



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:15 AM UTC

PDB ID : 6N55 / pdb_00006n55
Title : Crystal structure of human uridine-cytidine kinase 2 complexed with 2'-azidouridine
Authors : Cuthbert, B.J.; Nainar, S.; Spitale, R.C.; Goulding, C.W.
Deposited on : 2018-11-21
Resolution : 3.08 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

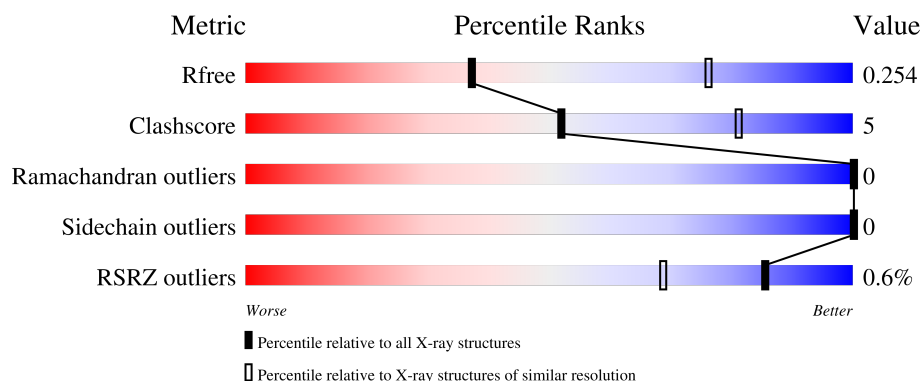
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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}	180053	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	255	 70% 9% 21%
1	B	255	 71% 10% 19%
1	C	255	 69% 14% 17%
1	D	255	 71% 13% 16%
1	E	255	 74% 10% 16%

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Mol	Chain	Length	Quality of chain
1	F	255	
1	G	255	
1	H	255	

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	PO4	C	301	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13198 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 Uridine-cytidine kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	1	0
			1569	1008	262	296	3			
1	B	206	Total	C	N	O	S	0	1	0
			1582	1015	260	304	3			
1	C	212	Total	C	N	O	S	0	1	0
			1647	1062	273	309	3			
1	D	213	Total	C	N	O	S	0	0	0
			1661	1067	275	316	3			
1	E	214	Total	C	N	O	S	0	1	0
			1658	1063	280	312	3			
1	F	212	Total	C	N	O	S	0	1	0
			1621	1037	271	310	3			
1	G	201	Total	C	N	O	S	0	0	0
			1475	950	249	273	3			
1	H	211	Total	C	N	O	S	0	0	0
			1542	991	259	289	3			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q9BZX2
A	-3	PRO	-	expression tag	UNP Q9BZX2
A	-2	LEU	-	expression tag	UNP Q9BZX2
A	-1	GLY	-	expression tag	UNP Q9BZX2
A	0	SER	-	expression tag	UNP Q9BZX2
B	-4	GLY	-	expression tag	UNP Q9BZX2
B	-3	PRO	-	expression tag	UNP Q9BZX2
B	-2	LEU	-	expression tag	UNP Q9BZX2
B	-1	GLY	-	expression tag	UNP Q9BZX2
B	0	SER	-	expression tag	UNP Q9BZX2
C	-4	GLY	-	expression tag	UNP Q9BZX2
C	-3	PRO	-	expression tag	UNP Q9BZX2
C	-2	LEU	-	expression tag	UNP Q9BZX2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP Q9BZX2
C	0	SER	-	expression tag	UNP Q9BZX2
D	-4	GLY	-	expression tag	UNP Q9BZX2
D	-3	PRO	-	expression tag	UNP Q9BZX2
D	-2	LEU	-	expression tag	UNP Q9BZX2
D	-1	GLY	-	expression tag	UNP Q9BZX2
D	0	SER	-	expression tag	UNP Q9BZX2
E	-4	GLY	-	expression tag	UNP Q9BZX2
E	-3	PRO	-	expression tag	UNP Q9BZX2
E	-2	LEU	-	expression tag	UNP Q9BZX2
E	-1	GLY	-	expression tag	UNP Q9BZX2
E	0	SER	-	expression tag	UNP Q9BZX2
F	-4	GLY	-	expression tag	UNP Q9BZX2
F	-3	PRO	-	expression tag	UNP Q9BZX2
F	-2	LEU	-	expression tag	UNP Q9BZX2
F	-1	GLY	-	expression tag	UNP Q9BZX2
F	0	SER	-	expression tag	UNP Q9BZX2
G	-4	GLY	-	expression tag	UNP Q9BZX2
G	-3	PRO	-	expression tag	UNP Q9BZX2
G	-2	LEU	-	expression tag	UNP Q9BZX2
G	-1	GLY	-	expression tag	UNP Q9BZX2
G	0	SER	-	expression tag	UNP Q9BZX2
H	-4	GLY	-	expression tag	UNP Q9BZX2
H	-3	PRO	-	expression tag	UNP Q9BZX2
H	-2	LEU	-	expression tag	UNP Q9BZX2
H	-1	GLY	-	expression tag	UNP Q9BZX2
H	0	SER	-	expression tag	UNP Q9BZX2

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



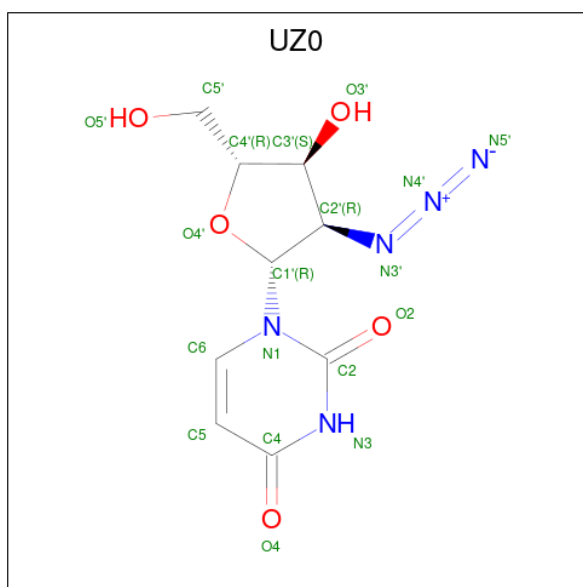
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 2'-azido-2'-deoxyuridine (CCD ID: UZ0) (formula: C₉H₁₁N₅O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			19	9	5	5		
4	E	1	Total	C	N	O	0	0
			19	9	5	5		
4	F	1	Total	C	N	O	0	0
			19	9	5	5		

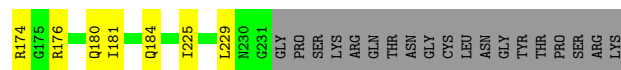
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total	O	0	0
			30	30		
5	B	25	Total	O	0	0
			25	25		
5	C	21	Total	O	0	0
			21	21		
5	D	25	Total	O	0	0
			25	25		
5	E	17	Total	O	0	0
			17	17		
5	F	28	Total	O	0	0
			28	28		
5	G	24	Total	O	0	0
			24	24		
5	H	14	Total	O	0	0
			14	14		



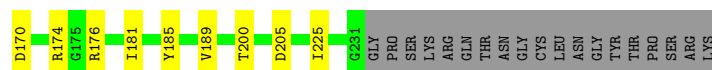
- Molecule 1: Uridine-cytidine kinase 2

Chain E: 74% 10% 16%



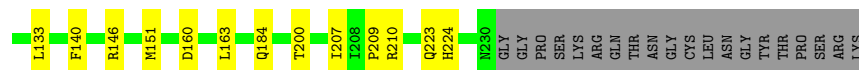
- Molecule 1: Uridine-cytidine kinase 2

Chain F: 73% 10% 17%



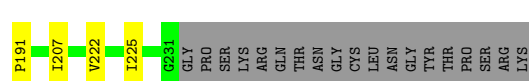
- Molecule 1: Uridine-cytidine kinase 2

Chain G: 2% 72% 7% 21%



- Molecule 1: Uridine-cytidine kinase 2

Chain H: 75% 7% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.75Å 85.76Å 153.37Å 90.00° 95.39° 90.00°	Depositor
Resolution (Å)	38.50 – 3.08 38.50 – 3.08	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.50-3.08) 98.3 (38.50-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 3.06Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.211 , 0.258 0.213 , 0.254	Depositor DCC
R_{free} test set	2214 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13198	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GOL, UZ0

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	0.09	0/1599	0.24	0/2167
1	B	0.09	0/1611	0.25	0/2185
1	C	0.09	0/1680	0.26	0/2278
1	D	0.13	0/1690	0.27	0/2293
1	E	0.11	0/1690	0.27	0/2290
1	F	0.10	0/1652	0.26	0/2243
1	G	0.09	0/1496	0.24	0/2034
1	H	0.09	0/1567	0.25	0/2137
All	All	0.10	0/12985	0.25	0/17627

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 [i](#)

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	1569	0	1547	15	0
1	B	1582	0	1534	18	0
1	C	1647	0	1641	22	0
1	D	1661	0	1649	27	0
1	E	1658	0	1649	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1621	0	1574	14	0
1	G	1475	0	1405	12	0
1	H	1542	0	1443	12	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
2	C	5	0	0	2	0
2	D	5	0	0	1	0
2	E	5	0	0	1	0
2	F	5	0	0	0	0
2	G	5	0	0	1	0
2	H	5	0	0	1	0
3	A	24	0	32	2	0
3	B	18	0	24	3	0
3	C	24	0	32	0	0
3	D	36	0	48	3	0
3	E	24	0	32	0	0
3	F	30	0	40	0	0
3	G	6	0	8	0	0
4	D	19	0	0	1	0
4	E	19	0	0	1	0
4	F	19	0	0	0	0
5	A	30	0	0	0	0
5	B	25	0	0	1	0
5	C	21	0	0	0	0
5	D	25	0	0	2	0
5	E	17	0	0	0	0
5	F	28	0	0	0	0
5	G	24	0	0	2	0
5	H	14	0	0	0	0
All	All	13198	0	12658	131	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 5.

All (131) 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:41:VAL:HG13	1:A:46:GLN:HB2	1.74	0.70
1:D:131:VAL:HG11	1:D:225:ILE:HD12	1.74	0.69
1:D:169:ARG:NH1	3:D:306:GOL:O2	2.28	0.66
1:D:68:LEU:HD12	1:D:72:GLN:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:ARG:HB2	1:F:181:ILE:HD11	1.78	0.65
1:E:160:ASP:HB2	1:G:163:LEU:HD12	1.77	0.65
1:D:65:TYR:OH	4:D:308:UZ0:O3'	2.13	0.65
1:B:207:ILE:HB	1:G:207:ILE:HB	1.79	0.63
1:B:112:TYR:HB2	3:B:304:GOL:H11	1.78	0.63
1:G:223:GLN:NE2	5:G:401:HOH:O	2.33	0.61
1:C:131:VAL:HG21	1:C:225:ILE:HG23	1.83	0.60
1:D:91:ASN:OD1	1:D:142:SER:OG	2.20	0.60
1:E:110:PRO:HB3	1:E:119:ARG:HD3	1.84	0.60
1:E:137:ILE:HG13	1:E:138:LEU:HG	1.83	0.59
1:B:131:VAL:HG21	1:B:225:ILE:HG23	1.85	0.59
1:D:41:VAL:HG13	1:D:46:GLN:HB2	1.84	0.59
1:C:46:GLN:HG3	1:C:56:VAL:HB	1.85	0.58
1:F:29:THR:HG21	1:F:166:ARG:HH11	1.69	0.58
1:E:174:ARG:HH22	4:E:306:UZ0:C2'	2.18	0.57
1:F:106:THR:HG22	1:F:128:PRO:HD3	1.86	0.57
1:D:19:GLU:N	5:D:401:HOH:O	2.36	0.56
1:H:131:VAL:HG21	1:H:225:ILE:HG23	1.87	0.56
1:A:207:ILE:HB	1:H:207:ILE:HB	1.88	0.56
1:H:46:GLN:OE1	1:H:56:VAL:N	2.32	0.56
1:C:41:VAL:HG13	1:C:46:GLN:HB2	1.89	0.55
1:B:46:GLN:HG3	1:B:56:VAL:HB	1.87	0.55
1:B:140:PHE:HB2	1:B:200:THR:HB	1.88	0.55
1:B:30:ALA:HB1	1:B:165:ARG:HB2	1.89	0.55
1:B:66:ARG:NH2	1:B:87:ASP:O	2.40	0.55
1:A:46:GLN:HG3	1:A:56:VAL:HB	1.89	0.54
1:E:180:GLN:O	1:E:184:GLN:HG3	2.07	0.54
1:F:67:VAL:HG12	1:F:118:SER:HA	1.90	0.54
1:F:131:VAL:HG21	1:F:225:ILE:HG23	1.90	0.53
1:A:131:VAL:HG21	1:A:225:ILE:HG23	1.90	0.53
1:E:176:ARG:HB2	1:E:181:ILE:HD11	1.89	0.53
1:C:29:THR:HG21	1:C:166:ARG:HH11	1.74	0.53
1:D:86:PRO:HG3	1:D:138:LEU:HD13	1.90	0.52
3:A:304:GOL:O1	3:A:304:GOL:O3	2.21	0.52
1:C:106:THR:HG23	1:C:127:TYR:HA	1.92	0.52
1:E:106:THR:HG23	1:E:127:TYR:HA	1.91	0.52
1:D:158:ASP:HB3	3:D:302:GOL:H12	1.92	0.52
1:E:131:VAL:HG21	1:E:225:ILE:HG23	1.91	0.52
1:D:110:PRO:HB3	1:D:119:ARG:HD3	1.92	0.51
1:D:46:GLN:HG3	1:D:56:VAL:HB	1.92	0.51
1:D:51:TYR:HA	1:D:54:LYS:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LYS:NZ	3:A:302:GOL:O3	2.35	0.51
1:D:142:SER:OG	3:D:303:GOL:O2	2.28	0.51
1:D:84:ASP:OD2	1:D:84:ASP:N	2.44	0.51
1:C:170:ASP:HB3	1:C:181:ILE:HD13	1.93	0.51
1:G:23:ILE:HB	1:G:133:LEU:HD23	1.94	0.50
1:B:101:ILE:HG21	1:B:132:VAL:HG21	1.93	0.50
1:C:99:LYS:O	1:C:103:GLU:HG3	2.12	0.50
1:F:170:ASP:HA	1:F:174:ARG:HG3	1.93	0.50
1:B:210:ARG:NH2	5:B:401:HOH:O	2.43	0.49
1:C:36:VAL:HG22	1:C:218:ILE:HD11	1.95	0.49
1:F:110:PRO:HB3	1:F:119:ARG:HD3	1.94	0.49
1:A:182:LEU:HD12	1:C:168:LEU:HG	1.95	0.49
1:D:68:LEU:HD23	1:D:117:HIS:HB3	1.94	0.49
1:A:30:ALA:HB1	1:A:165:ARG:HB2	1.95	0.49
1:D:146:ARG:NH1	5:D:403:HOH:O	2.42	0.49
1:D:221:ILE:O	1:D:225:ILE:HG12	2.13	0.48
1:F:109:ILE:HD12	1:F:126:VAL:HG21	1.95	0.48
1:H:160:ASP:N	1:H:160:ASP:OD1	2.46	0.48
1:E:32:GLY:N	2:E:301:PO4:O3	2.44	0.48
1:D:160:ASP:N	1:D:160:ASP:OD1	2.45	0.48
1:E:108:GLN:OE1	1:E:123:THR:OG1	2.32	0.48
1:D:30:ALA:HA	1:D:169:ARG:HH12	1.79	0.47
1:G:46:GLN:HG3	1:G:56:VAL:HB	1.95	0.47
1:G:184:GLN:NE2	5:G:403:HOH:O	2.43	0.47
1:E:30:ALA:HB1	1:E:165:ARG:HB2	1.96	0.47
1:F:46:GLN:HG3	1:F:56:VAL:HB	1.97	0.47
1:B:36:VAL:O	1:B:40:ILE:HG12	2.15	0.47
1:E:225:ILE:O	1:E:229:LEU:HD23	2.15	0.47
1:B:169:ARG:NH1	2:B:301:PO4:O2	2.28	0.47
1:D:131:VAL:HG21	1:D:225:ILE:HG23	1.96	0.47
1:E:23:ILE:HB	1:E:133:LEU:HD23	1.98	0.46
1:C:172:SER:HA	1:D:115:VAL:HG11	1.97	0.46
1:A:23:ILE:HB	1:A:133:LEU:HD23	1.98	0.46
1:G:160:ASP:N	1:G:160:ASP:OD1	2.49	0.46
1:C:33:LYS:N	2:C:301:PO4:O2	2.48	0.45
1:B:118:SER:H	3:B:304:GOL:H31	1.81	0.45
1:C:169:ARG:NH2	2:C:301:PO4:O3	2.49	0.45
1:G:140:PHE:HB2	1:G:200:THR:HB	1.98	0.45
1:H:40:ILE:HD13	1:H:222:VAL:HG23	1.98	0.45
1:F:160:ASP:OD1	1:F:160:ASP:N	2.49	0.45
1:A:140:PHE:HB2	1:A:200:THR:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LYS:O	1:C:102:THR:OG1	2.32	0.45
1:H:31:SER:HB3	1:H:162:ARG:HD3	2.00	0.44
1:B:230:ASN:O	1:B:230:ASN:ND2	2.50	0.44
1:D:23:ILE:HB	1:D:133:LEU:HD23	1.99	0.44
1:C:160:ASP:N	1:C:160:ASP:OD1	2.49	0.44
1:C:23:ILE:HB	1:C:133:LEU:HD23	1.99	0.44
1:F:31:SER:HB3	1:F:162:ARG:HD3	2.00	0.44
1:D:66:ARG:NH2	1:D:92:GLU:OE2	2.51	0.44
1:B:56:VAL:HG22	1:B:131:VAL:HB	1.99	0.43
1:C:31:SER:HB3	1:C:162:ARG:HD3	1.99	0.43
1:D:46:GLN:O	1:D:54:LYS:NZ	2.52	0.43
1:A:29:THR:HG21	1:A:166:ARG:HH11	1.82	0.43
1:E:46:GLN:HG3	1:E:56:VAL:HB	1.99	0.43
1:C:96:LYS:O	1:C:100:GLU:HG3	2.19	0.43
1:A:99:LYS:O	1:A:102:THR:OG1	2.36	0.43
1:B:30:ALA:O	1:B:165:ARG:HD2	2.19	0.43
1:G:140:PHE:HA	1:G:146:ARG:HG2	2.01	0.43
1:B:65:TYR:CD2	3:B:304:GOL:H2	2.54	0.42
1:G:33:LYS:N	2:G:301:PO4:O3	2.43	0.42
1:A:33:LYS:N	2:A:301:PO4:O2	2.44	0.42
1:C:66:ARG:NH2	1:C:92:GLU:OE1	2.51	0.42
1:H:23:ILE:HB	1:H:133:LEU:HD23	2.02	0.41
1:A:31:SER:HB3	1:A:162:ARG:HD3	2.01	0.41
1:B:171:ILE:HD11	1:B:178:LEU:HD13	2.01	0.41
1:G:209:PRO:O	1:G:210:ARG:HG2	2.21	0.41
1:H:86:PRO:HG3	1:H:138:LEU:HD13	2.02	0.41
1:F:185:TYR:HA	1:F:189:VAL:HB	2.02	0.41
1:H:22:LEU:HD23	1:H:132:VAL:HB	2.02	0.41
1:A:56:VAL:HG22	1:A:131:VAL:HB	2.03	0.41
1:D:30:ALA:N	2:D:301:PO4:O1	2.51	0.41
1:E:33:LYS:HD2	1:E:135:GLU:HG2	2.03	0.41
1:C:151:MET:HE3	1:C:151:MET:HB2	1.97	0.41
1:H:33:LYS:HB2	1:H:33:LYS:HE2	1.87	0.41
1:C:214:ASN:ND2	1:F:205:ASP:O	2.47	0.41
1:E:229:LEU:HD23	1:E:229:LEU:H	1.86	0.40
1:F:140:PHE:HB2	1:F:200:THR:HB	2.04	0.40
1:B:31:SER:HB3	1:B:162:ARG:HD3	2.03	0.40
1:C:190:LYS:HB3	1:C:191:PRO:HD3	2.03	0.40
1:G:151:MET:HE1	1:G:224:HIS:CD2	2.57	0.40
1:A:160:ASP:N	1:A:160:ASP:OD1	2.55	0.40
1:C:109:ILE:HA	1:C:110:PRO:HD3	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:ASN:HD22	1:D:91:ASN:C	2.29	0.40
1:D:151:MET:HE1	1:D:224:HIS:CD2	2.57	0.40
1:H:33:LYS:HD3	2:H:301:PO4:O4	2.22	0.40
1:H:190:LYS:HB3	1:H:191:PRO:HD3	2.04	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	196/255 (77%)	194 (99%)	2 (1%)	0	100	100
1	B	199/255 (78%)	196 (98%)	3 (2%)	0	100	100
1	C	211/255 (83%)	209 (99%)	2 (1%)	0	100	100
1	D	211/255 (83%)	208 (99%)	3 (1%)	0	100	100
1	E	213/255 (84%)	212 (100%)	1 (0%)	0	100	100
1	F	209/255 (82%)	207 (99%)	2 (1%)	0	100	100
1	G	193/255 (76%)	190 (98%)	3 (2%)	0	100	100
1	H	207/255 (81%)	201 (97%)	6 (3%)	0	100	100
All	All	1639/2040 (80%)	1617 (99%)	22 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	170/223 (76%)	170 (100%)	0	100	100
1	B	169/223 (76%)	169 (100%)	0	100	100
1	C	178/223 (80%)	178 (100%)	0	100	100
1	D	181/223 (81%)	181 (100%)	0	100	100
1	E	179/223 (80%)	179 (100%)	0	100	100
1	F	172/223 (77%)	172 (100%)	0	100	100
1	G	145/223 (65%)	145 (100%)	0	100	100
1	H	149/223 (67%)	149 (100%)	0	100	100
All	All	1343/1784 (75%)	1343 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	226	GLN
1	B	230	ASN
1	C	91	ASN
1	C	219	ASN
1	C	224	HIS
1	D	42	GLN
1	D	53	GLN
1	E	42	GLN
1	E	117	HIS
1	E	226	GLN
1	G	224	HIS
1	H	55	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

38 ligands are 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$
3	GOL	A	305	-	5,5,5	0.92	0	5,5,5	1.09	0
3	GOL	F	304	-	5,5,5	0.92	0	5,5,5	1.08	0
2	PO4	E	301	-	4,4,4	0.96	0	6,6,6	0.48	0
3	GOL	B	304	-	5,5,5	0.95	0	5,5,5	1.04	0
3	GOL	D	307	-	5,5,5	0.98	0	5,5,5	1.07	0
3	GOL	F	306	-	5,5,5	0.93	0	5,5,5	1.06	0
2	PO4	B	301	-	4,4,4	1.00	0	6,6,6	0.50	0
4	UZ0	F	307	-	19,20,20	1.64	3 (15%)	23,28,28	2.64	9 (39%)
4	UZ0	E	306	-	19,20,20	1.31	2 (10%)	23,28,28	2.85	11 (47%)
2	PO4	F	301	-	4,4,4	0.98	0	6,6,6	0.51	0
3	GOL	D	305	-	5,5,5	0.94	0	5,5,5	1.08	0
3	GOL	E	304	-	5,5,5	0.98	0	5,5,5	1.03	0
3	GOL	F	303	-	5,5,5	0.95	0	5,5,5	1.06	0
3	GOL	D	302	-	5,5,5	0.97	0	5,5,5	1.06	0
3	GOL	B	303	-	5,5,5	0.95	0	5,5,5	1.06	0
3	GOL	F	302	-	5,5,5	0.95	0	5,5,5	1.07	0
3	GOL	A	303	-	5,5,5	0.95	0	5,5,5	1.08	0
3	GOL	B	302	-	5,5,5	0.93	0	5,5,5	1.13	0
3	GOL	C	304	-	5,5,5	0.94	0	5,5,5	1.06	0
3	GOL	F	305	-	5,5,5	0.93	0	5,5,5	1.09	0
2	PO4	H	301	-	4,4,4	0.99	0	6,6,6	0.44	0
4	UZ0	D	308	-	19,20,20	1.66	2 (10%)	23,28,28	3.06	15 (65%)
2	PO4	D	301	-	4,4,4	0.99	0	6,6,6	0.44	0
2	PO4	A	301	-	4,4,4	0.97	0	6,6,6	0.49	0
3	GOL	D	303	-	5,5,5	0.95	0	5,5,5	1.06	0
3	GOL	G	302	-	5,5,5	0.92	0	5,5,5	1.07	0
3	GOL	A	304	-	5,5,5	0.93	0	5,5,5	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	E	305	-	5,5,5	0.95	0	5,5,5	1.06	0
3	GOL	E	302	-	5,5,5	0.95	0	5,5,5	1.04	0
3	GOL	C	302	-	5,5,5	0.93	0	5,5,5	1.09	0
3	GOL	D	304	-	5,5,5	0.92	0	5,5,5	1.07	0
3	GOL	C	305	-	5,5,5	0.97	0	5,5,5	1.04	0
3	GOL	C	303	-	5,5,5	0.95	0	5,5,5	1.07	0
3	GOL	D	306	-	5,5,5	0.98	0	5,5,5	1.01	0
2	PO4	C	301	-	4,4,4	1.02	0	6,6,6	0.42	0
2	PO4	G	301	-	4,4,4	0.98	0	6,6,6	0.49	0
3	GOL	E	303	-	5,5,5	0.96	0	5,5,5	1.06	0
3	GOL	A	302	-	5,5,5	0.91	0	5,5,5	1.07	0

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
3	GOL	A	305	-	-	0/4/4/4	-
3	GOL	F	304	-	-	2/4/4/4	-
3	GOL	B	304	-	-	0/4/4/4	-
3	GOL	D	307	-	-	0/4/4/4	-
3	GOL	F	306	-	-	0/4/4/4	-
4	UZ0	F	307	-	-	3/9/25/25	0/2/2/2
4	UZ0	E	306	-	-	4/9/25/25	0/2/2/2
3	GOL	D	305	-	-	2/4/4/4	-
3	GOL	E	304	-	-	2/4/4/4	-
3	GOL	F	303	-	-	2/4/4/4	-
3	GOL	D	302	-	-	0/4/4/4	-
3	GOL	B	303	-	-	0/4/4/4	-
3	GOL	F	302	-	-	0/4/4/4	-
3	GOL	A	303	-	-	0/4/4/4	-
3	GOL	B	302	-	-	0/4/4/4	-
3	GOL	C	304	-	-	1/4/4/4	-
3	GOL	F	305	-	-	2/4/4/4	-
4	UZ0	D	308	-	-	5/9/25/25	0/2/2/2
3	GOL	D	303	-	-	2/4/4/4	-
3	GOL	G	302	-	-	0/4/4/4	-
3	GOL	A	304	-	-	0/4/4/4	-
3	GOL	E	305	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	302	-	-	0/4/4/4	-
3	GOL	C	302	-	-	0/4/4/4	-
3	GOL	D	304	-	-	0/4/4/4	-
3	GOL	C	305	-	-	0/4/4/4	-
3	GOL	C	303	-	-	2/4/4/4	-
3	GOL	D	306	-	-	0/4/4/4	-
3	GOL	E	303	-	-	0/4/4/4	-
3	GOL	A	302	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	308	UZ0	N5'-N4'	-4.80	1.13	1.23
4	F	307	UZ0	N5'-N4'	-4.36	1.14	1.23
4	E	306	UZ0	N5'-N4'	-4.11	1.14	1.23
4	D	308	UZ0	N4'-N3'	-4.09	1.13	1.23
4	F	307	UZ0	N4'-N3'	-4.01	1.13	1.23
4	E	306	UZ0	N4'-N3'	-3.28	1.15	1.23
4	F	307	UZ0	C2-N1	-2.28	1.34	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	306	UZ0	C1'-N1-C2	6.77	129.75	117.59
4	D	308	UZ0	O4'-C1'-N1	6.33	122.70	108.36
4	F	307	UZ0	C4-N3-C2	-5.54	119.74	126.61
4	F	307	UZ0	N3-C2-N1	5.49	122.04	114.89
4	E	306	UZ0	C1'-N1-C6	-4.84	110.43	120.78
4	D	308	UZ0	C5'-C4'-C3'	-4.38	104.77	115.10
4	E	306	UZ0	C4-N3-C2	-4.29	121.28	126.61
4	F	307	UZ0	O2-C2-N1	-4.28	117.23	122.80
4	D	308	UZ0	O4'-C4'-C5'	4.28	118.26	109.22
4	E	306	UZ0	O4-C4-C5	-4.27	117.79	125.16
4	F	307	UZ0	C2'-N3'-N4'	4.19	124.78	115.61
4	D	308	UZ0	C4'-O4'-C1'	-4.08	100.45	109.47
4	D	308	UZ0	C6-N1-C2	-4.04	116.08	121.00
4	D	308	UZ0	C2'-N3'-N4'	3.98	124.32	115.61
4	D	308	UZ0	C1'-N1-C2	3.92	124.64	117.59
4	F	307	UZ0	C1'-C2'-N3'	3.85	127.23	112.96
4	E	306	UZ0	C5'-C4'-C3'	-3.84	106.02	115.10
4	D	308	UZ0	C1'-C2'-N3'	3.84	127.20	112.96
4	D	308	UZ0	N3-C2-N1	3.77	119.81	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	307	UZ0	O4-C4-C5	-3.61	118.94	125.16
4	F	307	UZ0	C5-C4-N3	3.51	119.72	114.80
4	E	306	UZ0	N3-C2-N1	3.43	119.35	114.89
4	E	306	UZ0	C1'-C2'-N3'	3.23	124.97	112.96
4	E	306	UZ0	O2-C2-N3	-2.97	116.02	121.49
4	E	306	UZ0	O4-C4-N3	2.96	123.56	119.27
4	E	306	UZ0	C5-C4-N3	2.75	118.64	114.80
4	D	308	UZ0	C6-C5-C4	-2.67	116.13	119.53
4	D	308	UZ0	C5-C6-N1	2.65	126.15	121.84
4	F	307	UZ0	C5'-C4'-C3'	-2.59	108.98	115.10
4	D	308	UZ0	C4-N3-C2	-2.57	123.42	126.61
4	D	308	UZ0	C5-C4-N3	2.53	118.35	114.80
4	E	306	UZ0	O4'-C4'-C3'	2.45	110.01	105.15
4	D	308	UZ0	O2-C2-N3	-2.43	117.00	121.49
4	D	308	UZ0	O4-C4-C5	-2.26	121.26	125.16
4	F	307	UZ0	O4'-C4'-C5'	2.07	113.58	109.22

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	303	GOL	O1-C1-C2-C3
3	D	305	GOL	O1-C1-C2-C3
3	E	304	GOL	O1-C1-C2-C3
3	F	303	GOL	O1-C1-C2-C3
3	F	304	GOL	O1-C1-C2-C3
4	D	308	UZ0	C2'-C1'-N1-C2
4	D	308	UZ0	C2'-C1'-N1-C6
4	E	306	UZ0	C2'-C1'-N1-C2
4	F	307	UZ0	C3'-C4'-C5'-O5'
4	E	306	UZ0	C2'-C1'-N1-C6
3	D	305	GOL	O1-C1-C2-O2
3	F	303	GOL	O1-C1-C2-O2
3	F	304	GOL	O1-C1-C2-O2
4	F	307	UZ0	O4'-C4'-C5'-O5'
3	E	305	GOL	O1-C1-C2-C3
3	F	305	GOL	C1-C2-C3-O3
3	C	303	GOL	O1-C1-C2-O2
3	F	305	GOL	O2-C2-C3-O3
4	F	307	UZ0	C1'-C2'-N3'-N4'
3	E	304	GOL	O1-C1-C2-O2
3	E	305	GOL	O1-C1-C2-O2

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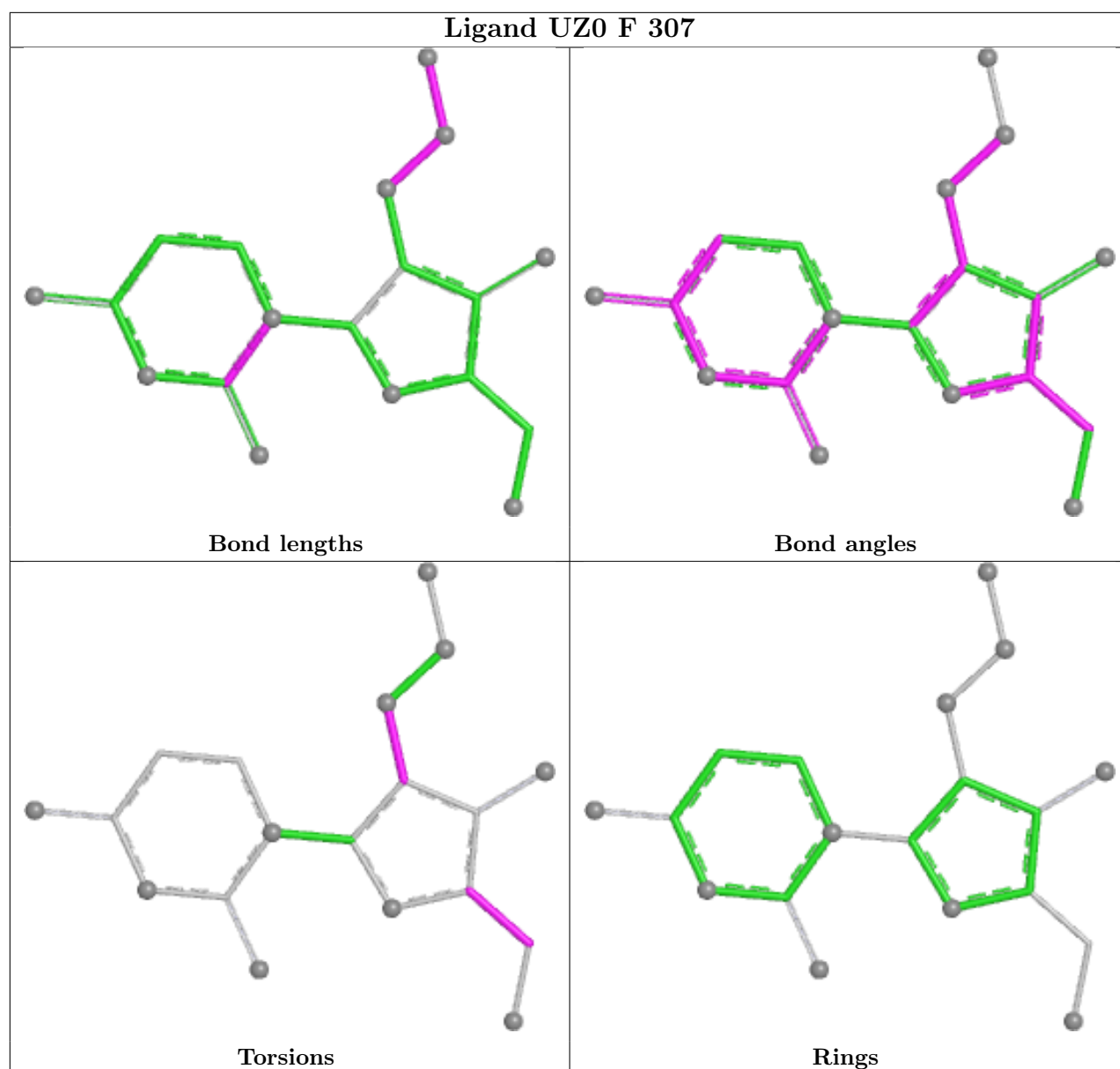
Mol	Chain	Res	Type	Atoms
4	D	308	UZ0	O4'-C1'-N1-C6
4	E	306	UZ0	C2'-N3'-N4'-N5'
3	D	303	GOL	O2-C2-C3-O3
4	E	306	UZ0	C3'-C2'-N3'-N4'
4	D	308	UZ0	O4'-C1'-N1-C2
3	D	303	GOL	C1-C2-C3-O3
4	D	308	UZ0	C3'-C2'-N3'-N4'
3	C	304	GOL	O1-C1-C2-O2

There are no ring outliers.

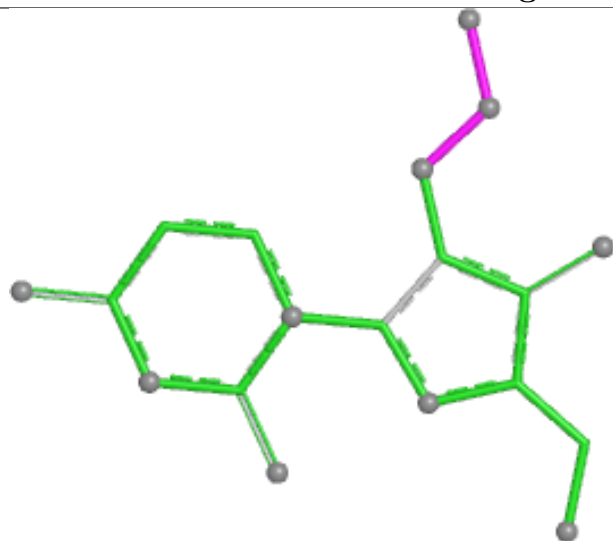
15 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	PO4	1	0
3	B	304	GOL	3	0
2	B	301	PO4	1	0
4	E	306	UZ0	1	0
3	D	302	GOL	1	0
2	H	301	PO4	1	0
4	D	308	UZ0	1	0
2	D	301	PO4	1	0
2	A	301	PO4	1	0
3	D	303	GOL	1	0
3	A	304	GOL	1	0
3	D	306	GOL	1	0
2	C	301	PO4	2	0
2	G	301	PO4	1	0
3	A	302	GOL	1	0

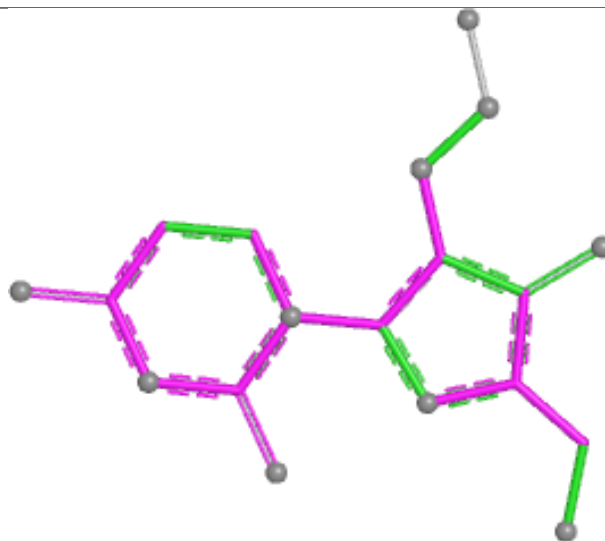
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



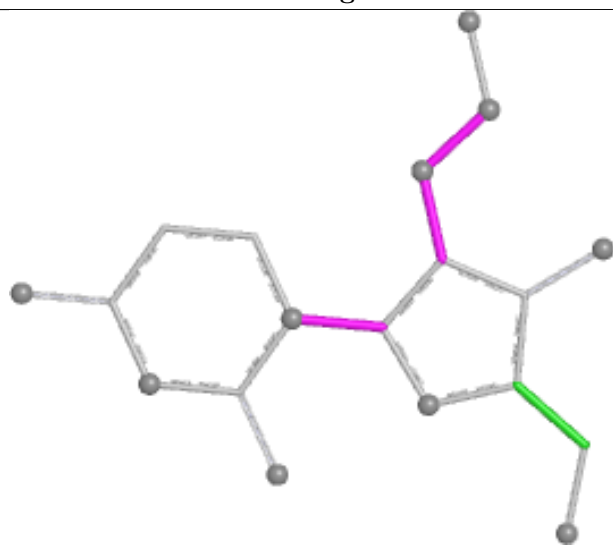
Ligand UZ0 E 306



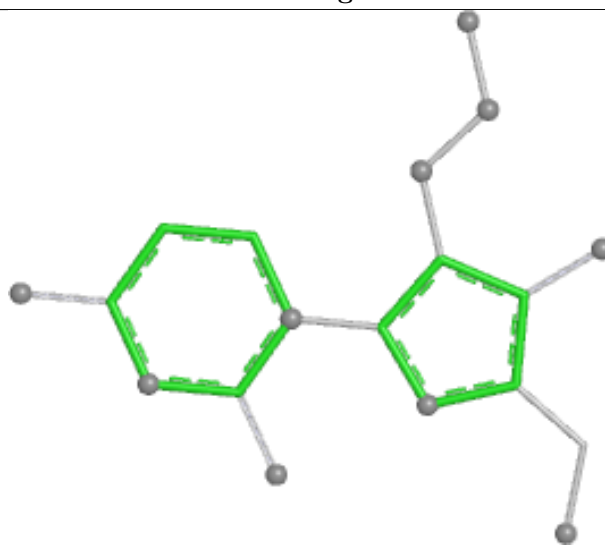
Bond lengths



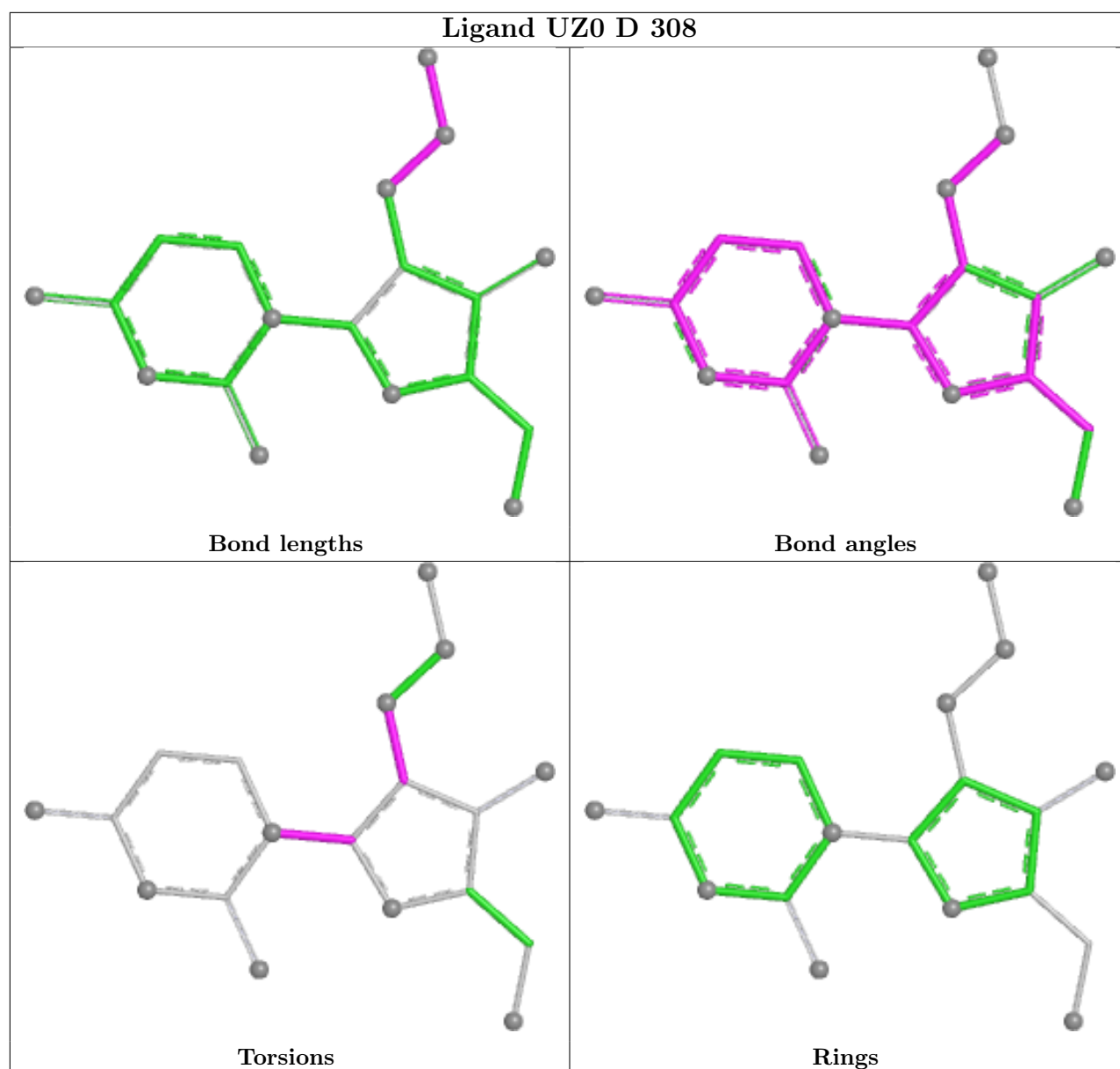
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	201/255 (78%)	-0.19	1 (0%) 87 72	45, 70, 116, 133	1 (0%)
1	B	206/255 (80%)	-0.20	2 (0%) 79 59	46, 71, 118, 133	1 (0%)
1	C	212/255 (83%)	-0.38	1 (0%) 87 72	46, 72, 98, 118	1 (0%)
1	D	213/255 (83%)	-0.27	0 100 100	48, 73, 98, 110	0
1	E	214/255 (83%)	-0.40	0 100 100	45, 68, 98, 121	1 (0%)
1	F	212/255 (83%)	-0.39	0 100 100	47, 67, 94, 123	1 (0%)
1	G	201/255 (78%)	-0.07	4 (1%) 65 42	50, 84, 121, 143	0
1	H	211/255 (82%)	-0.08	2 (0%) 81 61	56, 86, 139, 155	0
All	All	1670/2040 (81%)	-0.25	10 (0%) 85 69	45, 73, 115, 155	5 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	91	ASN	3.1
1	H	76	ALA	2.9
1	B	232	GLY	2.6
1	B	74	ALA	2.4
1	A	177	ASP	2.4
1	H	113	ASP	2.2
1	C	176	ARG	2.1
1	G	77	LEU	2.1
1	G	88	ALA	2.1
1	G	118	SER	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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
3	GOL	D	305	6/6	0.21	0.21	98,123,133,137	0
3	GOL	C	303	6/6	0.52	0.19	114,121,134,140	0
3	GOL	F	306	6/6	0.64	0.17	84,102,104,107	0
4	UZ0	D	308	19/19	0.66	0.15	76,87,96,98	19
4	UZ0	F	307	19/19	0.67	0.16	82,108,125,133	0
3	GOL	D	306	6/6	0.68	0.24	81,92,96,96	0
3	GOL	B	303	6/6	0.68	0.19	75,77,79,79	6
3	GOL	B	304	6/6	0.70	0.11	86,89,98,100	0
3	GOL	A	305	6/6	0.71	0.17	67,70,76,88	6
3	GOL	F	302	6/6	0.72	0.13	91,94,109,111	0
3	GOL	G	302	6/6	0.72	0.18	76,76,89,92	0
3	GOL	E	304	6/6	0.75	0.20	77,91,105,107	0
3	GOL	D	304	6/6	0.76	0.11	97,102,105,109	0
3	GOL	C	305	6/6	0.77	0.15	68,85,95,95	0
4	UZ0	E	306	19/19	0.78	0.12	97,112,120,125	0
3	GOL	D	302	6/6	0.82	0.13	74,82,92,96	0
3	GOL	D	307	6/6	0.84	0.18	94,103,108,110	0
3	GOL	A	304	6/6	0.85	0.36	76,83,87,93	6
2	PO4	E	301	5/5	0.86	0.08	58,67,76,81	0
3	GOL	A	302	6/6	0.87	0.15	75,79,85,90	6
3	GOL	A	303	6/6	0.87	0.14	68,89,105,112	0
3	GOL	B	302	6/6	0.88	0.15	63,68,72,73	6
3	GOL	C	302	6/6	0.88	0.16	78,80,89,93	6
3	GOL	E	303	6/6	0.89	0.12	68,71,87,95	0
3	GOL	D	303	6/6	0.90	0.11	66,71,75,82	0
3	GOL	E	302	6/6	0.90	0.16	82,91,101,101	0
2	PO4	F	301	5/5	0.91	0.07	68,68,75,90	0
2	PO4	D	301	5/5	0.91	0.06	55,62,66,71	0
3	GOL	F	304	6/6	0.91	0.14	66,71,86,92	0
3	GOL	C	304	6/6	0.91	0.17	66,68,78,79	0
2	PO4	H	301	5/5	0.92	0.06	67,71,73,74	0
3	GOL	F	303	6/6	0.92	0.09	59,71,77,78	0

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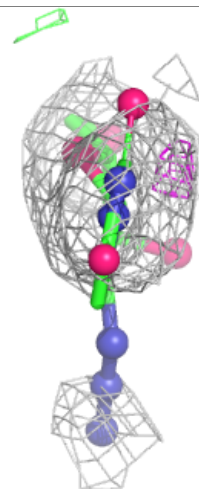
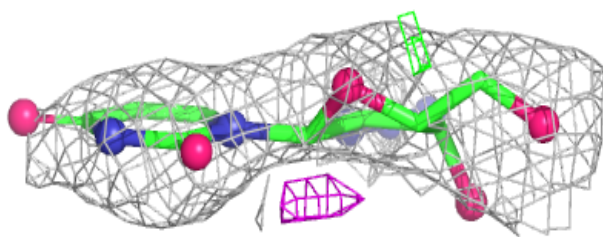
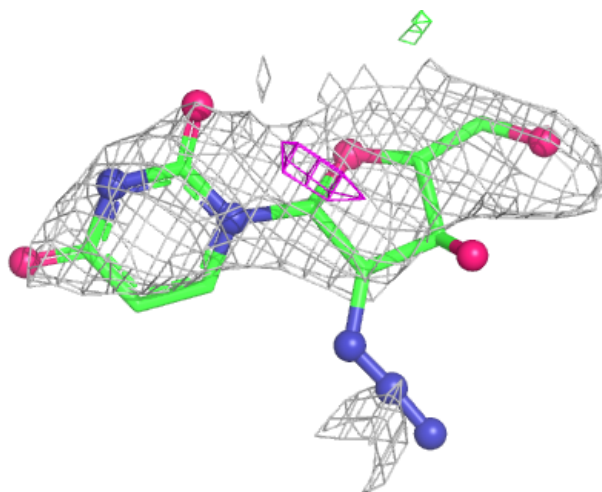
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	E	305	6/6	0.93	0.11	73,76,87,89	0
3	GOL	F	305	6/6	0.94	0.07	73,76,77,90	0
2	PO4	G	301	5/5	0.95	0.05	65,65,67,67	0
2	PO4	B	301	5/5	0.95	0.06	57,62,67,73	0
2	PO4	A	301	5/5	0.96	0.08	61,63,66,67	0
2	PO4	C	301	5/5	0.97	0.05	55,56,71,78	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.

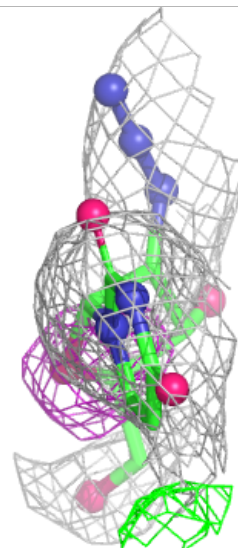
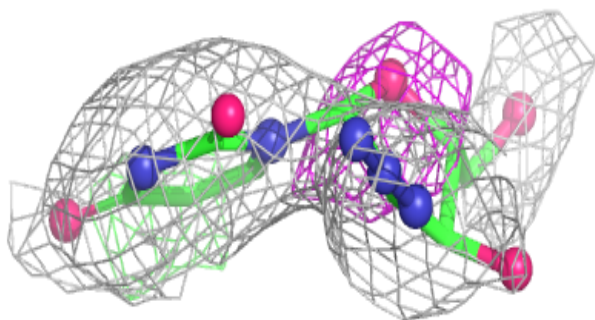
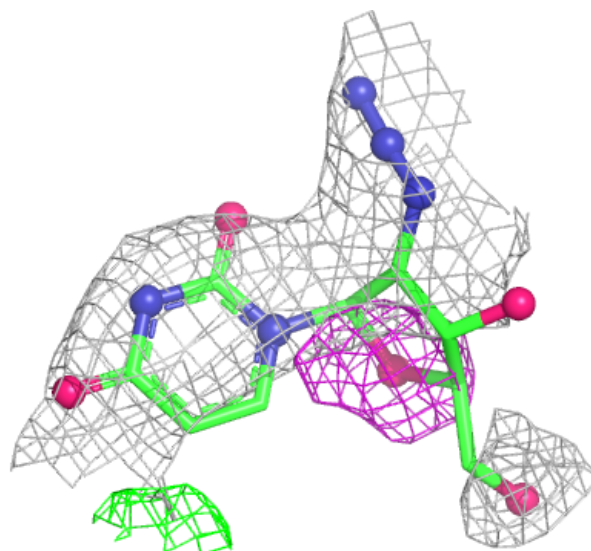
Electron density around UZ0 D 308:

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



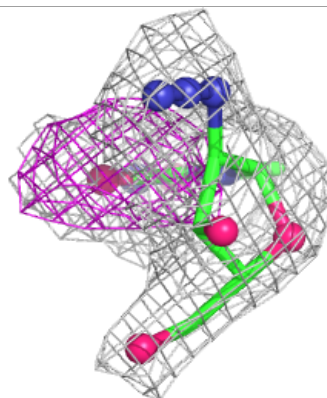
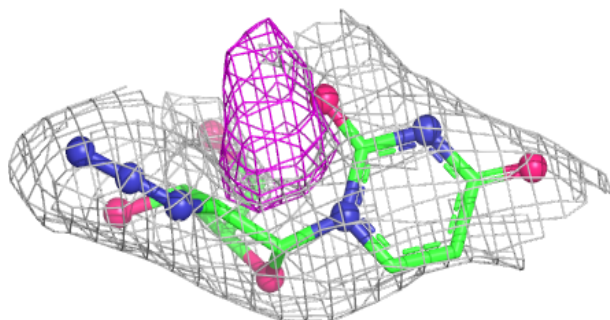
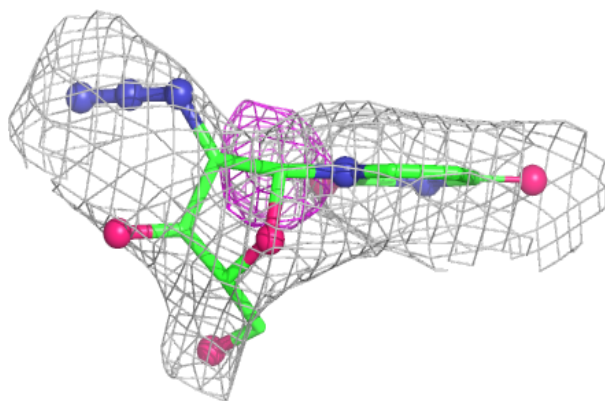
Electron density around UZ0 F 307:

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



Electron density around UZ0 E 306:

$2mF_o-DF_c$ (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.