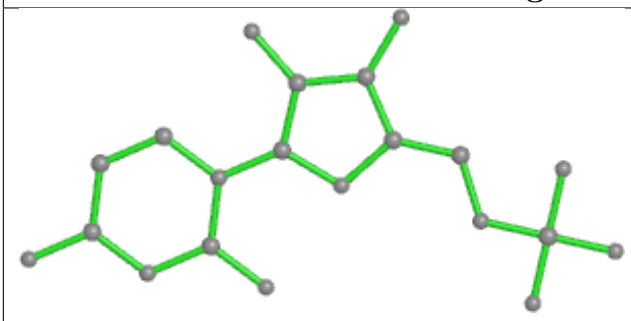
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	H2U	2	0
2	L	301	H2U	2	0
2	M	301	H2U	3	0

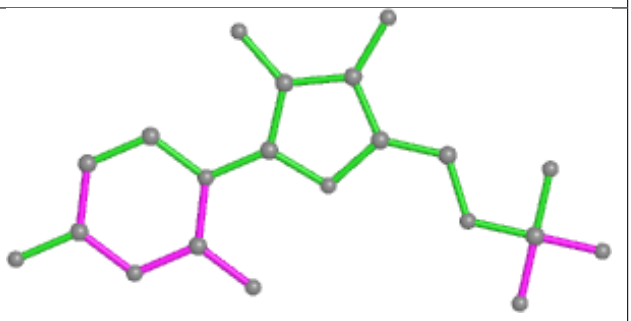
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



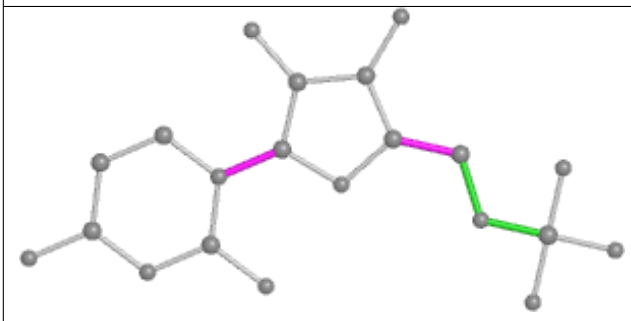
Ligand H2U F 301



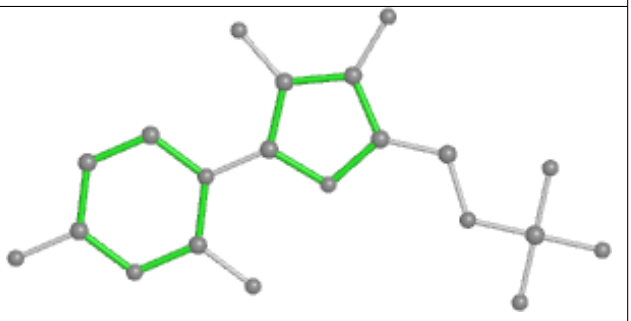
Bond lengths



Bond angles

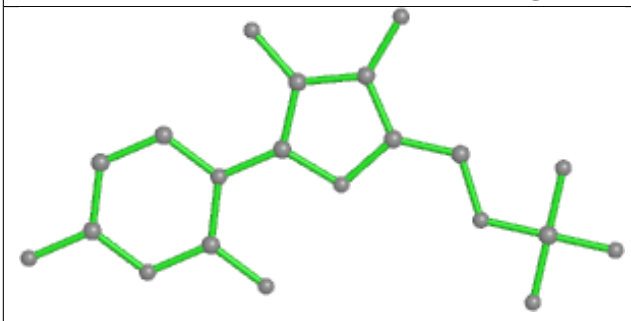


Torsions

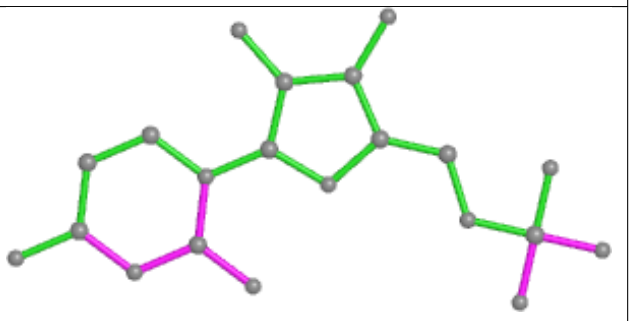


Rings

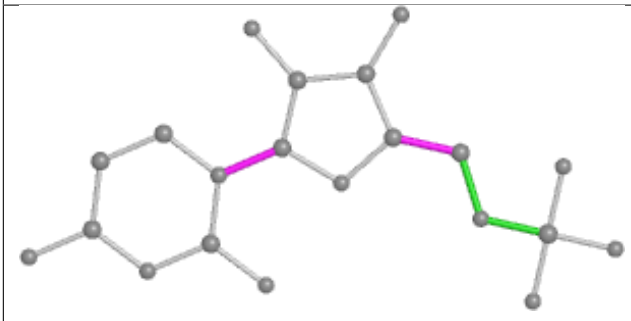
Ligand H2U L 301



Bond lengths



Bond angles



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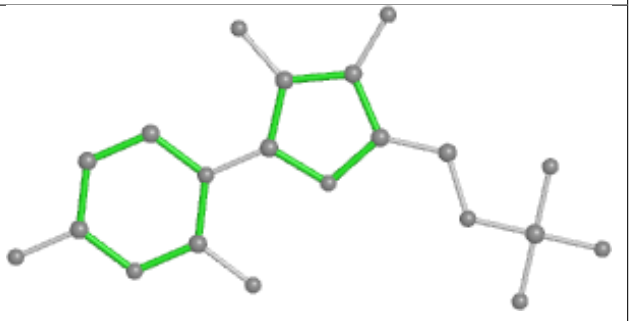
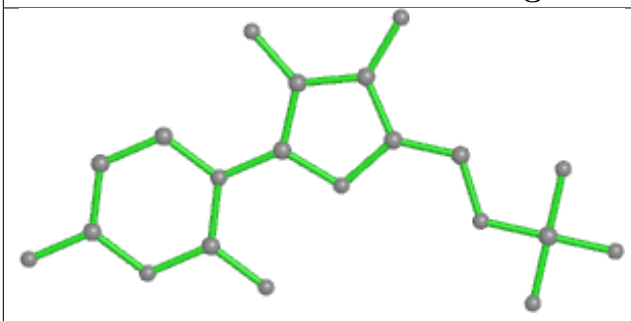


Rings

Ligand H2U A 301



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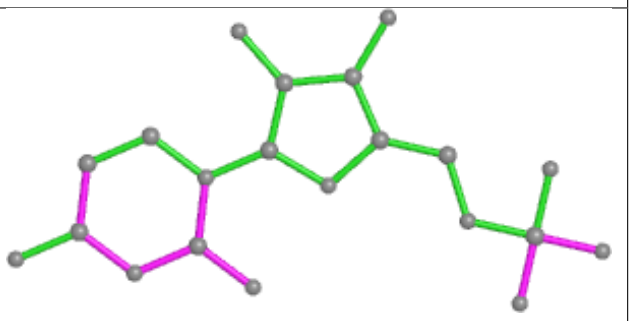
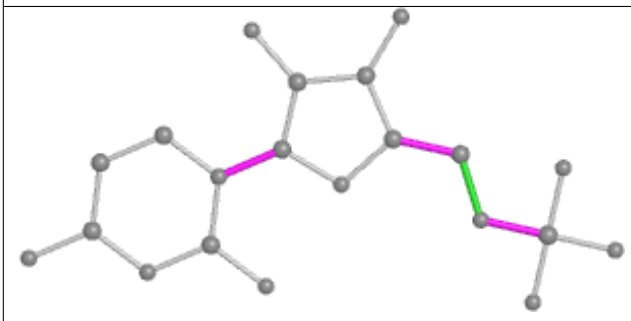
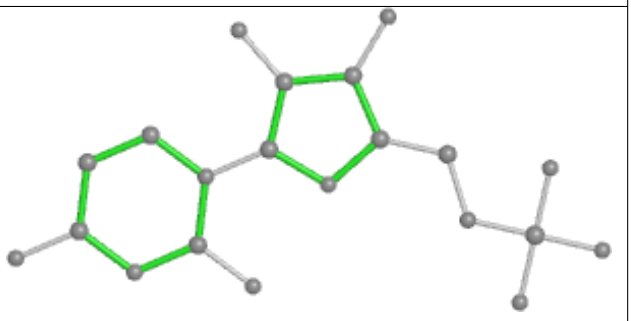


Bond angles

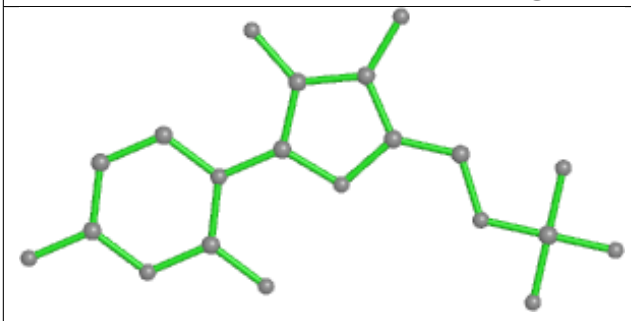


Torsions



Rings

Ligand H2U J 301



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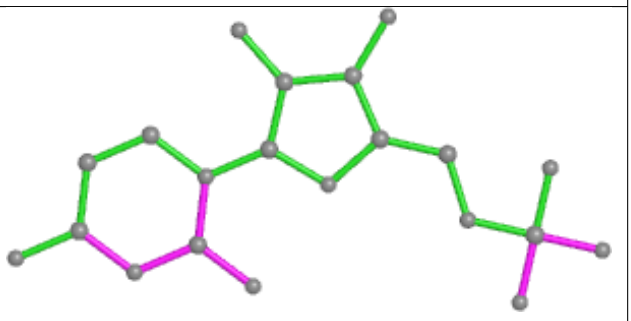
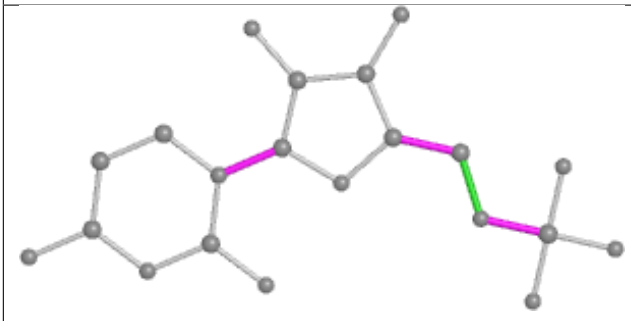


Bond angles



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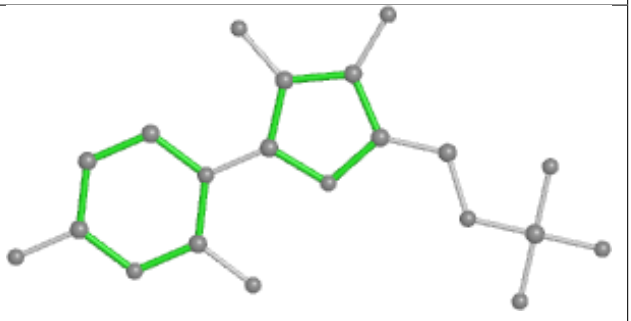
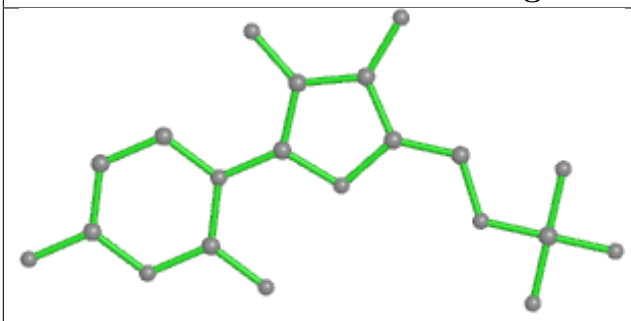


Rings

Ligand H2U G 301



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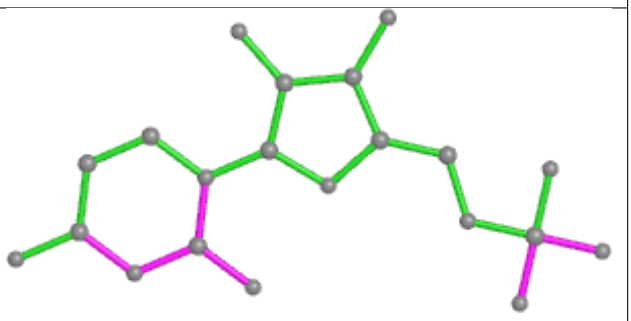
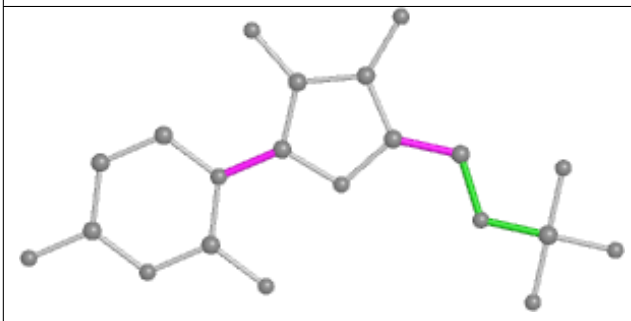


Bond angles



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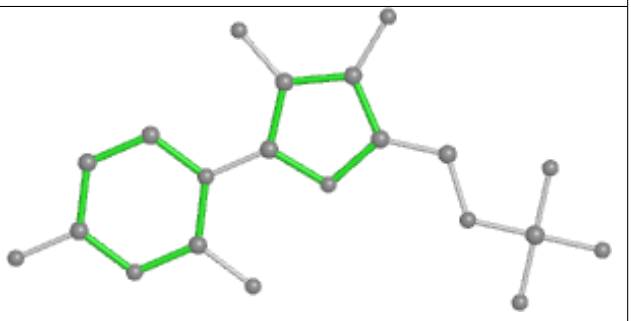
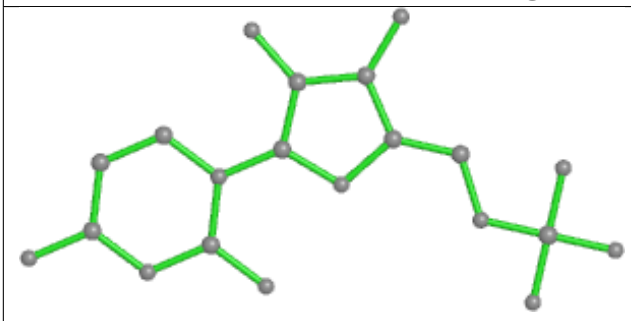
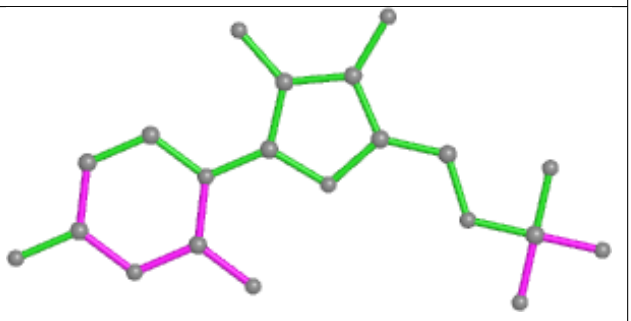


Rings

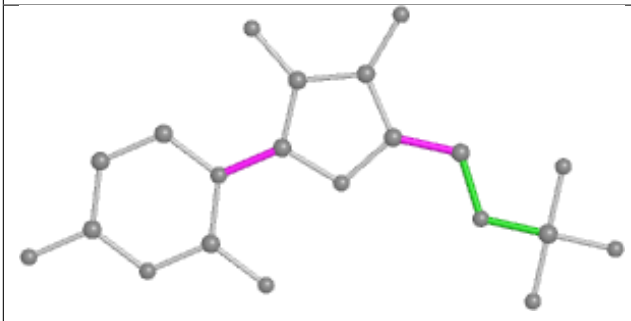
Ligand H2U K 301



Bond lengths



Bond angles



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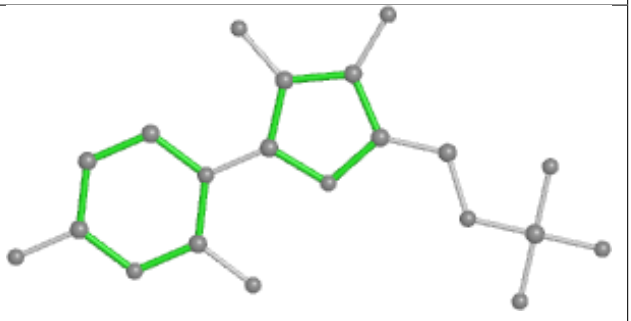
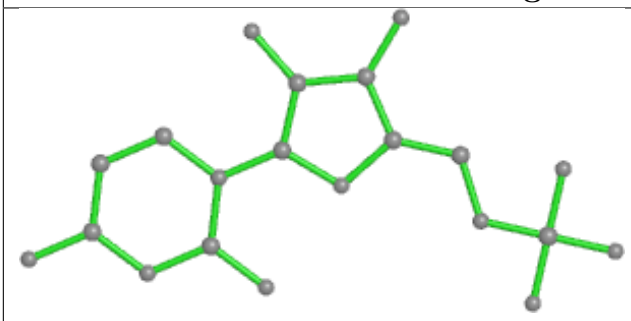
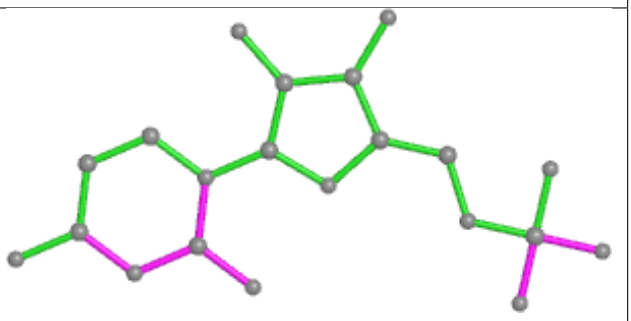
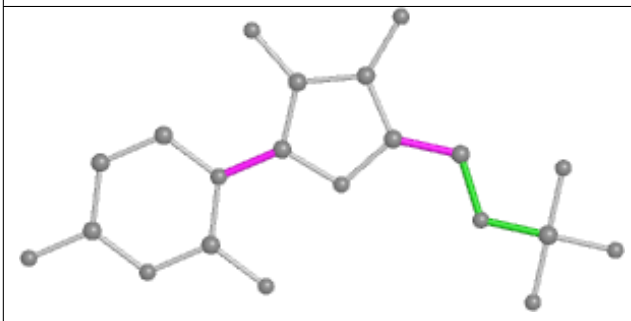
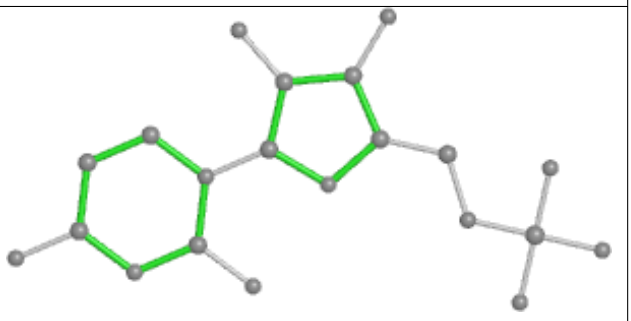
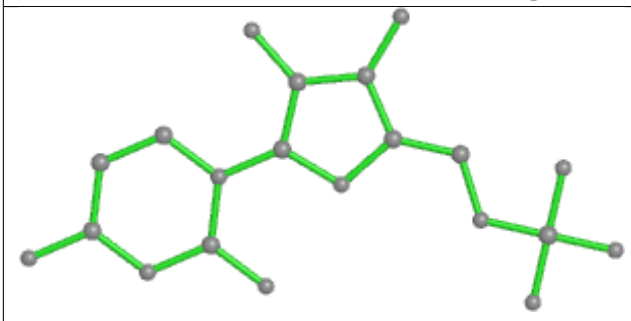
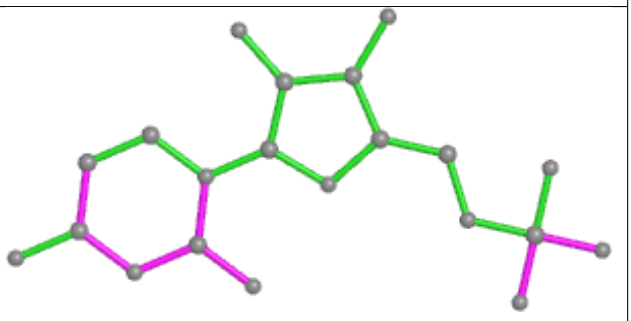
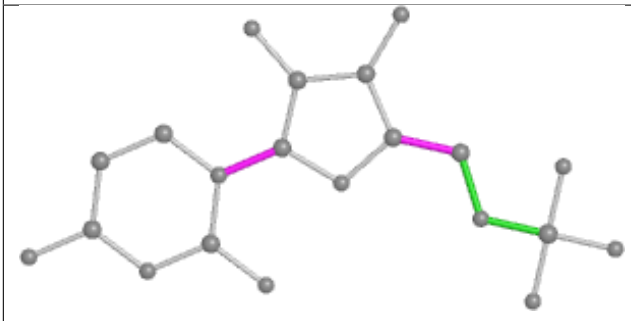
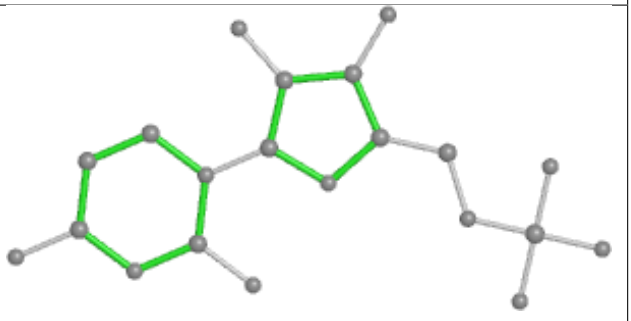
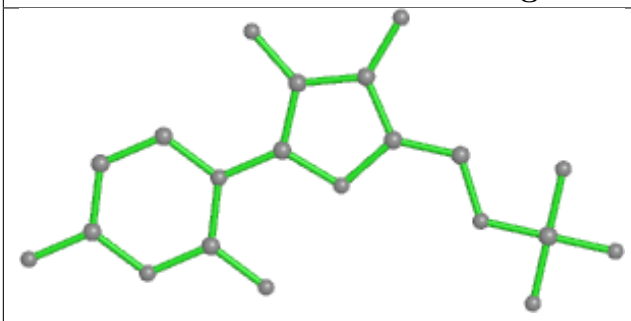
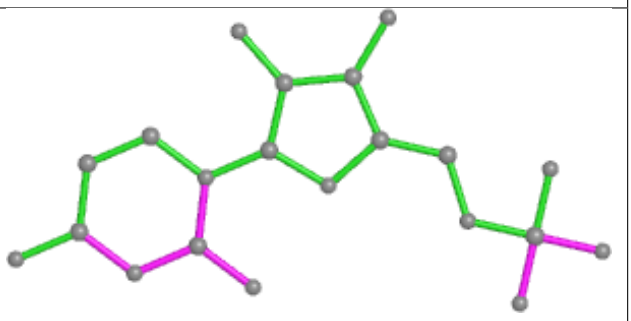
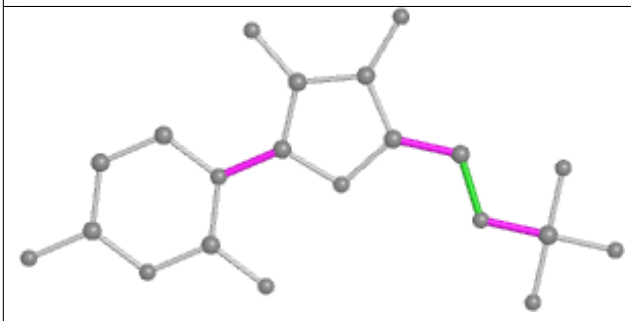
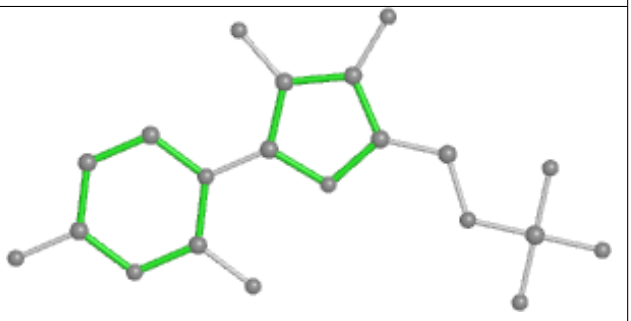
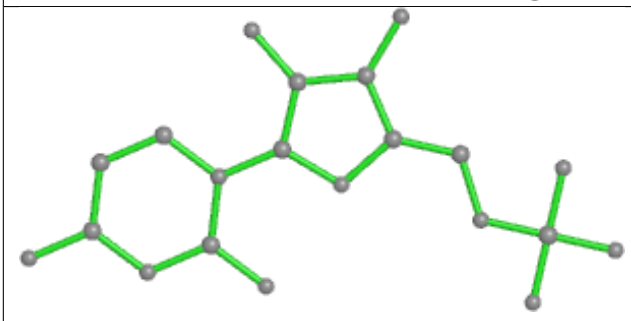
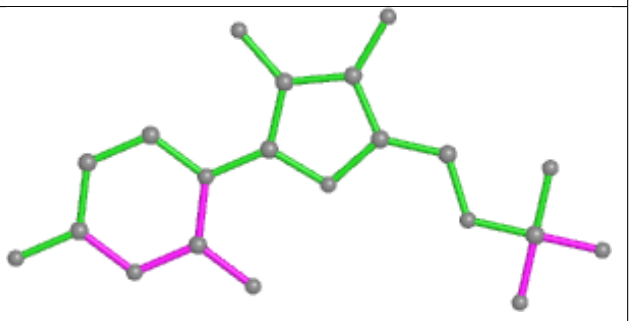
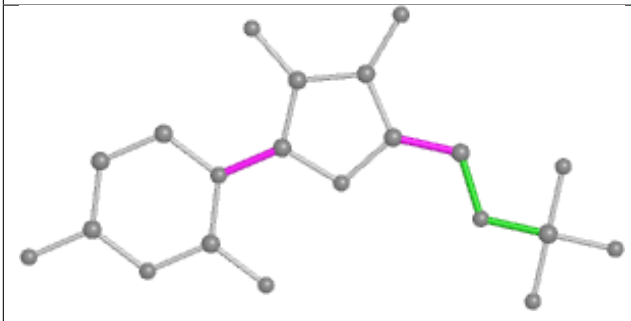
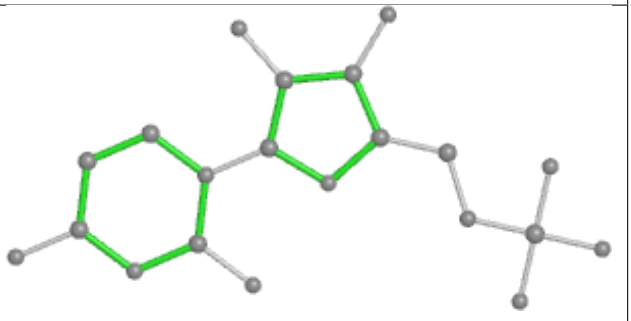


Rings

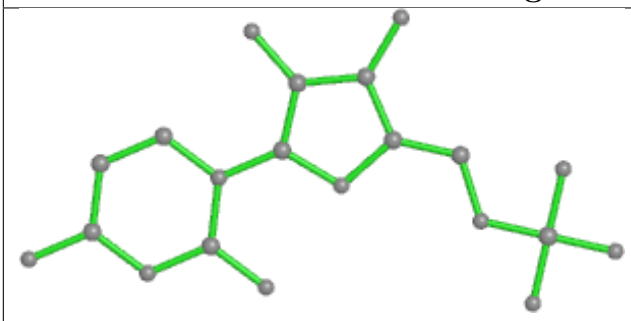
Ligand H2U H 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand H2U B 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

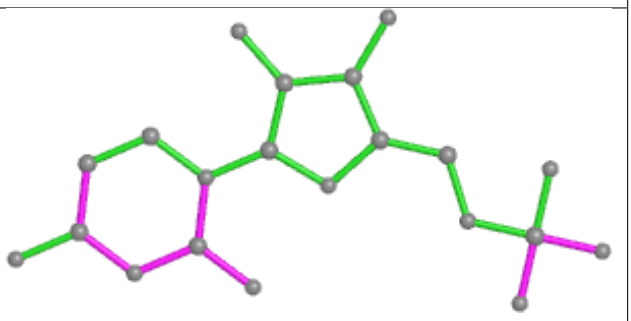
Ligand H2U M 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand H2U E 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

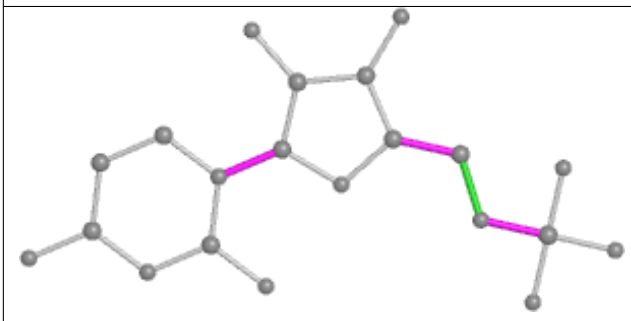
Ligand H2U C 301



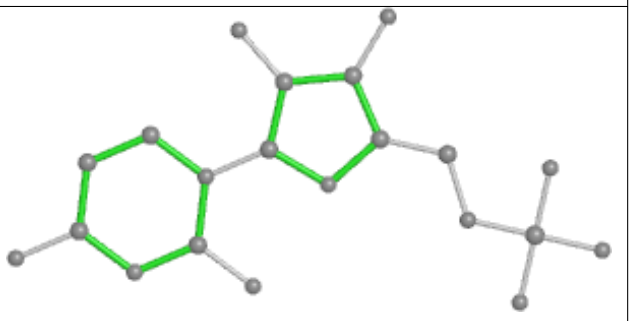
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	220/228 (96%)	-0.02	2 (0%) 84 88	27, 40, 65, 108	0
1	B	219/228 (96%)	0.34	8 (3%) 41 48	28, 53, 88, 146	0
1	C	225/228 (98%)	0.01	2 (0%) 84 88	30, 46, 84, 120	0
1	D	216/228 (94%)	0.46	18 (8%) 11 15	33, 58, 116, 143	0
1	E	217/228 (95%)	0.52	9 (4%) 37 44	49, 75, 102, 136	0
1	F	215/228 (94%)	0.57	20 (9%) 8 11	43, 73, 117, 146	0
1	G	213/228 (93%)	0.52	14 (6%) 18 23	54, 77, 114, 135	0
1	H	215/228 (94%)	0.40	7 (3%) 46 53	54, 76, 119, 145	0
1	I	197/228 (86%)	0.62	24 (12%) 4 6	40, 72, 125, 141	0
1	J	218/228 (95%)	0.22	6 (2%) 53 60	34, 66, 113, 145	0
1	K	216/228 (94%)	0.97	41 (18%) 1 1	67, 97, 127, 150	0
1	L	213/228 (93%)	1.17	49 (23%) 0 1	64, 100, 136, 153	0
1	M	218/228 (95%)	0.28	3 (1%) 75 80	33, 54, 90, 115	0
All	All	2802/2964 (94%)	0.46	203 (7%) 15 20	27, 69, 119, 153	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	137	GLY	6.4
1	L	159	THR	6.1
1	L	167	LEU	6.1
1	F	215	ALA	5.8
1	F	218	ILE	5.5
1	I	37	TYR	5.4
1	L	161	PRO	5.4
1	L	142	ILE	5.1
1	F	217	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	I	189	PRO	4.7
1	K	136	GLN	4.7
1	I	164	LEU	4.7
1	D	222	ILE	4.6
1	G	211	PRO	4.5
1	D	207	LEU	4.5
1	L	202	GLY	4.5
1	L	196	ALA	4.4
1	L	217	GLY	4.4
1	L	222	ILE	4.3
1	L	213	ALA	4.1
1	G	218	ILE	4.1
1	E	182	VAL	4.1
1	G	206	TYR	4.1
1	D	209	ASP	4.0
1	F	9	MET	4.0
1	K	171	ILE	4.0
1	L	155	VAL	3.9
1	B	8	VAL	3.8
1	B	222	ILE	3.8
1	F	208	ALA	3.8
1	K	103	ALA	3.8
1	K	142	ILE	3.8
1	D	195	PHE	3.7
1	E	167	LEU	3.7
1	K	149	LEU	3.7
1	F	206	TYR	3.6
1	F	15	LEU	3.6
1	L	171	ILE	3.6
1	E	224	ASP	3.5
1	A	6	VAL	3.5
1	K	225	LEU	3.5
1	L	182	VAL	3.5
1	L	187	GLY	3.5
1	G	207	LEU	3.4
1	I	160	ARG	3.4
1	G	209	ASP	3.4
1	K	105	SER	3.4
1	L	193	LEU	3.4
1	L	21	LEU	3.4
1	B	34	VAL	3.4
1	K	107	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	217	GLY	3.4
1	I	161	PRO	3.4
1	L	37	TYR	3.4
1	H	38	ILE	3.4
1	L	34	VAL	3.3
1	L	15	LEU	3.3
1	D	211	PRO	3.3
1	C	6	VAL	3.3
1	K	192	THR	3.3
1	G	38	ILE	3.2
1	E	218	ILE	3.2
1	F	211	PRO	3.2
1	L	144	ARG	3.2
1	F	36	GLU	3.2
1	D	37	TYR	3.2
1	L	127	SER	3.1
1	I	166	ARG	3.1
1	L	180	PRO	3.1
1	K	144	ARG	3.1
1	J	159	THR	3.1
1	G	208	ALA	3.0
1	D	8	VAL	3.0
1	C	5	ARG	3.0
1	J	191	GLU	3.0
1	E	34	VAL	2.9
1	D	220	GLU	2.9
1	K	38	ILE	2.9
1	L	135	ILE	2.9
1	I	199	ILE	2.9
1	E	223	LYS	2.9
1	L	164	LEU	2.9
1	L	139	ALA	2.9
1	L	184	ALA	2.9
1	L	205	ILE	2.8
1	I	157	PRO	2.8
1	H	218	ILE	2.8
1	K	124	THR	2.8
1	D	38	ILE	2.8
1	G	215	ALA	2.8
1	K	180	PRO	2.8
1	K	135	ILE	2.8
1	L	100	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	35	ARG	2.8
1	H	63	PHE	2.7
1	L	103	ALA	2.7
1	M	189	PRO	2.7
1	L	134	PHE	2.7
1	K	160	ARG	2.7
1	K	41	VAL	2.7
1	K	164	LEU	2.7
1	D	214	ALA	2.7
1	K	195	PHE	2.7
1	L	206	TYR	2.7
1	K	223	LYS	2.7
1	L	183	GLY	2.7
1	F	34	VAL	2.7
1	L	125	GLU	2.6
1	L	158	SER	2.6
1	L	176	PHE	2.6
1	D	223	LYS	2.6
1	K	10	ASP	2.6
1	K	169	GLU	2.6
1	L	208	ALA	2.6
1	K	193	LEU	2.6
1	I	34	VAL	2.6
1	K	143	ALA	2.6
1	K	181	GLY	2.5
1	K	207	LEU	2.5
1	A	223	LYS	2.5
1	F	207	LEU	2.5
1	K	167	LEU	2.5
1	I	190	GLY	2.5
1	K	134	PHE	2.4
1	D	206	TYR	2.4
1	I	169	GLU	2.4
1	K	15	LEU	2.4
1	K	206	TYR	2.4
1	D	213	ALA	2.4
1	I	30	VAL	2.4
1	J	222	ILE	2.4
1	J	225	LEU	2.4
1	F	209	ASP	2.4
1	B	191	GLU	2.4
1	K	63	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	171	ILE	2.4
1	G	14	ARG	2.4
1	F	181	GLY	2.3
1	K	152	LYS	2.3
1	L	38	ILE	2.3
1	D	189	PRO	2.3
1	J	180	PRO	2.3
1	K	168	ARG	2.3
1	F	10	ASP	2.3
1	K	210	ASN	2.3
1	H	31	THR	2.3
1	K	11	VAL	2.3
1	G	192	THR	2.3
1	I	167	LEU	2.3
1	L	185	GLN	2.3
1	G	205	ILE	2.3
1	B	225	LEU	2.3
1	L	149	LEU	2.3
1	K	106	VAL	2.3
1	F	13	ASN	2.3
1	I	210	ASN	2.3
1	L	219	ILE	2.3
1	I	207	LEU	2.2
1	L	207	LEU	2.2
1	H	37	TYR	2.2
1	L	11	VAL	2.2
1	D	215	ALA	2.2
1	I	15	LEU	2.2
1	F	129	PRO	2.2
1	M	195	PHE	2.2
1	K	222	ILE	2.2
1	L	169	GLU	2.2
1	K	186	GLY	2.2
1	E	210	ASN	2.2
1	I	218	ILE	2.2
1	L	160	ARG	2.2
1	I	129	PRO	2.2
1	I	205	ILE	2.2
1	F	201	VAL	2.2
1	L	195	PHE	2.2
1	K	196	ALA	2.2
1	F	37	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	30	VAL	2.1
1	D	218	ILE	2.1
1	L	190	GLY	2.1
1	E	14	ARG	2.1
1	I	31	THR	2.1
1	B	7	ASP	2.1
1	J	218	ILE	2.1
1	F	204	SER	2.1
1	L	132	GLU	2.1
1	M	181	GLY	2.1
1	D	10	ASP	2.1
1	D	13	ASN	2.1
1	F	16	ILE	2.1
1	I	36	GLU	2.1
1	I	162	GLU	2.1
1	I	220	GLU	2.1
1	H	208	ALA	2.1
1	K	100	PHE	2.1
1	I	35	ARG	2.0
1	B	116	MET	2.0
1	K	176	PHE	2.0
1	L	194	ARG	2.0
1	L	209	ASP	2.0
1	G	13	ASN	2.0
1	H	193	LEU	2.0
1	G	107	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

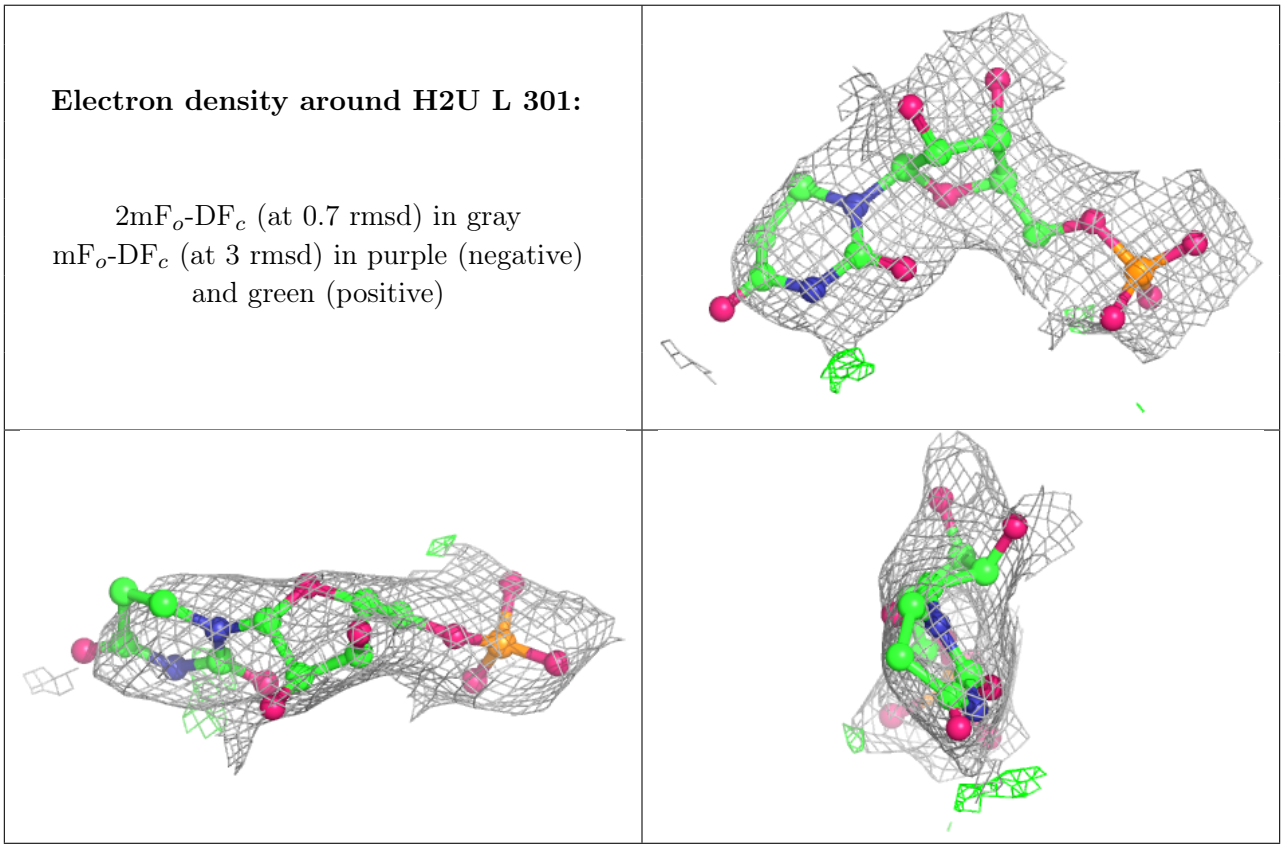
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	H2U	L	301	21/21	0.90	0.17	122,125,141,143	0
2	H2U	M	301	21/21	0.90	0.14	59,64,78,79	0
2	H2U	J	301	21/21	0.92	0.14	62,68,83,86	0
2	H2U	K	301	21/21	0.92	0.17	78,83,91,92	0
3	CL	A	302	1/1	0.92	0.10	78,78,78,78	1
2	H2U	F	301	21/21	0.93	0.15	69,74,84,87	0
2	H2U	G	301	21/21	0.94	0.13	71,74,82,84	0
2	H2U	D	301	21/21	0.94	0.16	55,59,71,73	0
2	H2U	H	301	21/21	0.95	0.12	70,75,82,85	0
2	H2U	B	301	21/21	0.97	0.11	42,44,52,56	0
2	H2U	E	301	21/21	0.97	0.11	62,70,73,74	0
2	H2U	A	301	21/21	0.98	0.13	32,34,36,38	0
2	H2U	C	301	21/21	0.98	0.13	35,38,45,47	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

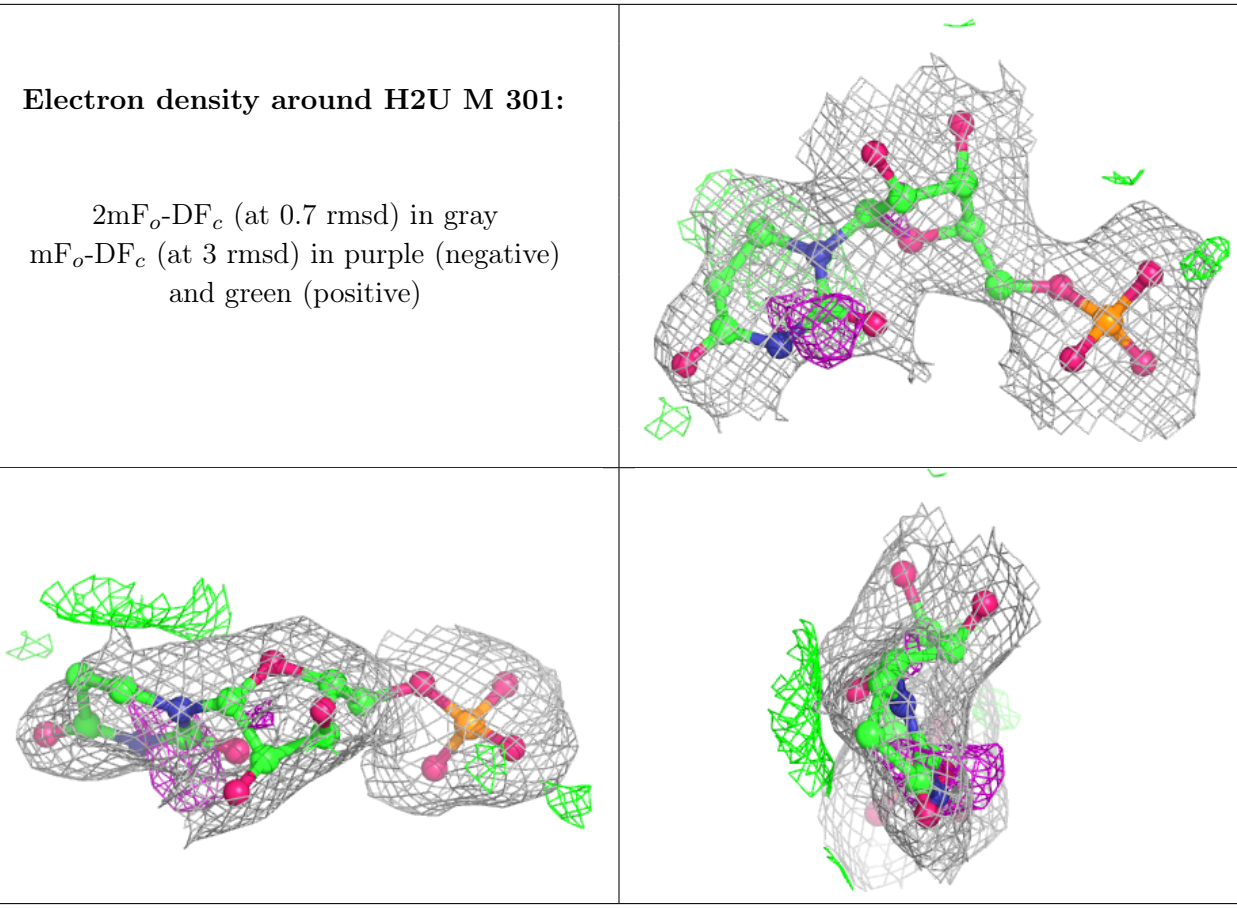
Electron density around H2U L 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



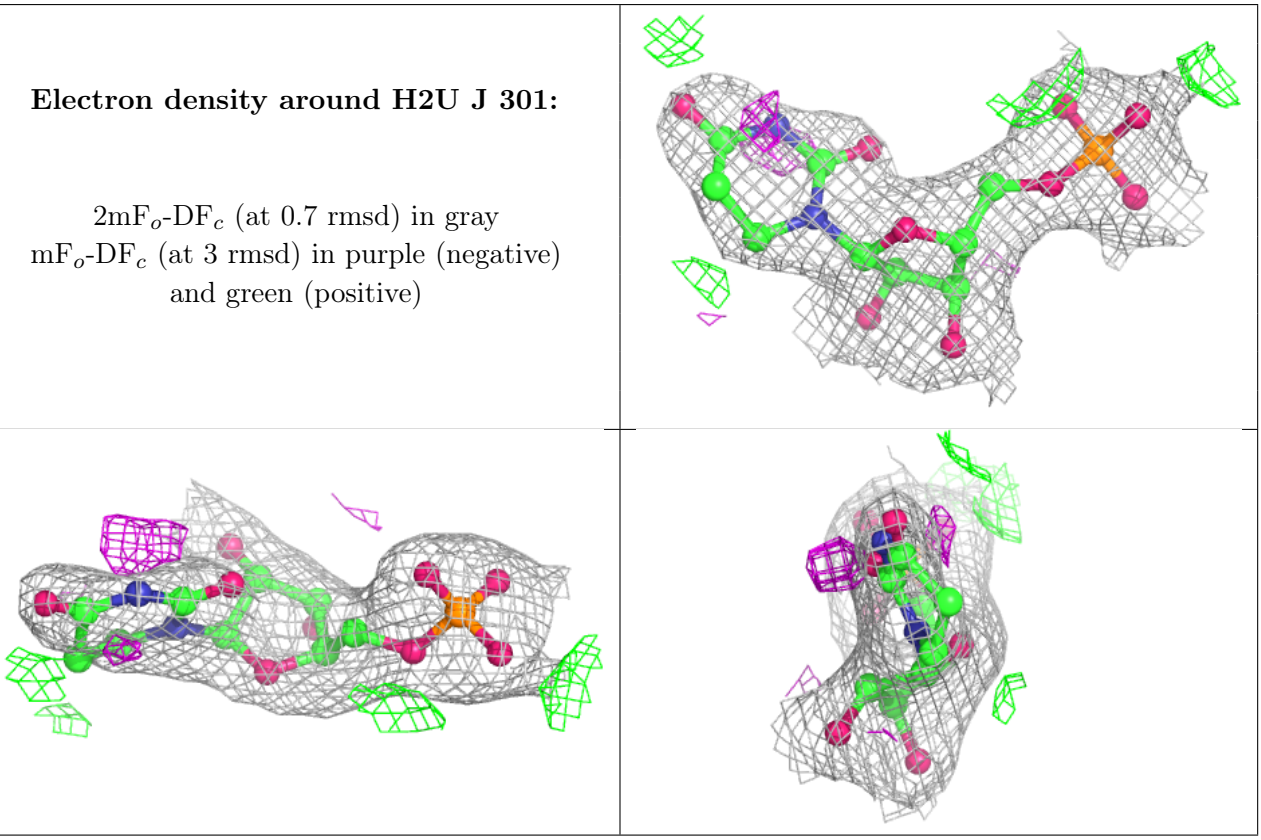
Electron density around H2U M 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



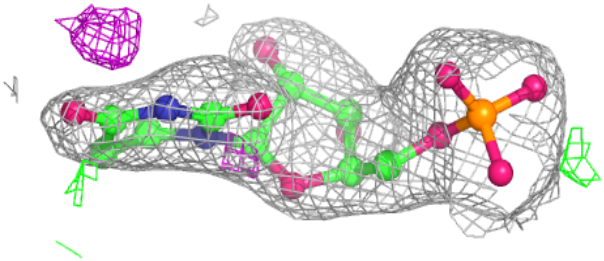
Electron density around H2U J 301:

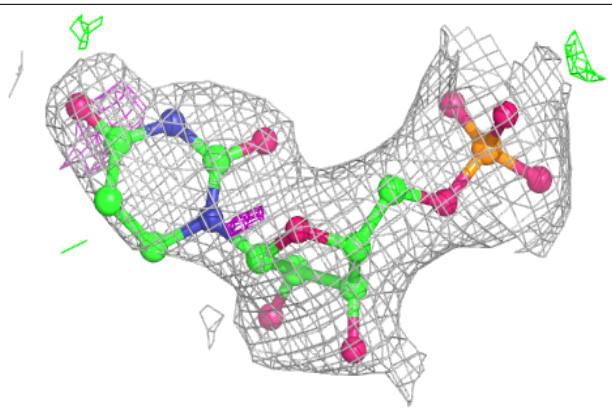
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

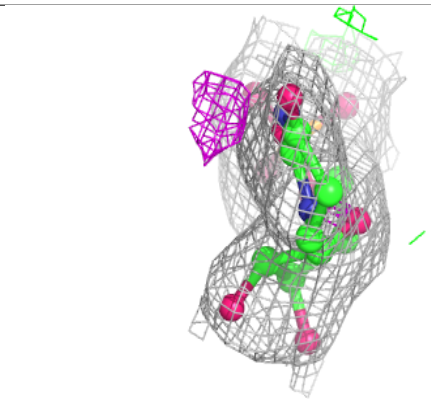


Electron density around H2U K 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

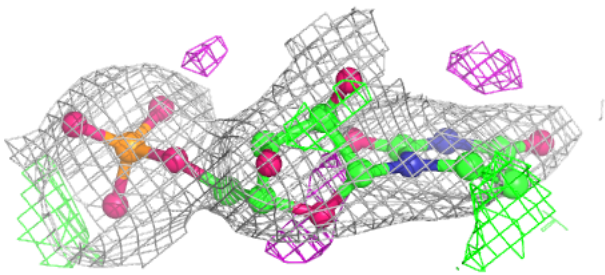


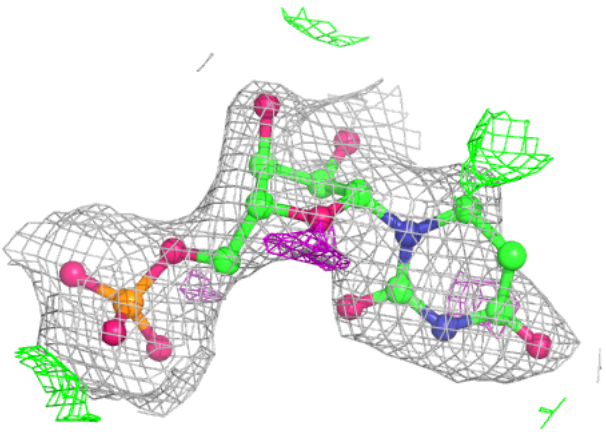


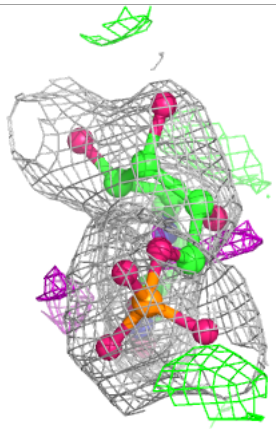


Electron density around H2U F 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

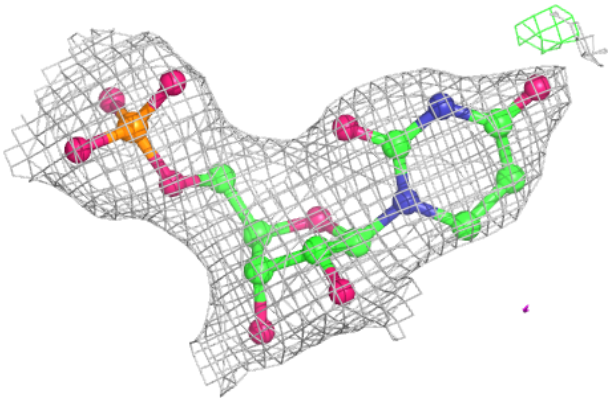


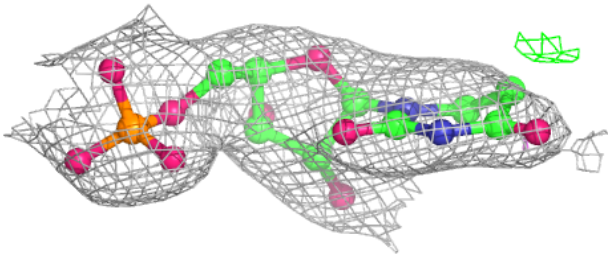


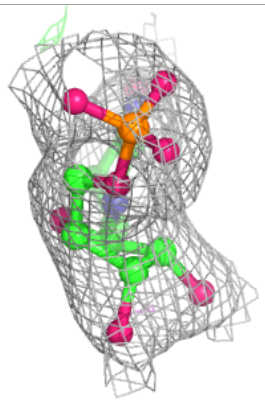


Electron density around H2U G 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

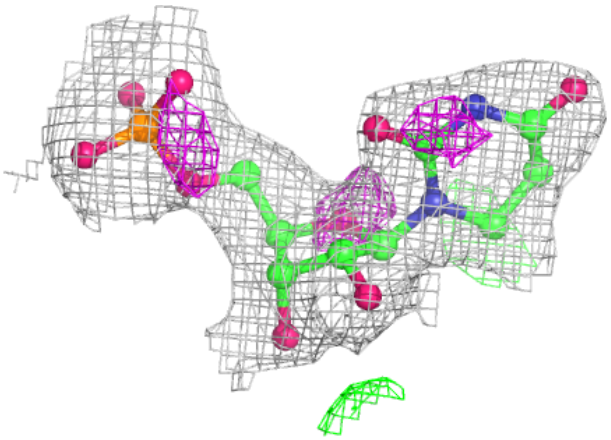


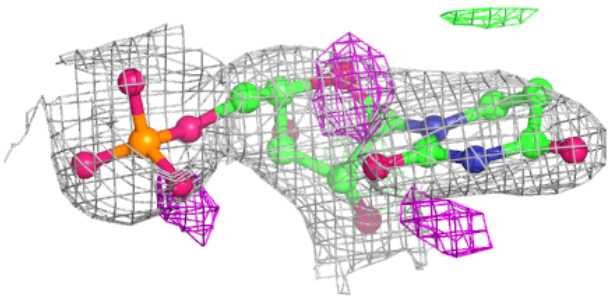


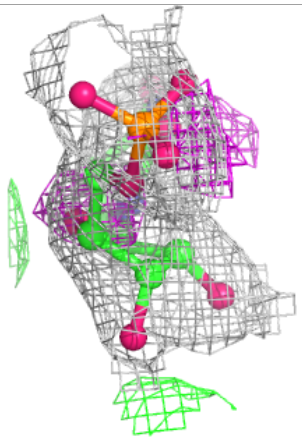


Electron density around H2U D 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

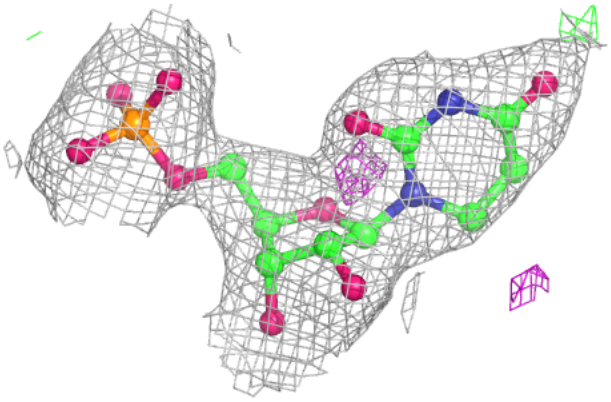


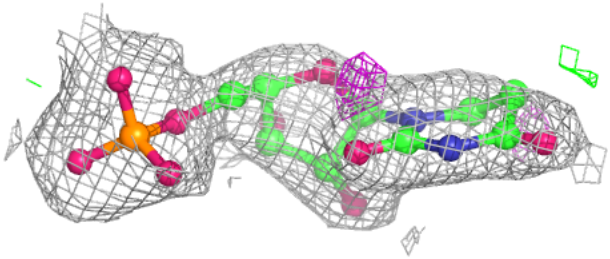


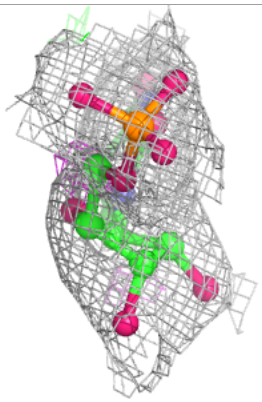


Electron density around H2U H 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

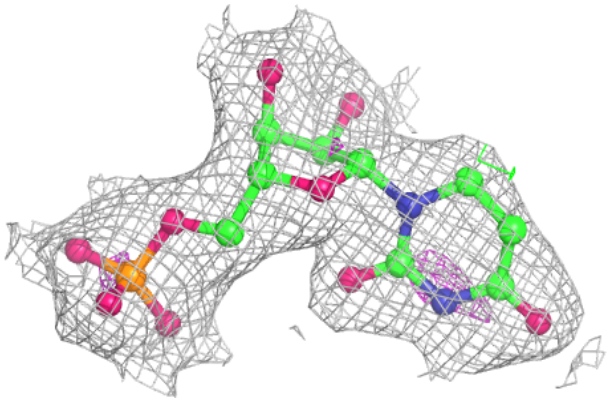


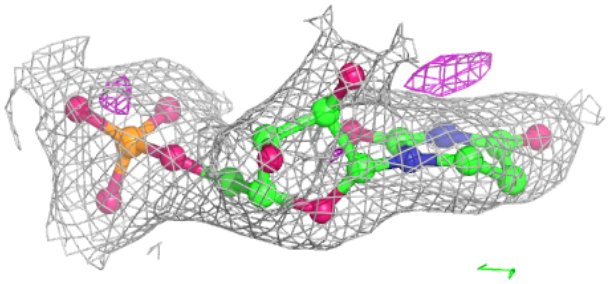


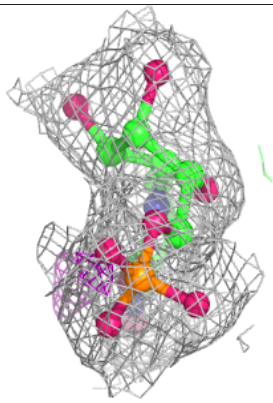


Electron density around H2U B 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

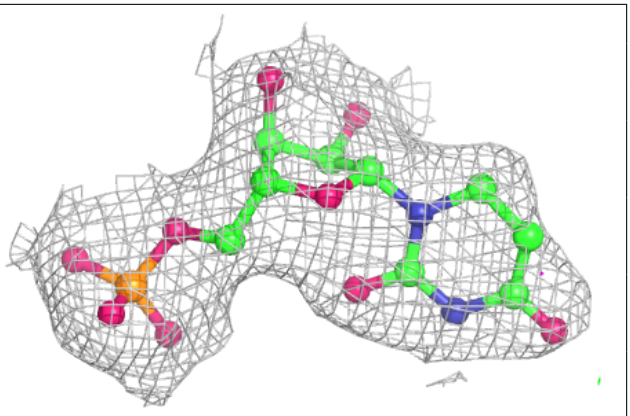


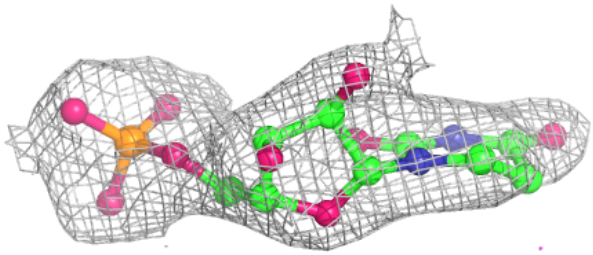


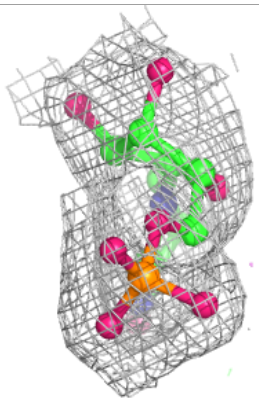


Electron density around H2U E 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

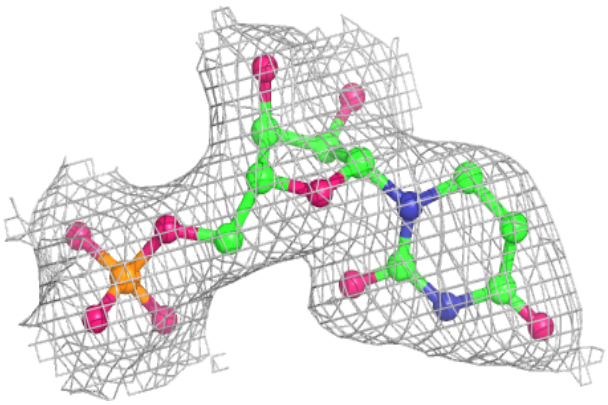


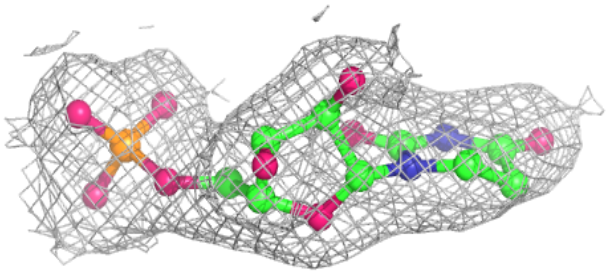


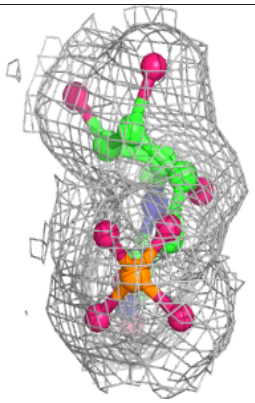


Electron density around H2U A 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

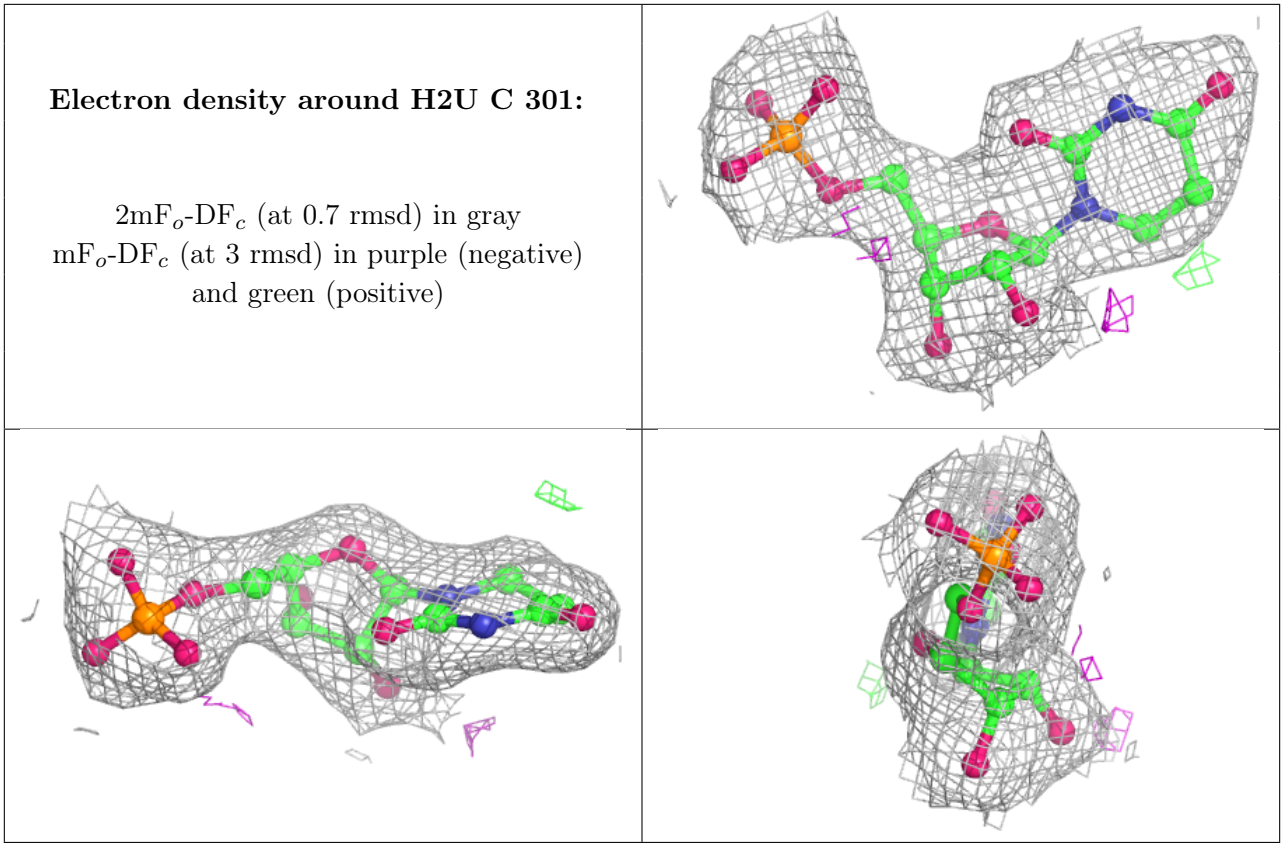






Electron density around H2U C 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.