



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2024 – 06:19 pm GMT

PDB ID : 6TRQ  
Title : S.c. Scavenger Decapping Enzyme DcpS in complex with the capped RNA dinucleotide m7G-GU  
Authors : Fuchs, A.-L.; Neu, A.; Sprangers, R.  
Deposited on : 2019-12-19  
Resolution : 2.94 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

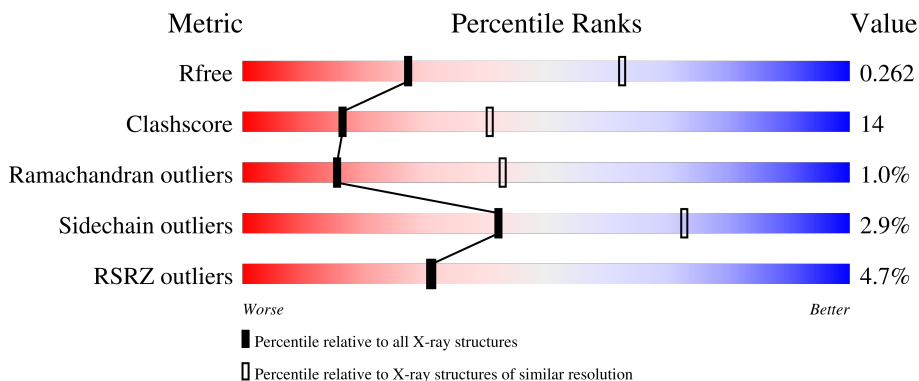
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.94 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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  $\geq 3$ , 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	345	 2% 69% 25% . .
1	B	345	 3% 69% 22% . 6%
1	C	345	 % 68% 26% . .
1	D	345	 11% 68% 23% . 8%

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	2PO	C	402	-	-	X	-
4	0G	A	403	X	-	-	-
4	0G	C	403	X	-	-	-
5	M7G	A	404	X	-	-	-
5	M7G	C	404	X	-	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10991 atoms, of which 74 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.

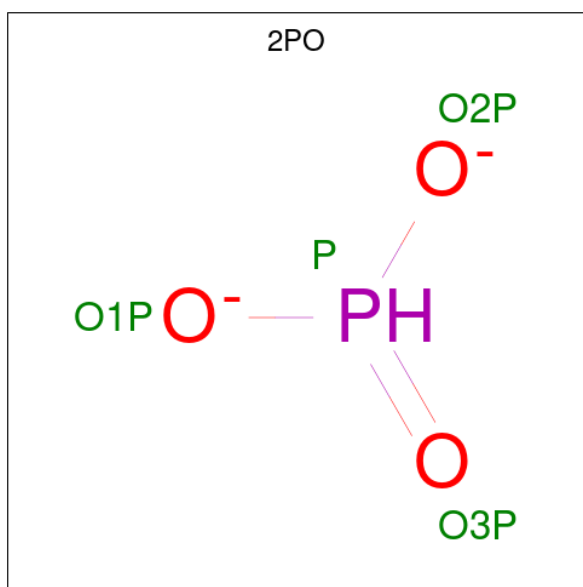
- Molecule 1 is a protein called m7GpppX diphosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	332	2722	1748	454	507	13	0	0	0
1	B	323	2657	1708	443	494	12	0	0	0
1	C	336	2758	1768	463	514	13	0	0	0
1	D	318	2616	1684	433	487	12	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

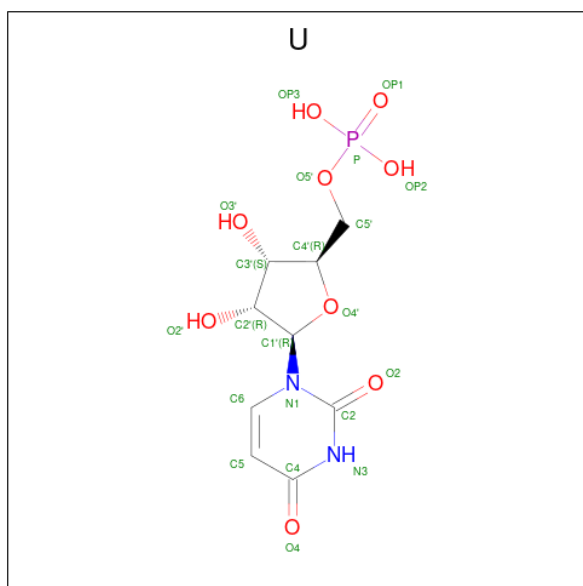
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLY	-	expression tag	UNP Q06151
A	7	MET	-	expression tag	UNP Q06151
A	268	ASN	HIS	engineered mutation	UNP Q06151
B	6	GLY	-	expression tag	UNP Q06151
B	7	MET	-	expression tag	UNP Q06151
B	268	ASN	HIS	engineered mutation	UNP Q06151
C	6	GLY	-	expression tag	UNP Q06151
C	7	MET	-	expression tag	UNP Q06151
C	268	ASN	HIS	engineered mutation	UNP Q06151
D	6	GLY	-	expression tag	UNP Q06151
D	7	MET	-	expression tag	UNP Q06151
D	268	ASN	HIS	engineered mutation	UNP Q06151

- Molecule 2 is PHOSPHONATE (three-letter code: 2PO) (formula: HO<sub>3</sub>P).



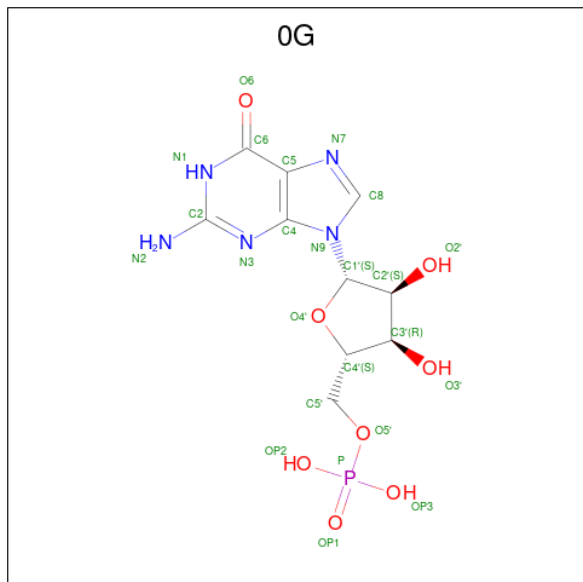
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 4 3 1	0	0
2	C	1	Total O P 4 3 1	0	0

- Molecule 3 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U) (formula:  $C_9H_{13}N_2O_9P$ ).



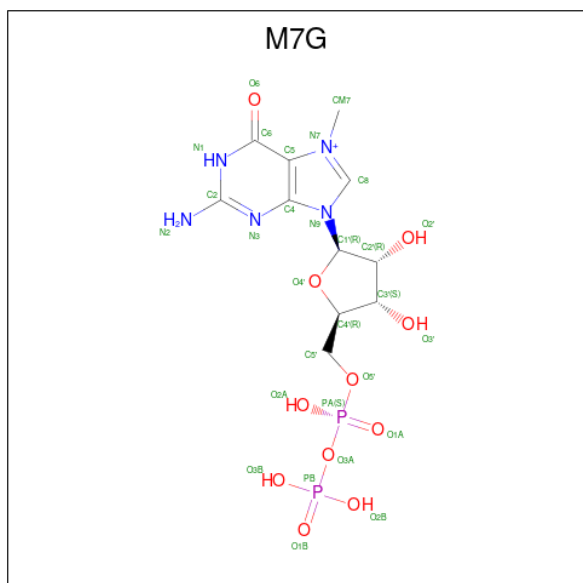
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H N O P 30 9 10 2 8 1	0	0
3	C	1	Total C H N O P 30 9 10 2 8 1	0	0

- Molecule 4 is L-GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 0G) (formula:  $C_{10}H_{14}N_5O_8P$ ).



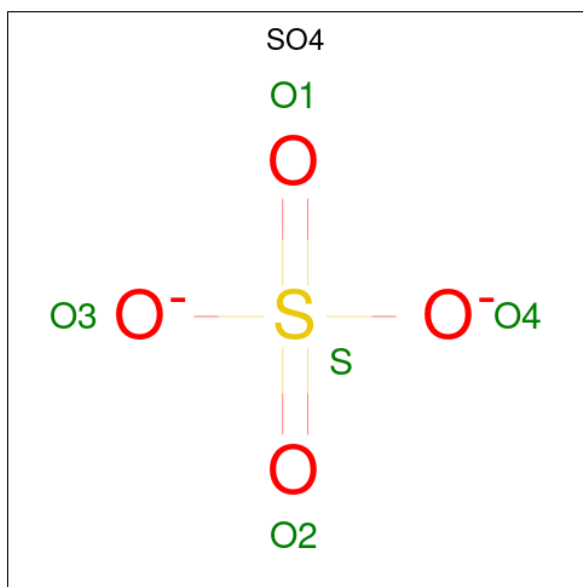
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
4	A	1	Total	C	H	N	O	P	0	0
			34	10	11	5	7	1		
4	C	1	Total	C	H	N	O	P	0	0
			34	10	11	5	7	1		

- Molecule 5 is 7N-METHYL-8-HYDROGUANOSINE-5'-DIPHOSPHATE (three-letter code: M7G) (formula:  $C_{11}H_{18}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	H	N	O	P	0	0
			45	11	16	5	11	2		
5	C	1	Total	C	H	N	O	P	0	0
			45	11	16	5	11	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	O S	0	0
			5	4 1		
6	D	1	Total	O S	0	0
			5	4 1		

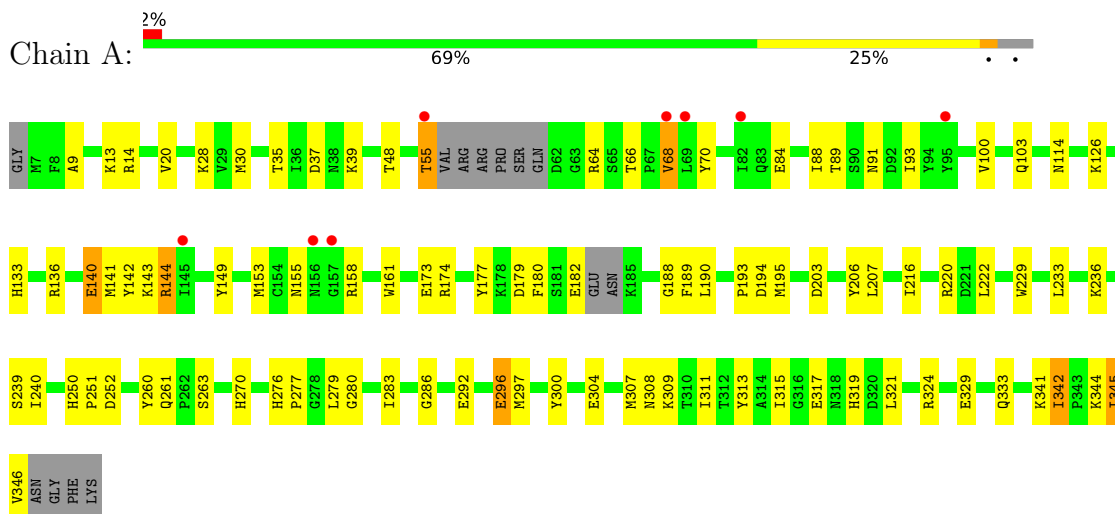
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	2	Total O	0	0
			2 2		

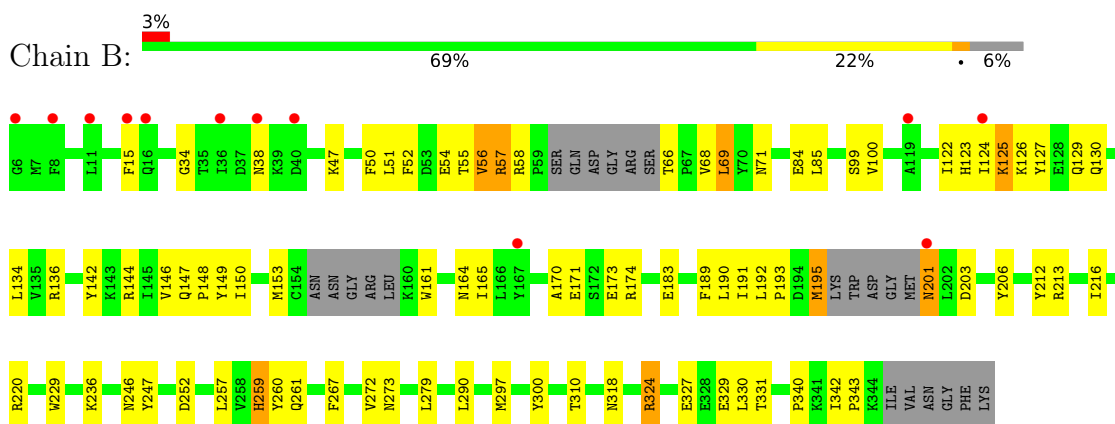
### 3 Residue-property plots [i](#)

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.

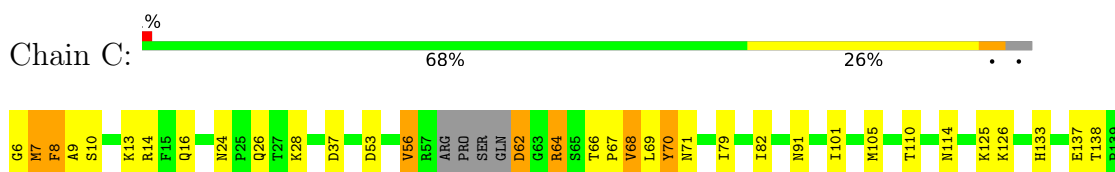
- Molecule 1: m7GpppX diphosphatase



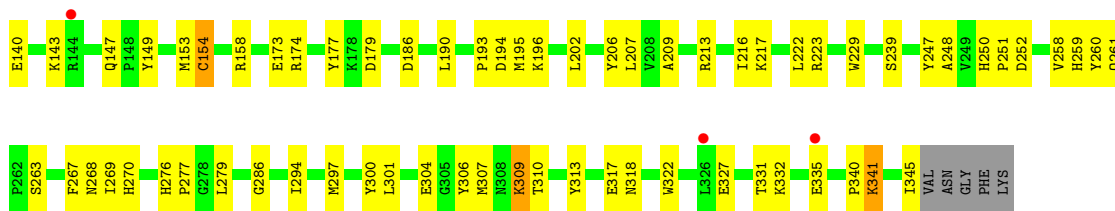
- Molecule 1: m7GpppX diphosphatase



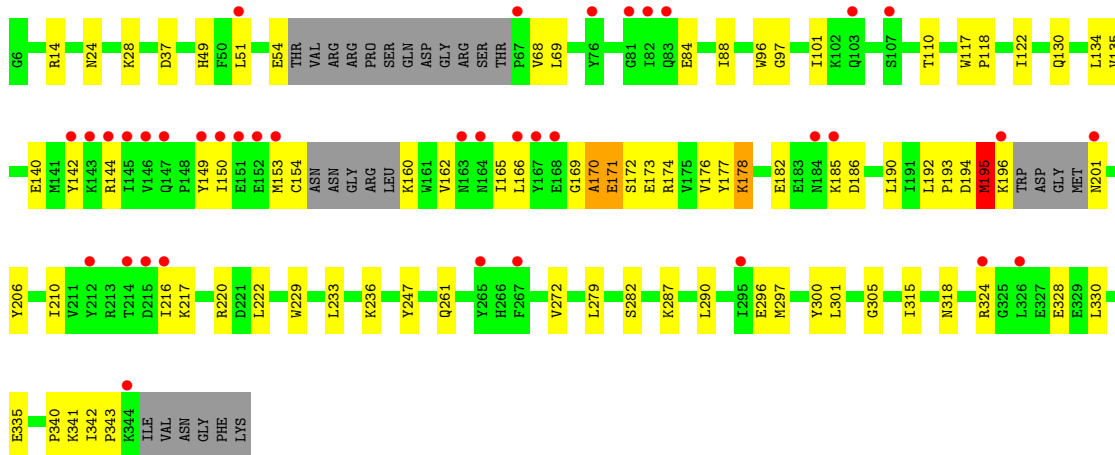
- Molecule 1: m7GpppX diphosphatase







• Molecule 1: m7GpppX diphosphatase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.76Å 104.10Å 189.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.31 – 2.94 47.31 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.31-2.94) 99.7 (47.31-2.94)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.96Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.204 , 0.263 0.203 , 0.262	Depositor DCC
$R_{free}$ test set	1872 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.1	Xtrriage
Anisotropy	0.794	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10991	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 0G, 2PO, M7G, SO4

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	0.43	1/2784 (0.0%)	0.78	3/3773 (0.1%)
1	B	0.38	0/2717	0.65	0/3681
1	C	0.41	0/2821	0.62	0/3822
1	D	0.39	0/2675	0.65	0/3621
All	All	0.40	1/10997 (0.0%)	0.68	3/14897 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	GLU	CB-CG	-5.37	1.42	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ARG	NE-CZ-NH1	-20.59	110.00	120.30
1	A	144	ARG	NE-CZ-NH2	15.34	127.97	120.30
1	A	144	ARG	CD-NE-CZ	-8.77	111.32	123.60

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	2722	0	2693	107	0
1	B	2657	0	2639	94	0
1	C	2758	0	2735	88	0
1	D	2616	0	2597	79	0
2	A	4	0	0	0	0
2	C	4	0	0	3	0
3	A	20	10	10	2	0
3	C	20	10	10	3	0
4	A	23	11	11	3	0
4	C	23	11	11	5	0
5	A	29	16	16	6	0
5	C	29	16	16	3	0
6	D	10	0	0	1	0
7	C	2	0	0	0	0
All	All	10917	74	10738	310	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 14.

All (310) 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:C:309:LYS:HE3	1:D:296:GLU:HG2	1.32	1.10
1:D:170:ALA:O	1:D:172:SER:N	1.94	1.00
1:D:140:GLU:OE2	1:D:144:ARG:NH1	1.96	0.98
1:B:165:ILE:HD13	1:B:170:ALA:HB3	1.46	0.97
1:D:282:SER:OG	6:D:401:SO4:O2	1.85	0.93
1:C:335:GLU:HG2	1:C:341:LYS:HE3	1.51	0.90
3:C:401:U:O2'	2:C:402:2PO:O1P	1.89	0.89
1:C:138:THR:HA	1:C:310:THR:HG22	1.54	0.88
1:A:296:GLU:OE1	1:B:310:THR:HB	1.76	0.84
1:A:140:GLU:OE2	1:A:144:ARG:NH1	2.11	0.83
1:B:55:THR:HG22	1:B:56:VAL:H	1.45	0.81
1:B:125:LYS:HG2	1:B:126:LYS:H	1.46	0.79
1:D:174:ARG:NH2	1:D:193:PRO:HB2	1.97	0.79
1:A:304:GLU:HG2	1:A:308:ASN:ND2	1.99	0.77
1:B:165:ILE:HD13	1:B:170:ALA:CB	2.14	0.77
1:D:154:CYS:O	1:D:160:LYS:HG3	1.85	0.76
1:A:9:ALA:O	1:A:13:LYS:HG3	1.85	0.76
1:D:272:VAL:HG11	1:D:279:LEU:HD11	1.65	0.76
1:C:309:LYS:CE	1:D:296:GLU:HG2	2.15	0.74
1:C:309:LYS:HD2	1:C:310:THR:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:MET:HE1	1:A:158:ARG:HD2	1.70	0.73
1:D:195:MET:SD	1:D:195:MET:N	2.57	0.72
1:D:14:ARG:NH1	1:D:37:ASP:OD2	2.22	0.72
1:D:272:VAL:HG11	1:D:279:LEU:CD1	2.19	0.72
1:A:173:GLU:HG2	1:A:174:ARG:HG2	1.73	0.71
1:D:335:GLU:CG	1:D:341:LYS:HE2	2.22	0.70
1:A:280:GLY:HA2	3:A:402:U:H3'	1.74	0.70
1:A:55:THR:HG23	1:A:68:VAL:HG21	1.75	0.69
1:A:345:ILE:HD13	1:D:51:LEU:HD21	1.73	0.69
1:C:14:ARG:NH1	1:C:37:ASP:OD2	2.25	0.68
1:C:309:LYS:HD2	1:C:310:THR:N	2.08	0.68
1:C:143:LYS:HD3	1:C:147:GLN:OE1	1.96	0.66
1:B:56:VAL:HG23	1:B:69:LEU:O	1.96	0.66
1:A:84:GLU:CB	1:A:100:VAL:HG12	2.26	0.65
1:A:84:GLU:HB3	1:A:100:VAL:HG12	1.78	0.65
1:D:176:VAL:HG23	1:D:193:PRO:HD3	1.79	0.65
1:A:55:THR:CG2	1:A:68:VAL:HG21	2.27	0.65
1:A:30:MET:HE3	1:B:50:PHE:HB2	1.77	0.65
1:A:133:HIS:NE2	1:A:317:GLU:HG3	2.12	0.65
1:D:178:LYS:HA	1:D:190:LEU:HB3	1.79	0.65
1:A:91:ASN:ND2	1:D:236:LYS:HG2	2.13	0.63
1:A:55:THR:HG23	1:A:68:VAL:CG2	2.28	0.63
1:A:55:THR:OG1	1:A:68:VAL:HG21	1.99	0.63
1:C:216:ILE:HD13	1:C:222:LEU:HD23	1.81	0.63
1:D:335:GLU:HG2	1:D:341:LYS:HE2	1.81	0.63
1:B:213:ARG:HD3	1:B:229:TRP:CH2	2.34	0.63
1:D:182:GLU:OE2	1:D:185:LYS:NZ	2.25	0.62
1:B:173:GLU:HG3	1:D:195:MET:CE	2.29	0.62
1:A:315:ILE:HD11	1:A:319:HIS:CG	2.34	0.62
1:B:56:VAL:HG23	1:B:69:LEU:HB2	1.82	0.62
1:B:216:ILE:HG22	1:B:267:PHE:HB2	1.81	0.62
1:B:125:LYS:HG2	1:B:126:LYS:N	2.15	0.62
1:B:56:VAL:HG22	1:B:58:ARG:H	1.65	0.61
1:A:342:ILE:HD13	1:B:247:TYR:CD2	2.34	0.61
1:C:69:LEU:O	1:C:70:TYR:HB2	1.99	0.61
1:A:91:ASN:HD21	1:D:236:LYS:HG2	1.65	0.61
1:D:68:VAL:O	1:D:69:LEU:HG	2.01	0.61
1:C:286:GLY:HA2	1:D:290:LEU:HD11	1.83	0.61
1:A:142:TYR:CE1	1:A:220:ARG:HG3	2.35	0.61
1:A:149:TYR:CZ	1:A:153:MET:HG3	2.35	0.60
1:B:201:ASN:N	1:B:201:ASN:ND2	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:MET:HE3	1:B:50:PHE:CB	2.31	0.60
1:B:327:GLU:O	1:B:331:THR:HG23	2.01	0.60
1:A:345:ILE:CD1	1:D:51:LEU:HD21	2.31	0.60
1:A:315:ILE:HD11	1:A:319:HIS:CD2	2.37	0.60
1:D:216:ILE:HD13	1:D:222:LEU:HD23	1.83	0.60
1:B:149:TYR:HD1	1:B:324:ARG:HH21	1.50	0.59
1:A:239:SER:HA	1:B:340:PRO:HD2	1.85	0.59
1:C:7:MET:O	1:C:10:SER:N	2.35	0.59
1:A:297:MET:HE1	1:B:297:MET:HE1	1.84	0.59
1:A:270:HIS:CE1	5:A:404:M7G:H5'1	2.38	0.59
1:A:304:GLU:HG2	1:A:308:ASN:HD21	1.66	0.59
1:B:150:ILE:O	1:B:153:MET:HB2	2.03	0.59
1:A:279:LEU:HD13	4:A:403:OG:N2	2.17	0.59
1:C:258:VAL:HG12	1:C:259:HIS:N	2.18	0.59
1:C:114:ASN:ND2	4:C:403:OG:N7	2.51	0.58
1:A:88:ILE:HG21	1:D:247:TYR:OH	2.03	0.58
1:A:297:MET:HA	1:A:297:MET:CE	2.31	0.58
1:A:342:ILE:CD1	1:B:247:TYR:HD2	2.16	0.58
1:A:70:TYR:OH	1:A:203:ASP:OD1	2.22	0.58
1:A:194:ASP:OD1	5:A:404:M7G:O2'	2.19	0.58
1:A:297:MET:HA	1:A:297:MET:HE3	1.85	0.58
1:D:68:VAL:O	1:D:68:VAL:HG23	2.04	0.58
1:A:14:ARG:NH1	1:A:37:ASP:OD2	2.37	0.58
1:B:55:THR:HG22	1:B:56:VAL:N	2.19	0.57
1:A:297:MET:CE	1:B:297:MET:CE	2.82	0.57
1:B:125:LYS:O	1:B:127:TYR:N	2.33	0.57
1:A:342:ILE:HD13	1:B:247:TYR:HD2	1.69	0.57
1:A:89:THR:HB	1:C:340:PRO:HG3	1.86	0.57
1:B:84:GLU:CB	1:B:100:VAL:HG12	2.35	0.57
1:C:174:ARG:NH2	1:C:193:PRO:HB2	2.19	0.57
1:C:177:TYR:CE2	1:C:179:ASP:HB2	2.40	0.56
1:A:344:LYS:O	1:A:344:LYS:HG3	2.04	0.56
1:C:194:ASP:OD2	5:C:404:M7G:H2'	2.05	0.56
1:A:30:MET:CE	1:B:50:PHE:HB2	2.35	0.56
1:B:54:GLU:O	1:B:54:GLU:HG2	2.04	0.56
1:B:189:PHE:HE2	1:B:191:ILE:HD11	1.71	0.56
1:B:201:ASN:N	1:D:201:ASN:HD22	2.04	0.56
1:D:154:CYS:C	1:D:160:LYS:HG3	2.25	0.56
1:A:153:MET:CE	1:A:158:ARG:HD2	2.34	0.56
1:B:57:ARG:HB3	1:B:71:ASN:ND2	2.21	0.55
1:A:297:MET:HE1	1:B:297:MET:CE	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:LEU:HD21	1:C:248:ALA:HB3	1.88	0.55
1:C:125:LYS:HB3	1:C:318:ASN:HB3	1.88	0.55
1:C:322:TRP:CE2	1:C:327:GLU:HB2	2.42	0.55
1:A:194:ASP:OD1	1:A:195:MET:N	2.40	0.55
1:D:153:MET:CE	1:D:153:MET:HA	2.37	0.55
1:A:297:MET:CE	1:A:297:MET:CA	2.83	0.54
1:A:297:MET:HE3	1:A:297:MET:CA	2.37	0.54
1:C:68:VAL:HG12	1:C:68:VAL:O	2.07	0.54
1:C:300:TYR:HB3	1:D:300:TYR:HB3	1.88	0.54
1:C:158:ARG:HG2	1:C:158:ARG:HH11	1.73	0.54
1:C:263:SER:OG	4:C:403:OG:OP1	2.15	0.54
1:A:189:PHE:HE1	1:A:236:LYS:HD3	1.72	0.54
1:C:223:ARG:NH1	1:C:304:GLU:HA	2.22	0.54
1:A:126:LYS:HZ1	1:A:263:SER:CB	2.20	0.54
1:B:84:GLU:HB3	1:B:100:VAL:HG12	1.88	0.54
1:B:173:GLU:HG3	1:D:195:MET:HE3	1.88	0.53
1:A:158:ARG:HG3	1:A:158:ARG:HH11	1.73	0.53
1:A:220:ARG:CZ	1:A:311:ILE:HD12	2.38	0.53
1:C:110:THR:HG21	1:D:101:ILE:HB	1.90	0.53
1:C:62:ASP:OD1	1:C:62:ASP:N	2.41	0.53
1:D:122:ILE:HD12	1:D:122:ILE:H	1.73	0.53
1:A:216:ILE:HD13	1:A:222:LEU:CD2	2.39	0.53
1:B:189:PHE:C	1:B:212:TYR:HE1	2.12	0.53
1:A:30:MET:HE2	1:B:52:PHE:CZ	2.44	0.52
1:B:165:ILE:CD1	1:B:171:GLU:HG3	2.40	0.52
1:C:239:SER:HA	1:D:340:PRO:HD2	1.91	0.52
1:C:137:GLU:OE1	1:C:260:TYR:OH	2.24	0.52
1:C:133:HIS:NE2	1:C:317:GLU:HG3	2.25	0.52
1:C:79:ILE:HB	1:C:82:ILE:CD1	2.40	0.51
1:B:195:MET:SD	1:D:173:GLU:HG3	2.50	0.51
1:C:261:GLN:HG2	1:C:313:TYR:CE2	2.45	0.51
1:C:270:HIS:CE1	5:C:404:M7G:H5'1	2.45	0.51
1:C:304:GLU:OE2	1:C:304:GLU:N	2.40	0.51
1:A:103:GLN:HB3	1:B:100:VAL:HG23	1.92	0.51
1:A:177:TYR:CD1	1:A:240:ILE:HD13	2.46	0.51
1:B:56:VAL:CG2	1:B:69:LEU:HB2	2.40	0.51
1:A:229:TRP:CZ2	1:A:233:LEU:HD11	2.46	0.51
1:C:190:LEU:HD12	1:C:190:LEU:C	2.32	0.50
1:C:279:LEU:HD22	4:C:403:OG:N2	2.26	0.50
1:C:28:LYS:HD2	1:C:28:LYS:N	2.26	0.50
1:D:135:VAL:HG23	1:D:315:ILE:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:PHE:CE2	1:A:182:GLU:HG3	2.46	0.50
1:B:173:GLU:HG3	1:D:195:MET:HE1	1.94	0.49
1:C:297:MET:SD	1:D:297:MET:SD	3.10	0.49
1:D:122:ILE:HD12	1:D:122:ILE:N	2.28	0.49
1:A:30:MET:CE	1:B:50:PHE:CB	2.90	0.49
1:A:297:MET:HE3	1:A:297:MET:O	2.12	0.49
1:B:129:GLN:OE1	1:B:129:GLN:HA	2.12	0.49
1:B:272:VAL:HG11	1:B:279:LEU:HD11	1.95	0.49
1:C:56:VAL:HA	1:C:67:PRO:HA	1.94	0.49
1:C:193:PRO:HA	1:C:207:LEU:HD23	1.95	0.49
1:A:48:THR:O	1:B:47:LYS:HE3	2.13	0.49
1:D:165:ILE:HD11	1:D:171:GLU:CG	2.42	0.49
1:B:122:ILE:HD12	1:B:122:ILE:H	1.78	0.49
1:C:149:TYR:CZ	1:C:153:MET:HG3	2.47	0.49
1:D:166:LEU:HD21	1:D:210:ILE:HG22	1.95	0.49
1:A:220:ARG:NH1	1:A:309:LYS:O	2.41	0.48
1:B:125:LYS:CG	1:B:126:LYS:H	2.21	0.48
1:C:6:GLY:O	1:C:7:MET:HB3	2.13	0.48
1:A:133:HIS:CD2	1:A:317:GLU:HG3	2.49	0.48
1:A:179:ASP:O	1:A:188:GLY:HA3	2.13	0.48
1:B:144:ARG:NH2	1:B:329:GLU:OE2	2.41	0.48
1:B:189:PHE:HA	1:B:212:TYR:CD1	2.47	0.48
1:C:133:HIS:CD2	1:C:317:GLU:HG3	2.49	0.48
1:A:141:MET:SD	1:A:329:GLU:HG2	2.54	0.48
1:A:216:ILE:HD13	1:A:222:LEU:HD23	1.95	0.48
1:B:51:LEU:HD21	1:C:345:ILE:CD1	2.43	0.48
1:A:28:LYS:HE2	1:B:47:LYS:O	2.14	0.48
1:C:24:ASN:OD1	1:C:26:GLN:HB2	2.14	0.48
1:C:126:LYS:HZ3	1:C:263:SER:CB	2.26	0.48
1:A:252:ASP:CB	1:B:330:LEU:HD21	2.44	0.48
1:C:6:GLY:O	1:C:7:MET:CB	2.61	0.48
1:D:130:GLN:OE1	1:D:318:ASN:HB2	2.14	0.48
1:A:304:GLU:HG2	1:A:308:ASN:CG	2.34	0.48
1:B:142:TYR:CE1	1:B:220:ARG:HG3	2.49	0.48
1:B:236:LYS:HE2	1:C:91:ASN:HD21	1.78	0.48
1:C:126:LYS:NZ	1:C:263:SER:HB3	2.29	0.48
1:A:300:TYR:HB3	1:B:300:TYR:HB3	1.94	0.47
1:B:190:LEU:C	1:B:190:LEU:HD12	2.35	0.47
1:C:101:ILE:HB	1:D:110:THR:HG21	1.96	0.47
1:A:149:TYR:CE1	1:A:153:MET:HG3	2.49	0.47
1:A:345:ILE:CG2	1:A:346:VAL:HG23	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ARG:HG2	1:C:158:ARG:NH1	2.30	0.47
1:C:8:PHE:CE2	1:D:97:GLY:HA3	2.49	0.47
1:C:53:ASP:OD2	1:C:71:ASN:HB3	2.14	0.47
1:A:35:THR:HA	1:A:39:LYS:O	2.15	0.47
1:B:161:TRP:O	1:B:164:ASN:HB2	2.14	0.47
1:D:142:TYR:CE1	1:D:220:ARG:HG3	2.50	0.47
1:D:149:TYR:HD1	1:D:324:ARG:NH1	2.12	0.47
1:B:66:THR:O	1:B:69:LEU:HG	2.15	0.47
1:A:143:LYS:HE3	1:A:307:MET:CE	2.44	0.46
1:A:189:PHE:CE1	1:A:236:LYS:HD3	2.50	0.46
1:A:64:ARG:NH2	1:B:342:ILE:HD13	2.30	0.46
1:B:189:PHE:HE1	1:B:236:LYS:HD3	1.79	0.46
1:C:9:ALA:O	1:C:13:LYS:HG2	2.15	0.46
1:A:190:LEU:HD12	1:A:190:LEU:C	2.35	0.46
1:A:193:PRO:HA	1:A:207:LEU:HD23	1.97	0.46
1:D:272:VAL:CG1	1:D:279:LEU:HD11	2.39	0.46
1:B:15:PHE:CZ	1:B:34:GLY:HA3	2.51	0.46
1:B:122:ILE:HD12	1:B:122:ILE:N	2.31	0.46
1:D:192:LEU:HD12	1:D:193:PRO:O	2.15	0.46
1:A:346:VAL:HG11	1:B:246:ASN:O	2.16	0.45
1:B:124:ILE:C	1:B:125:LYS:O	2.52	0.45
1:C:250:HIS:HB3	1:C:251:PRO:HD2	1.97	0.45
1:C:258:VAL:HG12	1:C:259:HIS:H	1.81	0.45
1:D:28:LYS:HD2	1:D:28:LYS:N	2.32	0.45
1:B:189:PHE:HA	1:B:212:TYR:HD1	1.80	0.45
1:D:88:ILE:HG13	1:D:97:GLY:HA2	1.98	0.45
1:A:270:HIS:CE1	5:A:404:M7G:C5'	2.99	0.45
1:D:142:TYR:CD1	1:D:220:ARG:HG3	2.51	0.45
1:D:192:LEU:HD12	1:D:192:LEU:C	2.37	0.45
1:A:297:MET:SD	1:B:297:MET:SD	3.15	0.45
3:A:402:U:H5''	3:A:402:U:C6	2.51	0.45
1:C:16:GLN:HA	1:C:16:GLN:OE1	2.17	0.45
1:C:286:GLY:CA	1:D:290:LEU:HD11	2.46	0.45
1:C:195:MET:HG3	1:D:96:TRP:CD2	2.51	0.45
1:A:286:GLY:HA2	1:B:290:LEU:HD11	1.99	0.45
1:B:134:LEU:HD23	1:B:134:LEU:HA	1.62	0.45
1:C:294:ILE:HD13	1:C:306:TYR:OH	2.16	0.45
1:A:48:THR:O	1:B:47:LYS:HG3	2.17	0.45
1:B:125:LYS:C	1:B:127:TYR:H	2.19	0.45
1:B:149:TYR:HA	1:B:324:ARG:NH2	2.32	0.45
1:B:192:LEU:HD12	1:B:193:PRO:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:LEU:HD23	1:D:134:LEU:HA	1.68	0.45
1:D:296:GLU:O	1:D:296:GLU:HG3	2.15	0.44
1:A:321:LEU:HA	1:A:324:ARG:HB2	2.00	0.44
1:A:84:GLU:CB	1:A:100:VAL:CG1	2.94	0.44
1:B:165:ILE:HD11	1:B:171:GLU:HG3	1.99	0.44
3:C:401:U:O2'	2:C:402:2PO:P	2.74	0.44
1:C:216:ILE:HD13	1:C:222:LEU:CD2	2.46	0.44
1:C:270:HIS:CE1	5:C:404:M7G:C5'	3.00	0.44
1:D:117:TRP:HA	1:D:118:PRO:HA	1.84	0.44
1:D:150:ILE:HG21	1:D:217:LYS:HD3	2.00	0.44
1:A:55:THR:CB	1:A:68:VAL:HG21	2.47	0.44
1:C:28:LYS:HA	1:D:49:HIS:ND1	2.33	0.44
3:C:401:U:HO2'	2:C:402:2PO:P	2.29	0.44
1:C:209:ALA:HB3	1:C:269:ILE:HB	2.00	0.44
1:A:345:ILE:HG22	1:A:346:VAL:HG23	2.00	0.44
1:D:177:TYR:O	1:D:178:LYS:HB3	2.18	0.44
1:A:194:ASP:OD1	5:A:404:M7G:C2'	2.66	0.43
5:A:404:M7G:PB	5:A:404:M7G:H5'2	2.58	0.43
1:D:178:LYS:HA	1:D:190:LEU:CB	2.46	0.43
1:C:301:LEU:HD13	1:C:306:TYR:HA	2.00	0.43
1:A:114:ASN:ND2	4:A:403:OG:N7	2.66	0.43
1:A:136:ARG:O	1:A:333:GLN:NE2	2.35	0.43
1:B:203:ASP:HA	1:B:273:ASN:ND2	2.33	0.43
1:A:342:ILE:CD1	1:B:247:TYR:CD2	2.98	0.43
1:A:345:ILE:HD13	1:D:51:LEU:CD2	2.45	0.43
1:B:147:GLN:HB3	1:B:148:PRO:HD3	2.00	0.43
1:C:79:ILE:HB	1:C:82:ILE:HD12	2.01	0.43
1:B:257:LEU:CD1	1:B:259:HIS:HE1	2.32	0.43
4:C:403:OG:H2'	4:C:403:OG:N3	2.34	0.43
1:C:173:GLU:HG2	1:C:174:ARG:HG2	2.00	0.43
1:D:261:GLN:O	1:D:287:LYS:NZ	2.41	0.43
1:C:7:MET:O	1:C:9:ALA:N	2.51	0.42
1:A:292:GLU:OE2	1:B:136:ARG:HD3	2.19	0.42
1:B:142:TYR:CD1	1:B:146:VAL:HB	2.54	0.42
1:C:252:ASP:CB	1:D:330:LEU:HD21	2.48	0.42
1:D:165:ILE:HD11	1:D:171:GLU:CD	2.39	0.42
1:A:279:LEU:HD13	4:A:403:OG:C2	2.49	0.42
1:C:126:LYS:HZ1	1:C:263:SER:HB3	1.84	0.42
1:C:154:CYS:SG	1:C:217:LYS:HD2	2.60	0.42
1:C:247:TYR:CD2	1:D:342:ILE:HD11	2.53	0.42
1:C:277:PRO:HG2	1:D:24:ASN:OD1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:MET:SD	1:D:297:MET:CE	3.07	0.42
1:D:165:ILE:HD13	1:D:170:ALA:HB3	2.01	0.42
1:A:30:MET:HE2	1:B:52:PHE:HZ	1.85	0.42
1:C:252:ASP:HB3	1:D:330:LEU:HD21	2.00	0.42
1:D:185:LYS:HG2	1:D:186:ASP:OD1	2.19	0.42
1:D:216:ILE:HD13	1:D:222:LEU:CD2	2.50	0.42
1:A:30:MET:HE3	1:B:50:PHE:CG	2.54	0.42
1:A:297:MET:CE	1:B:297:MET:HE3	2.49	0.42
1:B:236:LYS:HE2	1:C:91:ASN:OD1	2.19	0.42
1:C:105:MET:HE2	1:D:84:GLU:HB3	2.02	0.42
1:C:331:THR:O	1:C:335:GLU:HG3	2.18	0.42
1:A:261:GLN:HG2	1:A:313:TYR:CE2	2.55	0.42
1:C:213:ARG:HD3	1:C:229:TRP:CZ2	2.55	0.42
1:A:158:ARG:HH11	1:A:158:ARG:CG	2.33	0.41
1:A:84:GLU:HB2	1:A:100:VAL:CG1	2.49	0.41
1:C:7:MET:O	1:C:8:PHE:C	2.58	0.41
1:A:341:LYS:O	1:A:342:ILE:O	2.38	0.41
1:B:85:LEU:HD23	1:B:99:SER:HB3	2.01	0.41
1:C:332:LYS:HD2	1:C:332:LYS:HA	1.80	0.41
1:D:301:LEU:HB3	1:D:305:GLY:O	2.21	0.41
1:D:54:GLU:O	1:D:54:GLU:HG2	2.19	0.41
1:C:309:LYS:HE2	1:C:310:THR:O	2.20	0.41
1:A:93:ILE:HD11	1:B:123:HIS:CE1	2.55	0.41
1:B:51:LEU:HD21	1:C:345:ILE:HD12	2.01	0.41
1:A:20:VAL:O	1:B:68:VAL:HA	2.20	0.41
1:A:161:TRP:CE2	5:A:404:M7G:HM73	2.55	0.41
1:C:335:GLU:HG2	1:C:341:LYS:CE	2.35	0.41
1:B:57:ARG:HH22	1:B:58:ARG:NH1	2.19	0.41
1:B:173:GLU:HG2	1:B:174:ARG:HG2	2.02	0.41
1:B:201:ASN:N	1:B:201:ASN:HD22	2.19	0.41
1:C:64:ARG:H	1:C:64:ARG:HG2	1.63	0.41
1:C:196:LYS:HE2	4:C:403:OG:H5'	2.01	0.41
1:D:150:ILE:CG2	1:D:217:LYS:HD3	2.50	0.41
1:D:169:GLY:O	1:D:170:ALA:O	2.39	0.41
1:D:194:ASP:O	1:D:195:MET:C	2.59	0.41
1:B:252:ASP:OD1	1:B:252:ASP:N	2.54	0.41
1:A:277:PRO:O	1:A:283:ILE:HD11	2.21	0.40
1:D:229:TRP:CZ2	1:D:233:LEU:HD11	2.56	0.40
1:B:260:TYR:HA	1:B:261:GLN:HA	1.85	0.40
1:B:130:GLN:OE1	1:B:318:ASN:HB2	2.21	0.40
1:A:250:HIS:HB3	1:A:251:PRO:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:TYR:CZ	1:A:261:GLN:NE2	2.89	0.40
1:C:216:ILE:HG22	1:C:267:PHE:HB2	2.03	0.40
1:A:30:MET:HE2	1:A:30:MET:HB2	1.93	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	326/345 (94%)	312 (96%)	12 (4%)	2 (1%)	25	56
1	B	315/345 (91%)	302 (96%)	11 (4%)	2 (1%)	25	56
1	C	332/345 (96%)	315 (95%)	14 (4%)	3 (1%)	17	46
1	D	310/345 (90%)	292 (94%)	12 (4%)	6 (2%)	8	26
All	All	1283/1380 (93%)	1221 (95%)	49 (4%)	13 (1%)	15	43

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	125	LYS
1	C	7	MET
1	C	8	PHE
1	D	162	VAL
1	D	170	ALA
1	D	171	GLU
1	D	195	MET
1	D	343	PRO
1	A	342	ILE
1	D	178	LYS
1	B	343	PRO
1	C	70	TYR

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Mol	Chain	Res	Type
1	A	155	ASN

### 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	302/314 (96%)	295 (98%)	7 (2%)	50 78
1	B	296/314 (94%)	286 (97%)	10 (3%)	37 68
1	C	306/314 (98%)	292 (95%)	14 (5%)	27 57
1	D	291/314 (93%)	287 (99%)	4 (1%)	67 86
All	All	1195/1256 (95%)	1160 (97%)	35 (3%)	42 73

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	THR
1	A	66	THR
1	A	68	VAL
1	A	206	TYR
1	A	276	HIS
1	A	296	GLU
1	A	345	ILE
1	B	38	ASN
1	B	56	VAL
1	B	57	ARG
1	B	69	LEU
1	B	183	GLU
1	B	195	MET
1	B	201	ASN
1	B	206	TYR
1	B	259	HIS
1	B	324	ARG
1	C	56	VAL
1	C	62	ASP
1	C	64	ARG

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Mol	Chain	Res	Type
1	C	66	THR
1	C	68	VAL
1	C	140	GLU
1	C	154	CYS
1	C	186	ASP
1	C	206	TYR
1	C	268	ASN
1	C	276	HIS
1	C	307	MET
1	C	309	LYS
1	C	341	LYS
1	D	195	MET
1	D	196	LYS
1	D	206	TYR
1	D	328	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	201	ASN

### 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](#)

10 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
4	0G	C	403	3,5	18,25,26	0.90	1 (5%)	19,37,40	1.86	3 (15%)
3	U	C	401	4,2	18,21,22	1.37	4 (22%)	26,30,33	2.22	7 (26%)
6	SO4	D	402	-	4,4,4	0.11	0	6,6,6	0.25	0
5	M7G	C	404	4,1	26,31,31	2.60	3 (11%)	28,49,49	1.25	5 (17%)
2	2PO	C	402	3	0,3,3	-	-	0,3,3	-	-
4	0G	A	403	3,1,5	18,25,26	1.46	2 (11%)	19,37,40	2.30	7 (36%)
6	SO4	D	401	-	4,4,4	0.08	0	6,6,6	0.43	0
3	U	A	402	4,2	18,21,22	1.35	4 (22%)	26,30,33	2.27	8 (30%)
2	2PO	A	401	3	0,3,3	-	-	0,3,3	-	-
5	M7G	A	404	4	26,31,31	2.54	5 (19%)	28,49,49	1.48	6 (21%)

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
4	0G	C	403	3,5	1/1/5/5	0/3/25/26	0/3/3/3
3	U	C	401	4,2	-	0/7/25/26	0/2/2/2
5	M7G	C	404	4,1	3/3/6/6	7/12/32/32	0/3/3/3
4	0G	A	403	3,1,5	1/1/5/5	3/3/25/26	0/3/3/3
3	U	A	402	4,2	-	3/7/25/26	0/2/2/2
5	M7G	A	404	4	3/3/6/6	7/12/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	404	M7G	C8-N9	8.21	1.48	1.33
5	C	404	M7G	C8-N7	8.18	1.48	1.33
5	A	404	M7G	C8-N9	7.93	1.47	1.33
5	A	404	M7G	C8-N7	7.89	1.47	1.33
5	C	404	M7G	C5-C4	4.49	1.48	1.39
4	A	403	0G	O4'-C1'	4.24	1.47	1.41
5	A	404	M7G	C5-C4	4.20	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	U	C4-N3	-2.52	1.34	1.38
5	A	404	M7G	O4'-C1'	2.49	1.44	1.41
3	A	402	U	C5-C4	-2.46	1.38	1.43
3	A	402	U	C4-N3	-2.46	1.34	1.38
3	A	402	U	C2-N3	-2.41	1.33	1.38
4	A	403	0G	C6-N1	-2.38	1.34	1.37
3	C	401	U	C2-N1	2.34	1.42	1.38
3	A	402	U	C2-N1	2.29	1.42	1.38
3	C	401	U	C5-C4	-2.16	1.38	1.43
3	C	401	U	C2-N3	-2.12	1.34	1.38
4	C	403	0G	C6-N1	-2.04	1.34	1.37
5	A	404	M7G	C6-N1	-2.02	1.34	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	U	C4-N3-C2	-5.70	119.06	126.58
4	A	403	0G	C5'-C4'-C3'	5.14	134.45	115.18
4	C	403	0G	O4'-C1'-C2'	-4.97	99.66	106.93
3	A	402	U	C5-C4-N3	4.70	121.87	114.84
4	A	403	0G	O4'-C1'-C2'	-4.45	100.42	106.93
3	C	401	U	N3-C2-N1	4.41	120.75	114.89
3	A	402	U	C3'-C2'-C1'	4.30	109.59	101.43
3	C	401	U	C5-C4-N3	4.27	121.23	114.84
3	A	402	U	C4-N3-C2	-4.19	121.05	126.58
3	A	402	U	O4'-C1'-C2'	-3.95	98.02	106.64
3	C	401	U	O4-C4-C5	-3.93	118.25	125.16
3	A	402	U	O3'-C3'-C4'	3.66	121.62	111.05
4	A	403	0G	C3'-C2'-C1'	-3.65	95.48	100.98
3	A	402	U	O4-C4-C5	-3.58	118.86	125.16
3	A	402	U	C2'-C1'-N1	3.50	123.13	113.22
3	C	401	U	C2'-C3'-C4'	3.16	108.78	102.64
4	A	403	0G	C8-N7-C5	3.11	108.91	102.99
5	A	404	M7G	C3'-C2'-C1'	2.86	105.28	100.98
3	A	402	U	N3-C2-N1	2.74	118.53	114.89
5	A	404	M7G	O4'-C4'-C3'	2.74	110.54	105.11
4	C	403	0G	C8-N7-C5	2.74	108.21	102.99
3	C	401	U	O2-C2-N1	-2.68	119.23	122.79
5	C	404	M7G	PA-O3A-PB	-2.67	123.66	132.83
5	A	404	M7G	CM7-N7-C8	-2.55	113.16	125.43
4	A	403	0G	O4'-C4'-C3'	-2.53	100.10	105.11
5	C	404	M7G	C3'-C2'-C1'	2.50	104.74	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	404	M7G	O3B-PB-O3A	2.46	112.89	104.64
3	C	401	U	O4'-C1'-N1	2.43	113.91	108.36
5	C	404	M7G	O4'-C4'-C3'	2.43	109.92	105.11
5	C	404	M7G	O3'-C3'-C2'	-2.42	103.99	111.82
5	C	404	M7G	CM7-N7-C8	-2.41	113.85	125.43
4	A	403	0G	C2'-C3'-C4'	2.32	107.14	102.64
4	A	403	0G	C5-C6-N1	2.17	117.79	113.95
4	C	403	0G	C5'-C4'-C3'	2.12	123.12	115.18
5	A	404	M7G	O3'-C3'-C2'	-2.07	105.14	111.82
5	A	404	M7G	N2-C2-N3	-2.04	115.77	119.74

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	403	0G	C1'
4	C	403	0G	C1'
5	A	404	M7G	C2'
5	A	404	M7G	C4'
5	A	404	M7G	C3'
5	C	404	M7G	C2'
5	C	404	M7G	C4'
5	C	404	M7G	C3'

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404	M7G	C5'-O5'-PA-O1A
5	A	404	M7G	C5'-O5'-PA-O3A
5	A	404	M7G	PA-O3A-PB-O3B
5	C	404	M7G	C5'-O5'-PA-O3A
3	A	402	U	C2'-C1'-N1-C6
3	A	402	U	C2'-C1'-N1-C2
5	A	404	M7G	C5'-O5'-PA-O2A
5	C	404	M7G	C5'-O5'-PA-O1A
5	A	404	M7G	C3'-C4'-C5'-O5'
5	C	404	M7G	C4'-C5'-O5'-PA
4	A	403	0G	C4'-C5'-O5'-P
5	C	404	M7G	PA-O3A-PB-O1B
3	A	402	U	C4'-C5'-O5'-P
4	A	403	0G	O4'-C4'-C5'-O5'
4	A	403	0G	C3'-C4'-C5'-O5'
5	A	404	M7G	C4'-C5'-O5'-PA

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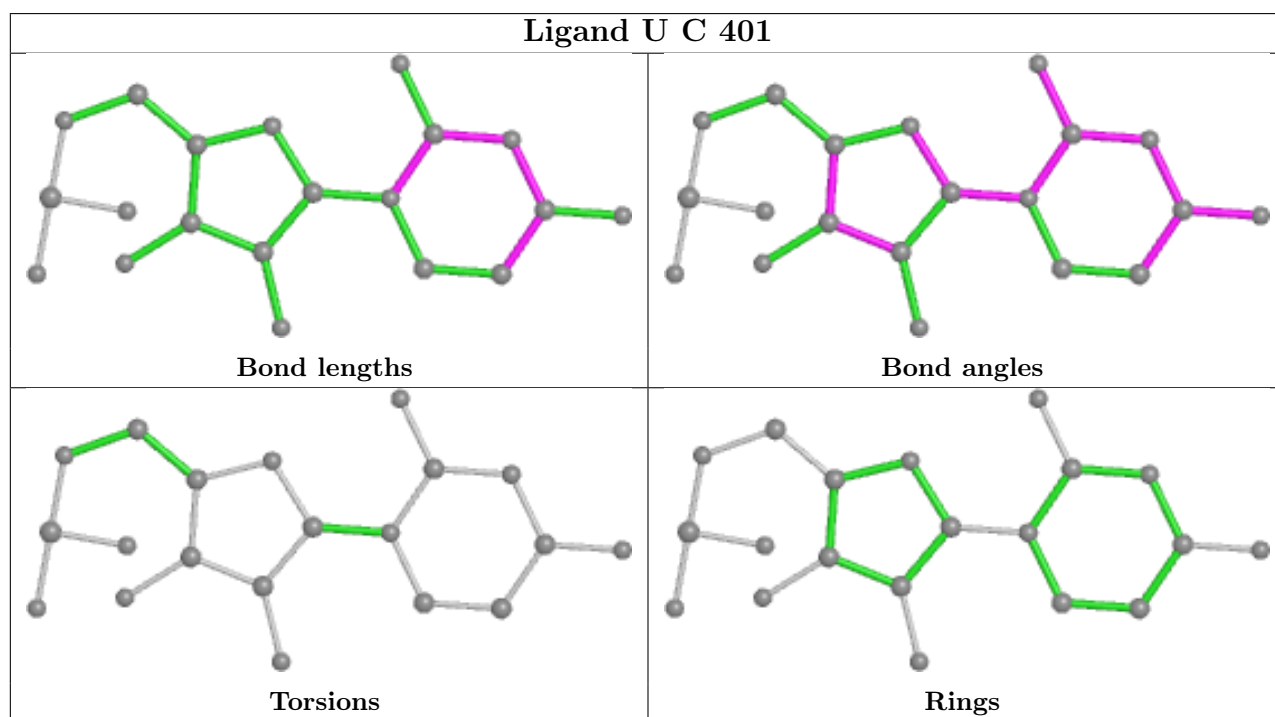
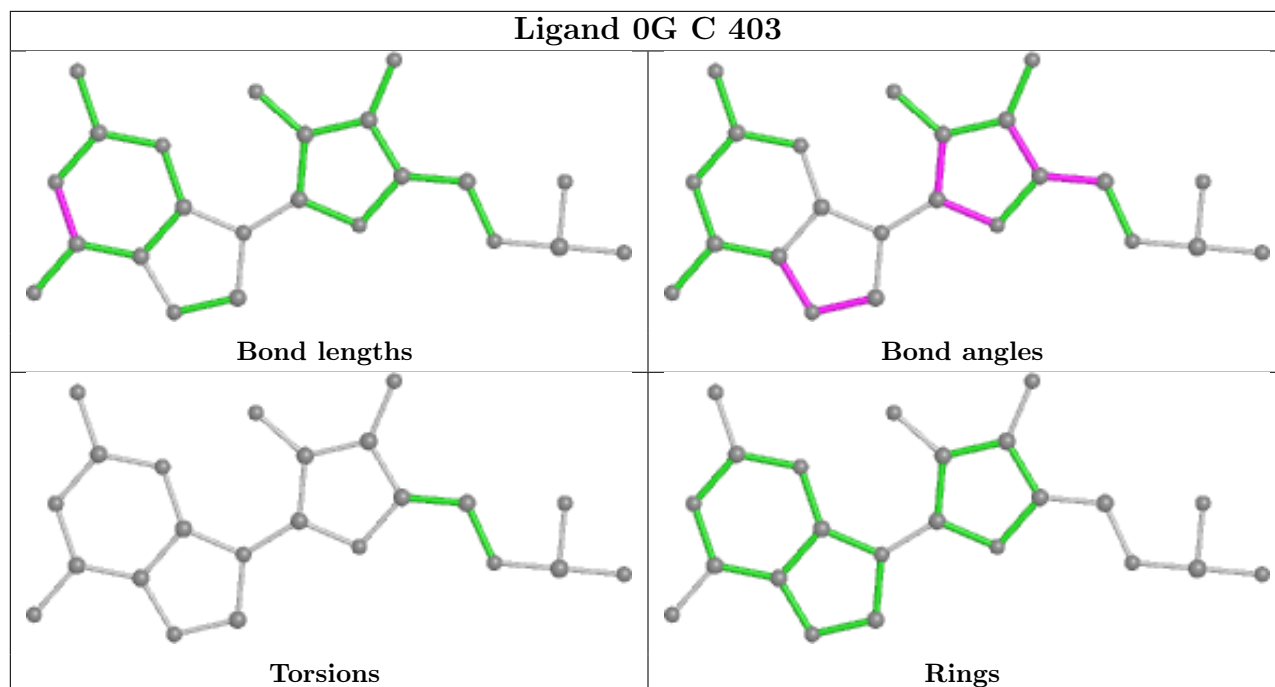
Mol	Chain	Res	Type	Atoms
5	A	404	M7G	PA-O3A-PB-O2B
5	C	404	M7G	PA-O3A-PB-O2B
5	C	404	M7G	PA-O3A-PB-O3B
5	C	404	M7G	C5'-O5'-PA-O2A

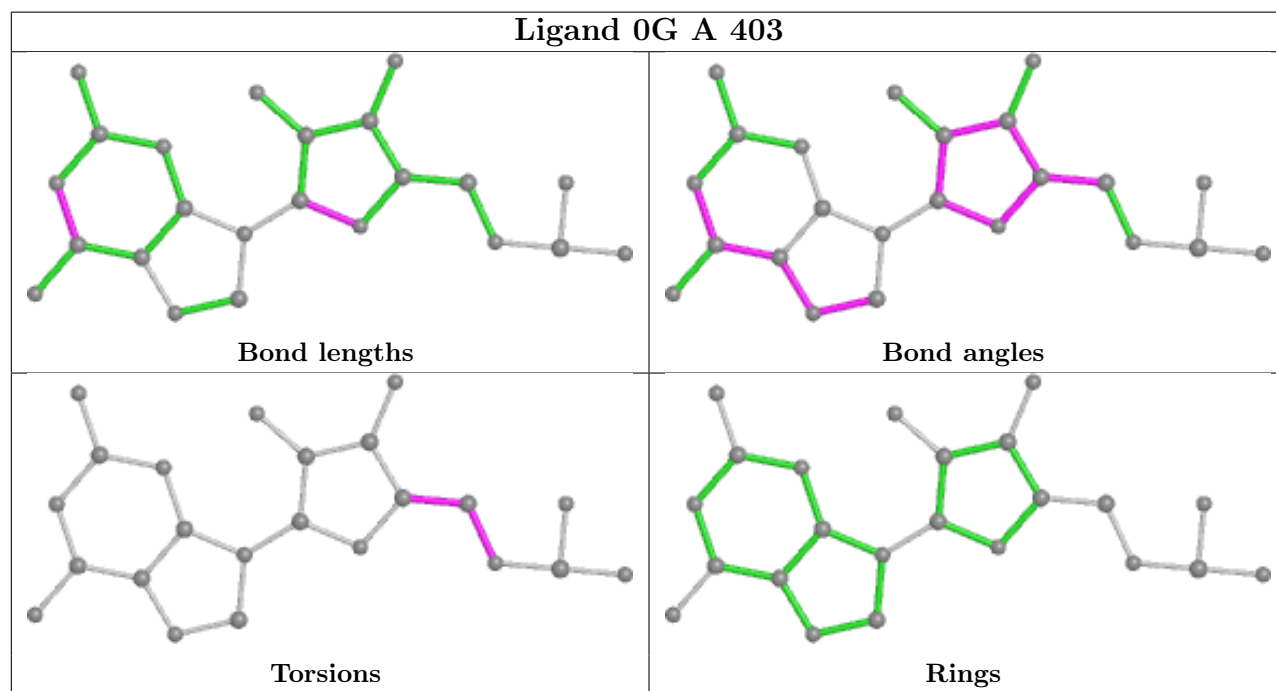
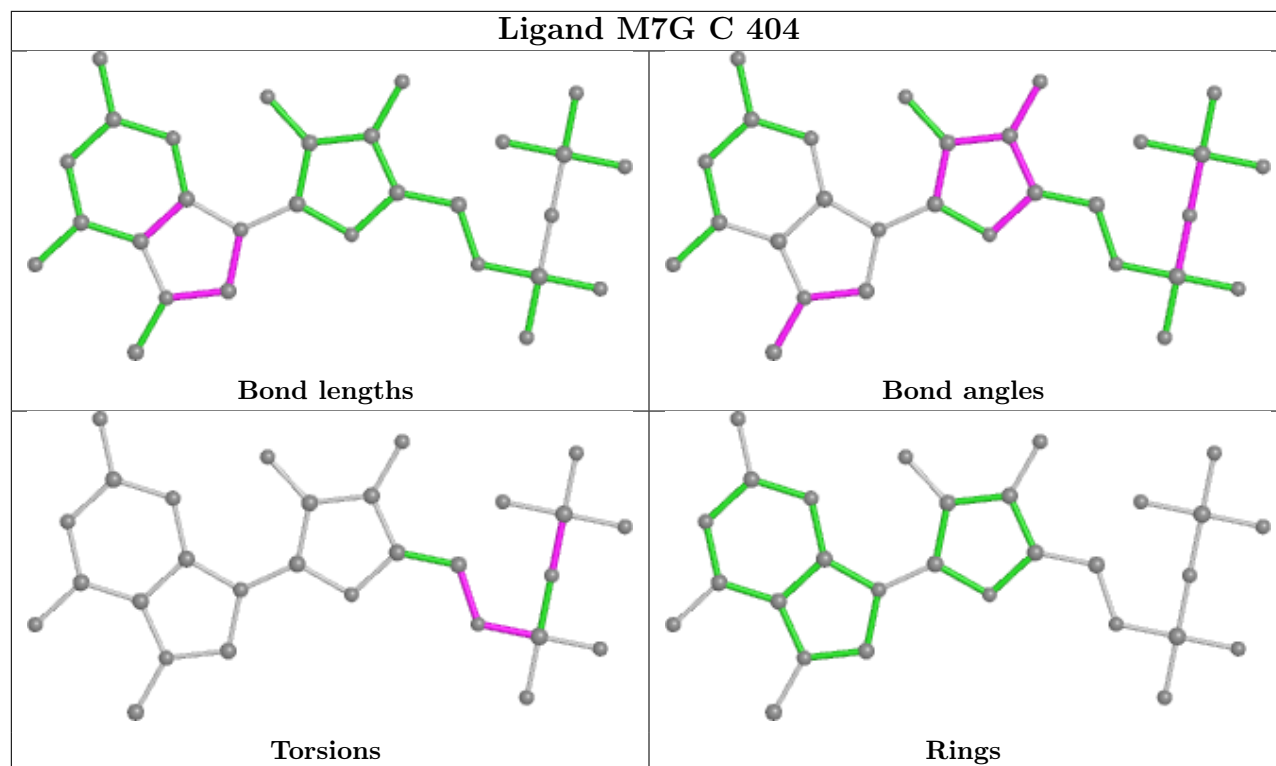
There are no ring outliers.

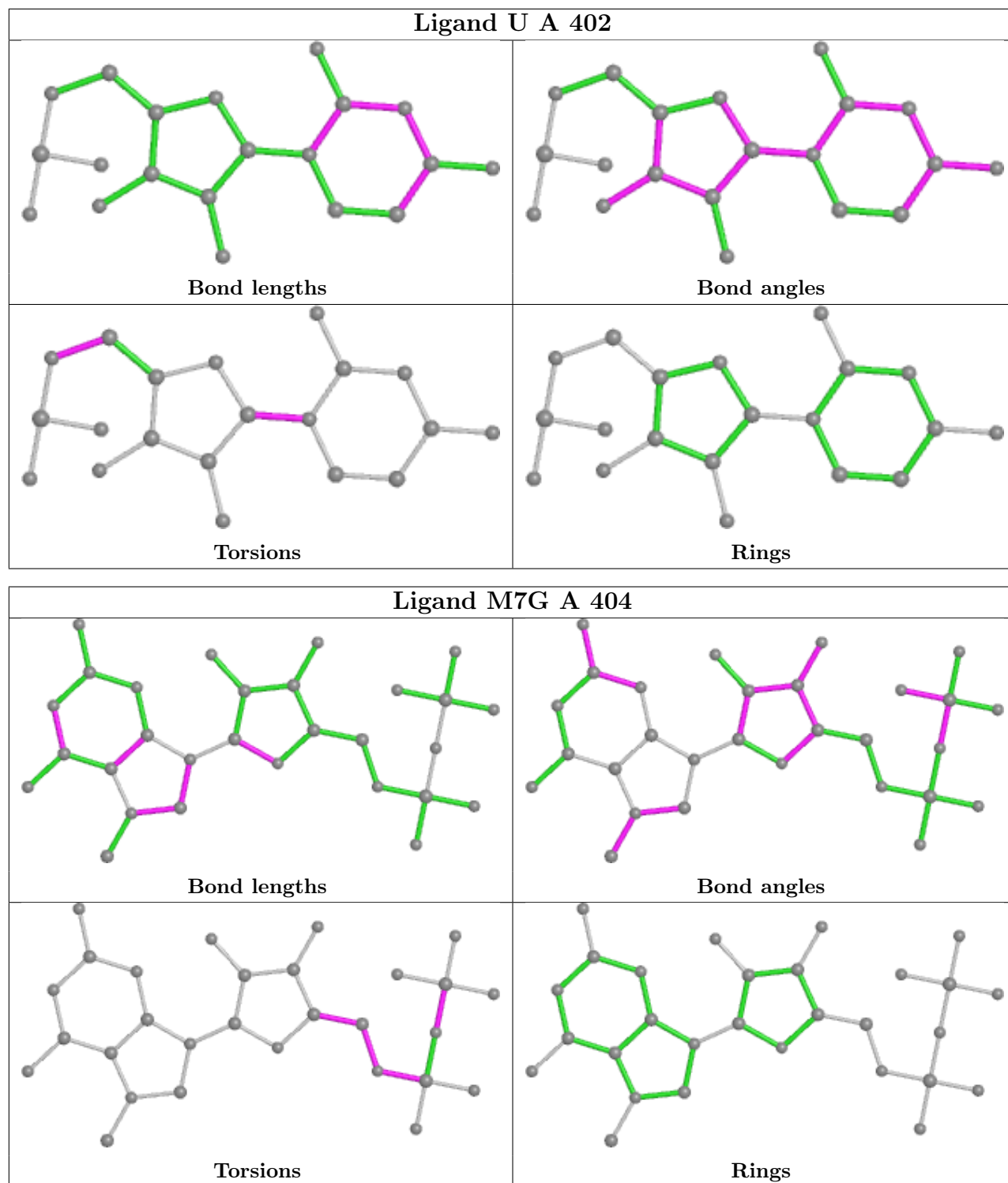
8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403	0G	5	0
3	C	401	U	3	0
5	C	404	M7G	3	0
2	C	402	2PO	3	0
4	A	403	0G	3	0
6	D	401	SO4	1	0
3	A	402	U	2	0
5	A	404	M7G	6	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.







## 5.7 Other polymers [\(i\)](#)

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	332/345 (96%)	0.07	8 (2%) 59 59	44, 69, 115, 152	0
1	B	323/345 (93%)	0.12	12 (3%) 41 40	44, 75, 121, 146	0
1	C	336/345 (97%)	0.13	3 (0%) 84 85	45, 81, 126, 161	0
1	D	318/345 (92%)	0.66	38 (11%) 4 3	49, 87, 138, 167	0
All	All	1309/1380 (94%)	0.24	61 (4%) 31 31	44, 77, 127, 167	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	166	LEU	5.4
1	D	144	ARG	5.1
1	D	265	TYR	4.8
1	D	145	ILE	4.8
1	D	150	ILE	4.3
1	D	152	GLU	4.0
1	D	142	TYR	3.8
1	D	168	GLU	3.6
1	D	184	ASN	3.6
1	D	216	ILE	3.5
1	D	167	TYR	3.4
1	D	82	ILE	3.2
1	B	8	PHE	3.2
1	B	6	GLY	3.2
1	D	215	ASP	3.1
1	D	196	LYS	3.1
1	B	11	LEU	3.1
1	B	15	PHE	3.0
1	D	295	ILE	2.9
1	D	151	GLU	2.8
1	D	149	TYR	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	326	LEU	2.8
1	D	164	ASN	2.7
1	D	163	ASN	2.7
1	D	185	LYS	2.7
1	D	201	ASN	2.7
1	B	167	TYR	2.6
1	C	326	LEU	2.6
1	A	95	TYR	2.6
1	A	156	ASN	2.6
1	B	201	ASN	2.6
1	A	82	ILE	2.5
1	A	55	THR	2.5
1	B	38	ASN	2.5
1	D	153	MET	2.5
1	D	324	ARG	2.4
1	D	83	GLN	2.4
1	D	103	GLN	2.4
1	D	143	LYS	2.4
1	B	40	ASP	2.4
1	D	267	PHE	2.4
1	B	36	ILE	2.4
1	D	212	TYR	2.3
1	B	124	ILE	2.3
1	D	81	GLY	2.3
1	D	76	TYR	2.3
1	A	69	LEU	2.3
1	A	68	VAL	2.3
1	D	147	GLN	2.3
1	C	335	GLU	2.3
1	B	16	GLN	2.2
1	C	144	ARG	2.2
1	D	67	PRO	2.2
1	D	146	VAL	2.2
1	B	119	ALA	2.1
1	D	214	THR	2.1
1	A	157	GLY	2.1
1	D	344	LYS	2.1
1	D	51	LEU	2.0
1	D	107	SER	2.0
1	A	145	ILE	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](#)

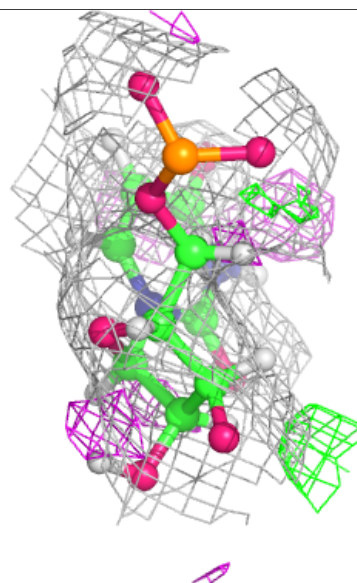
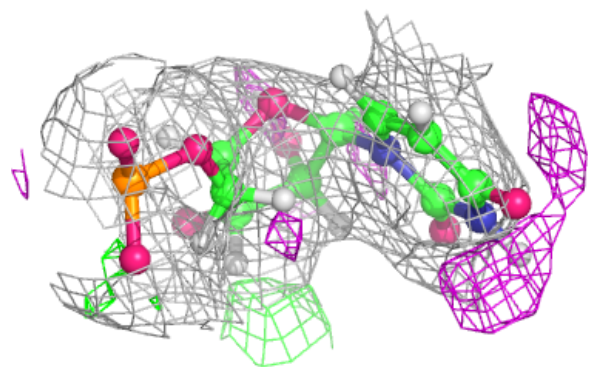
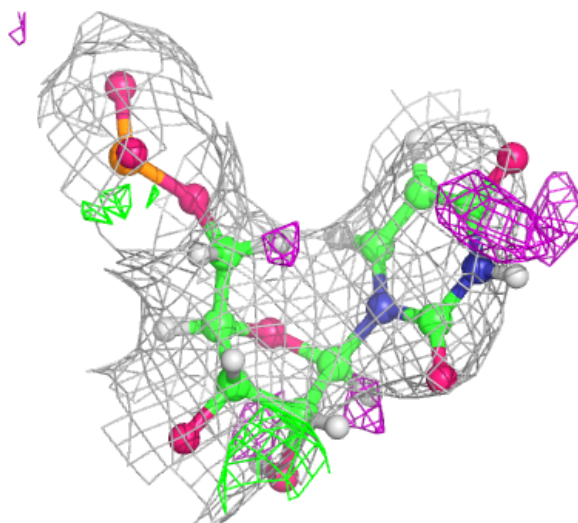
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	U	A	402	20/21	0.88	0.23	58,114,152,172	0
2	2PO	A	401	4/4	0.91	0.18	137,142,143,145	0
6	SO4	D	402	5/5	0.93	0.26	112,120,124,136	0
3	U	C	401	20/21	0.94	0.17	73,102,133,136	0
2	2PO	C	402	4/4	0.94	0.20	103,109,111,116	0
4	0G	C	403	23/24	0.95	0.19	65,107,130,138	0
6	SO4	D	401	5/5	0.95	0.16	92,95,108,111	0
4	0G	A	403	23/24	0.95	0.16	63,97,126,131	0
5	M7G	A	404	29/29	0.96	0.16	43,60,91,129	0
5	M7G	C	404	29/29	0.96	0.19	43,88,113,128	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.

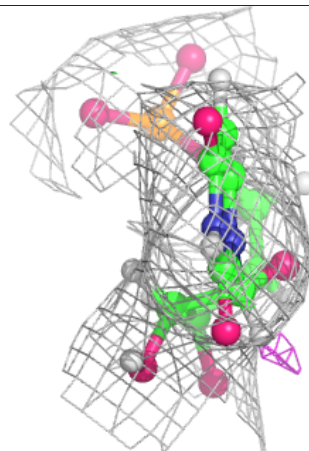
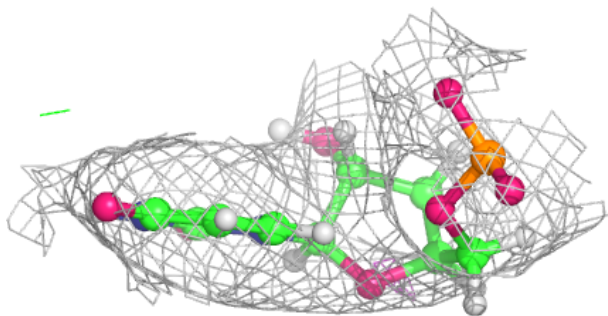
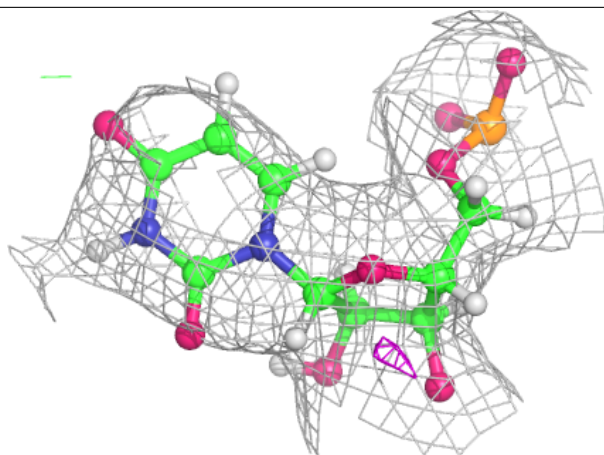
**Electron density around U A 402:**

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

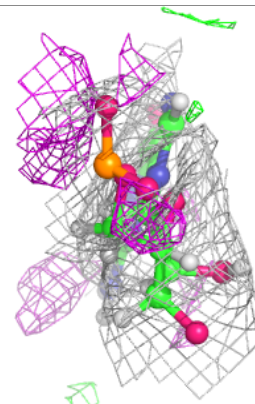
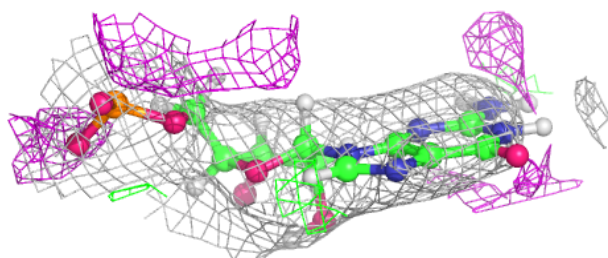
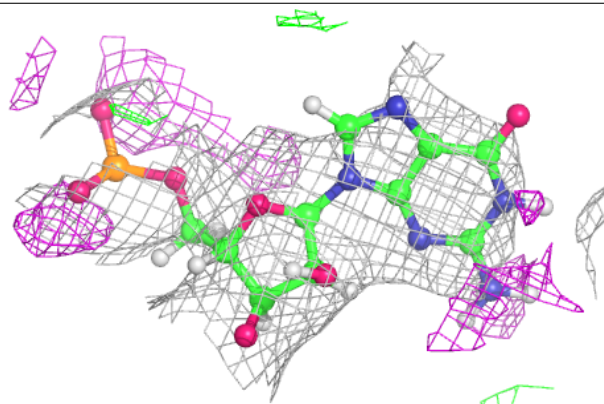


**Electron density around U C 401:**

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

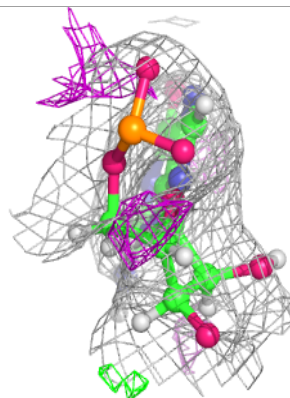
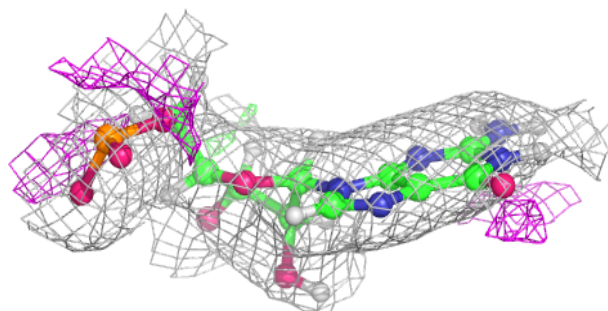
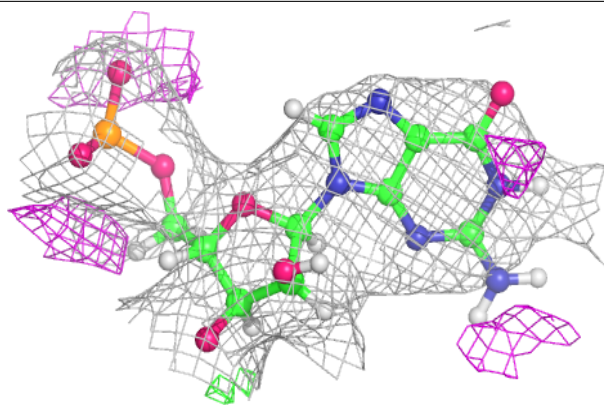
**Electron density around OG C 403:**

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

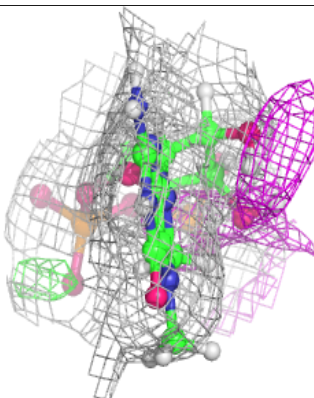
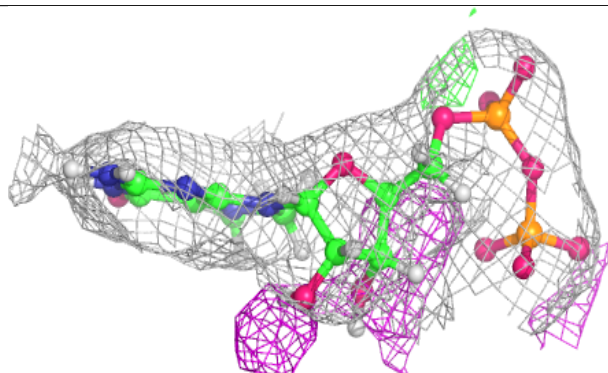
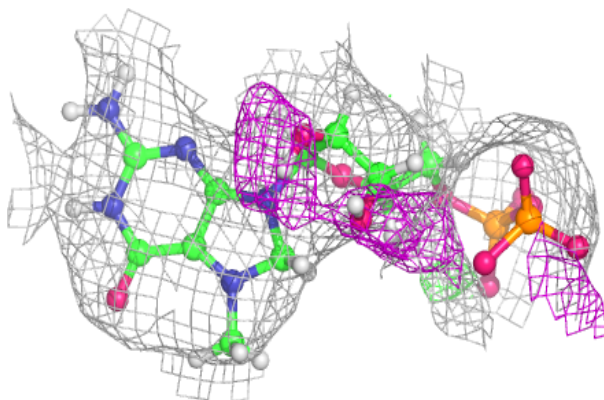


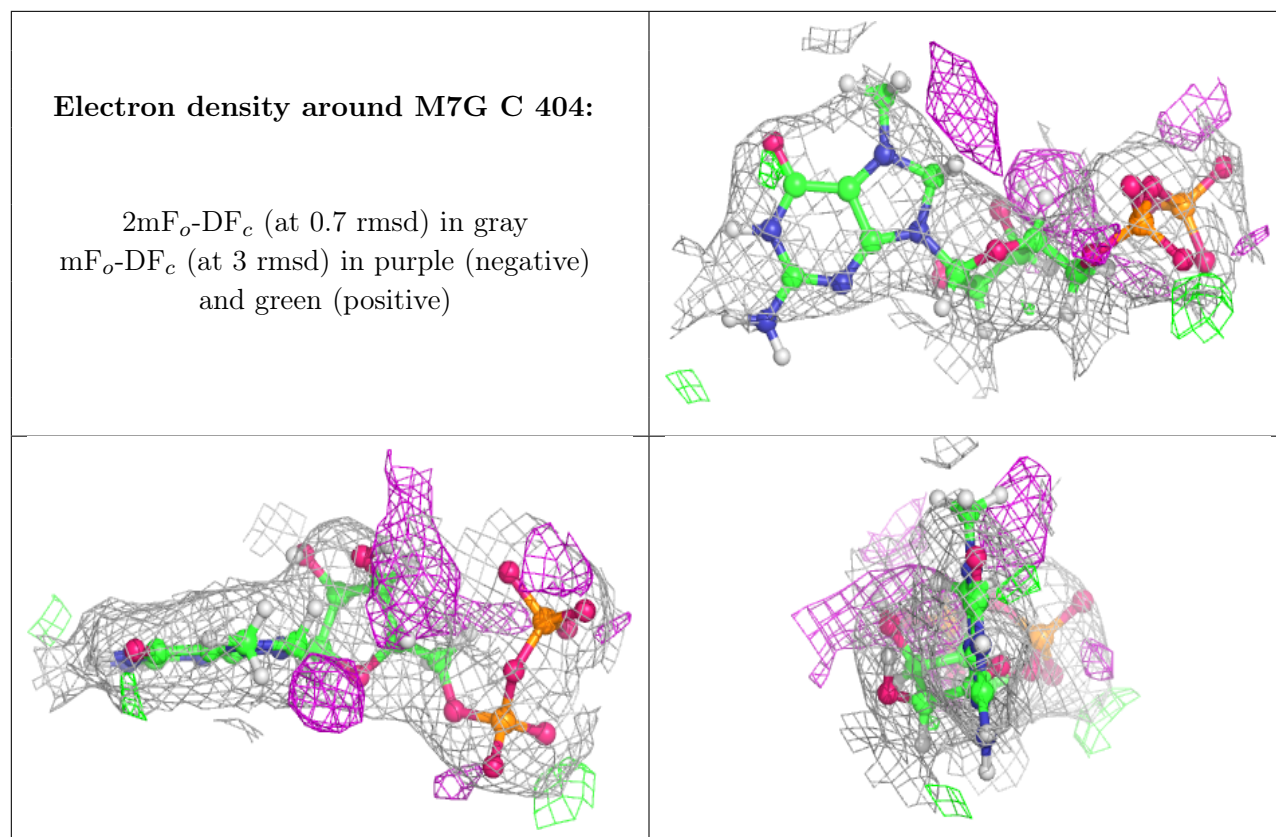
**Electron density around 0G A 403:**

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

**Electron density around M7G A 404:**

$2mF_o-DF_c$  (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.