Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2022 – 01:17 pm BST

PDB ID	:	7OP9
Title	:	Purine nucleoside phosphorylase(DeoD-type) from H. pylori with 2,6-dichloropurine
Authors	:	Narczyk, M.; Stefanic, Z.
Deposited on	:	2021-05-31
Resolution	:	1.50 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 following versions of software and data (see references ⓘ) were used in the production of this report:

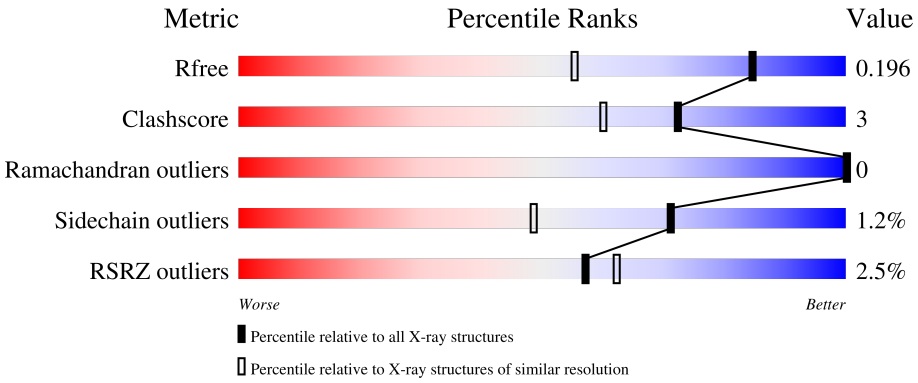
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28

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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	233	4% 91% 9%
1	B	233	2% 91% 9%
1	C	233	% 90% 10%
1	D	233	2% 90% 9%
1	E	233	2% 93% 6%

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Mol	Chain	Length	Quality of chain
1	F	233	4% 90% 9%
1	G	233	% 93% 7%
1	H	233	3% 89% 10%
1	I	233	2% 92% 7%
1	J	233	% 91% 8%
1	K	233	3% 93% 7%
1	L	233	4% 93% 6%

2 Entry composition (i)

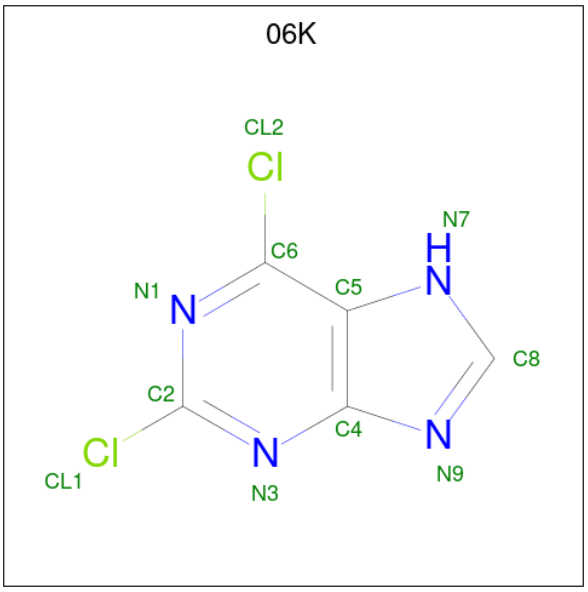
There are 5 unique types of molecules in this entry. The entry contains 24635 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Purine nucleoside phosphorylase DeoD-type.

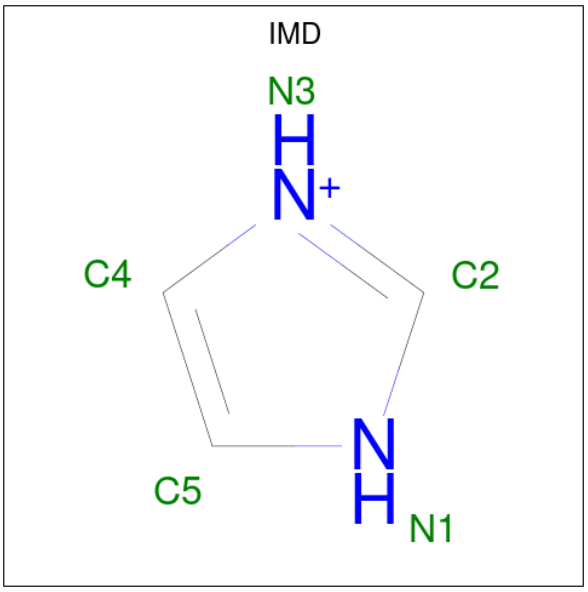
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	2	0
			1811	1153	302	337	19			
1	B	233	Total	C	N	O	S	0	2	0
			1811	1153	302	337	19			
1	C	233	Total	C	N	O	S	0	3	0
			1816	1157	302	337	20			
1	D	233	Total	C	N	O	S	0	3	0
			1816	1157	302	337	20			
1	E	233	Total	C	N	O	S	0	2	0
			1811	1153	302	337	19			
1	F	233	Total	C	N	O	S	0	3	0
			1816	1157	302	337	20			
1	G	233	Total	C	N	O	S	0	3	0
			1816	1157	302	337	20			
1	H	233	Total	C	N	O	S	0	3	0
			1814	1155	302	338	19			
1	I	233	Total	C	N	O	S	0	2	0
			1811	1153	302	337	19			
1	J	233	Total	C	N	O	S	0	2	0
			1811	1153	302	337	19			
1	K	233	Total	C	N	O	S	0	3	0
			1816	1157	302	337	20			
1	L	233	Total	C	N	O	S	0	3	0
			1816	1157	302	337	20			

- Molecule 2 is 2,6-bis(chloranyl)-7H-purine (three-letter code: 06K) (formula: $C_5H_2Cl_2N_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			11	5	2	4		
2	B	1	Total	C	Cl	N	0	0
			11	5	2	4		
2	C	1	Total	C	Cl	N	0	0
			11	5	2	4		
2	D	1	Total	C	Cl	N	0	0
			11	5	2	4		
2	E	1	Total	C	Cl	N	0	0
			11	5	2	4		
2	F	1	Total	C	Cl	N	0	0
			11	5	2	4		
2	G	1	Total	C	Cl	N	0	0
			11	5	2	4		
2	H	1	Total	C	Cl	N	0	0
			11	5	2	4		
2	I	1	Total	C	Cl	N	0	0
			11	5	2	4		
2	J	1	Total	C	Cl	N	0	0
			11	5	2	4		
2	K	1	Total	C	Cl	N	0	0
			11	5	2	4		
2	L	1	Total	C	Cl	N	0	0
			11	5	2	4		

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 5 3 2	0	0
3	B	1	Total C N 5 3 2	0	0
3	C	1	Total C N 5 3 2	0	0
3	D	1	Total C N 5 3 2	0	0
3	E	1	Total C N 5 3 2	0	0
3	E	1	Total C N 5 3 2	0	0
3	F	1	Total C N 5 3 2	0	0
3	G	1	Total C N 5 3 2	0	0
3	H	1	Total C N 5 3 2	0	0
3	I	1	Total C N 5 3 2	0	0
3	J	1	Total C N 5 3 2	0	0
3	K	1	Total C N 5 3 2	0	0
3	L	1	Total C N 5 3 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0
4	I	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0
4	K	1	Total Mg 1 1	0	0
4	L	1	Total Mg 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	222	Total O 222 222	0	0
5	B	259	Total O 259 259	0	0
5	C	229	Total O 229 229	0	0
5	D	221	Total O 221 221	0	0
5	E	228	Total O 228 228	0	0
5	F	203	Total O 203 203	0	0
5	G	217	Total O 217 217	0	0
5	H	217	Total O 217 217	0	0

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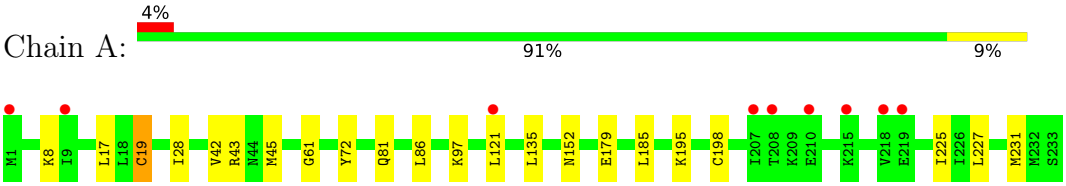
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	243	Total O 243 243	0	0
5	J	225	Total O 225 225	0	0
5	K	199	Total O 199 199	0	0
5	L	198	Total O 198 198	0	0

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.

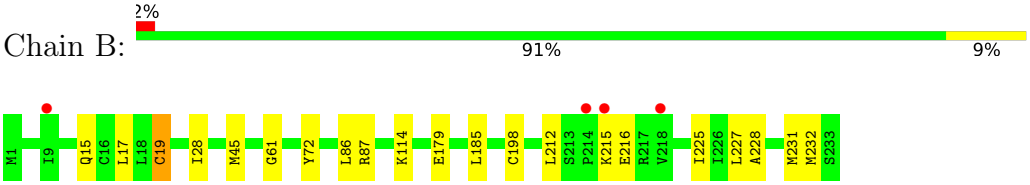
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain A:



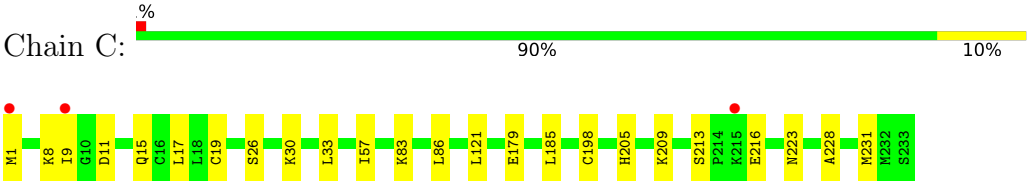
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain B:



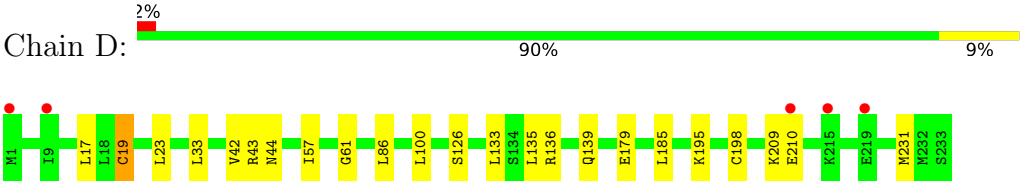
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain C:



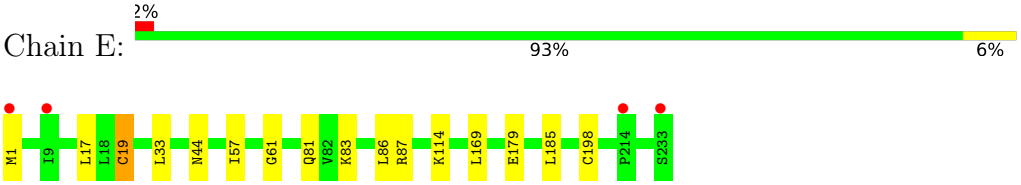
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain D:



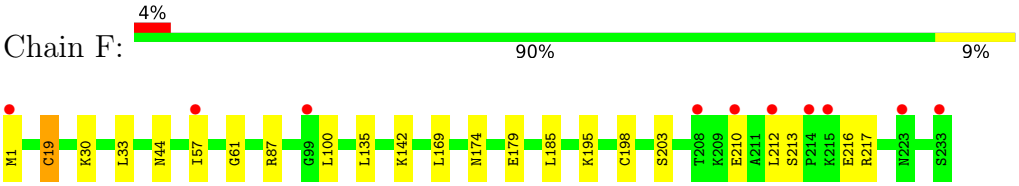
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain E:



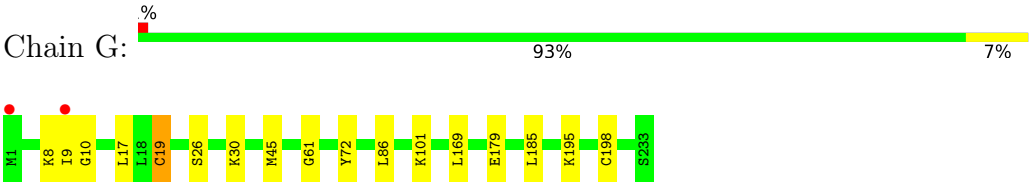
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain F:



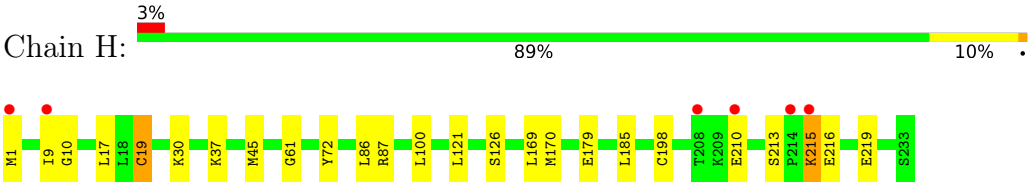
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain G:



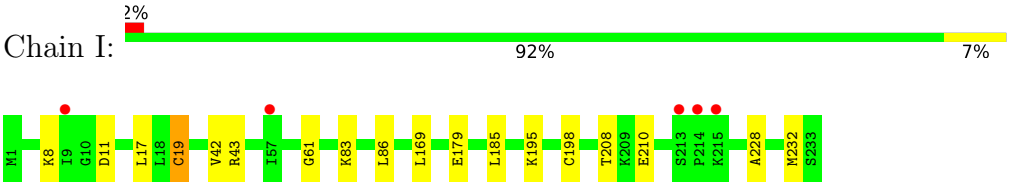
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain H:



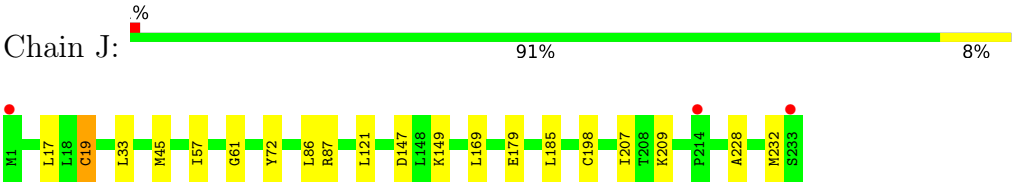
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain I:



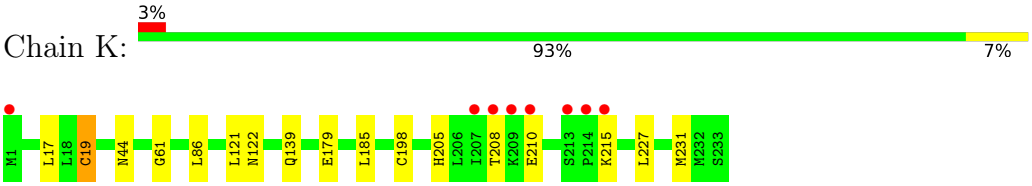
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain J:



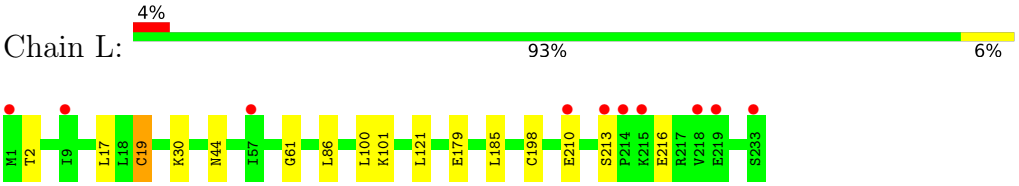
• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain K:



• Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	93.42Å 93.43Å 95.46Å 81.91° 79.35° 60.09°	Depositor
Resolution (Å)	42.59 – 1.50 42.58 – 1.50	Depositor EDS
% Data completeness (in resolution range)	94.8 (42.59-1.50) 94.9 (42.58-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.173 , 0.196 0.174 , 0.196	Depositor DCC
R_{free} test set	2013 reflections (0.48%)	wwPDB-VP
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.755	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.089 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	24635	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: IMD, MG, OCS, 06K

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	0.37	0/1838	0.62	0/2472
1	B	0.36	0/1838	0.63	0/2472
1	C	0.35	0/1846	0.65	0/2482
1	D	0.36	0/1846	0.62	0/2482
1	E	0.36	0/1838	0.65	0/2472
1	F	0.35	0/1846	0.62	0/2482
1	G	0.35	0/1846	0.63	0/2482
1	H	0.36	0/1844	0.67	1/2480 (0.0%)
1	I	0.35	0/1838	0.66	0/2472
1	J	0.37	0/1838	0.63	0/2472
1	K	0.35	0/1846	0.63	0/2482
1	L	0.35	0/1846	0.64	0/2482
All	All	0.36	0/22110	0.64	1/29732 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	170	MET	CG-SD-CE	-7.76	87.78	100.20

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	1811	0	1846	15	0
1	B	1811	0	1846	11	0
1	C	1816	0	1855	14	0
1	D	1816	0	1855	13	0
1	E	1811	0	1846	10	0
1	F	1816	0	1855	16	0
1	G	1816	0	1855	11	0
1	H	1814	0	1851	16	0
1	I	1811	0	1846	12	0
1	J	1811	0	1846	12	0
1	K	1816	0	1855	10	0
1	L	1816	0	1855	9	0
2	A	11	0	0	0	0
2	B	11	0	0	0	0
2	C	11	0	0	0	0
2	D	11	0	0	0	0
2	E	11	0	0	0	0
2	F	11	0	0	0	0
2	G	11	0	0	0	0
2	H	11	0	0	0	0
2	I	11	0	0	0	0
2	J	11	0	0	0	0
2	K	11	0	0	0	0
2	L	11	0	0	0	0
3	A	5	0	5	1	0
3	B	5	0	5	1	0
3	C	5	0	5	1	0
3	D	5	0	5	1	0
3	E	10	0	10	1	0
3	F	5	0	5	1	0
3	G	5	0	5	1	0
3	H	5	0	5	1	0
3	I	5	0	5	1	0
3	J	5	0	5	1	0
3	K	5	0	5	1	0
3	L	5	0	5	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	222	0	0	4	1
5	B	259	0	0	3	1
5	C	229	0	0	4	0
5	D	221	0	0	2	0
5	E	228	0	0	5	0
5	F	203	0	0	4	0
5	G	217	0	0	3	0
5	H	217	0	0	5	0
5	I	243	0	0	3	0
5	J	225	0	0	2	0
5	K	199	0	0	3	0
5	L	198	0	0	3	0
All	All	24635	0	22276	151	1

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 (151) 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:H:215:LYS:NZ	5:H:402:HOH:O	2.13	0.81
1:H:126:SER:OG	5:H:401:HOH:O	1.99	0.80
1:C:33:LEU:HD21	1:C:57:ILE:HD11	1.66	0.78
1:K:139:GLN:NE2	5:K:402:HOH:O	2.21	0.73
3:A:302:IMD:H5	5:D:546:HOH:O	1.90	0.71
1:C:83:LYS:NZ	5:C:402:HOH:O	2.24	0.70
5:A:531:HOH:O	3:D:302:IMD:H5	1.91	0.70
1:I:83:LYS:NZ	5:I:401:HOH:O	2.24	0.70
5:B:482:HOH:O	3:E:302:IMD:H5	1.92	0.69
1:E:87:ARG:NH1	5:E:401:HOH:O	2.24	0.69
5:C:464:HOH:O	3:F:302:IMD:H5	1.92	0.68
1:E:81:GLN:NE2	5:E:404:HOH:O	2.26	0.67
3:H:302:IMD:H5	5:K:526:HOH:O	1.93	0.67
1:K:122:ASN:OD1	5:K:401:HOH:O	2.12	0.66
5:G:515:HOH:O	3:J:302:IMD:H5	1.95	0.66
1:J:207:ILE:O	1:J:209:LYS:NZ	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:567:HOH:O	3:L:302:IMD:H5	1.97	0.65
1:I:208:THR:OG1	1:I:210:GLU:OE1	2.15	0.64
1:K:185:LEU:HD23	1:K:198[B]:CYS:SG	2.39	0.63
1:H:121:LEU:HD21	1:J:169:LEU:HD23	1.82	0.62
1:F:33:LEU:HD22	1:F:57:ILE:HD11	1.80	0.62
1:J:185:LEU:HD23	1:J:198[B]:CYS:SG	2.40	0.62
3:I:302:IMD:H5	5:L:540:HOH:O	2.00	0.61
1:A:185:LEU:HD23	1:A:198[B]:CYS:SG	2.41	0.60
1:G:26:SER:O	1:G:30:LYS:HG2	2.01	0.60
1:D:136:ARG:HD2	1:D:231:MET:HG2	1.84	0.60
1:A:227:LEU:O	1:A:231:MET:HG2	2.03	0.59
1:L:185:LEU:HD23	1:L:198[B]:CYS:SG	2.43	0.59
3:B:302:IMD:H5	5:E:534:HOH:O	2.02	0.58
1:G:185:LEU:HD23	1:G:198[B]:CYS:SG	2.43	0.58
1:D:185:LEU:HD23	1:D:198[B]:CYS:SG	2.44	0.58
1:F:174:ASN:ND2	5:F:403:HOH:O	2.31	0.57
1:H:100:LEU:HD11	1:H:210:GLU:HB3	1.86	0.57
1:H:185:LEU:HD23	1:H:198[B]:CYS:SG	2.44	0.57
1:H:213:SER:OG	1:H:216:GLU:HG3	2.04	0.57
1:K:227:LEU:O	1:K:231:MET:HG2	2.03	0.57
1:C:205:HIS:NE2	5:C:401:HOH:O	2.20	0.57
1:F:30:LYS:NZ	5:F:401:HOH:O	2.27	0.57
1:F:203:SER:HA	1:F:212:LEU:HD12	1.87	0.57
1:F:100:LEU:HD11	1:F:210:GLU:HB3	1.87	0.57
1:A:121:LEU:HD21	1:F:169:LEU:HD23	1.87	0.57
1:J:228:ALA:O	1:J:232:MET:HG3	2.05	0.57
1:G:9:ILE:HD12	1:G:10:GLY:H	1.70	0.56
1:K:17:LEU:HD12	1:K:86:LEU:O	2.04	0.56
1:F:185:LEU:HD23	1:F:198[B]:CYS:SG	2.47	0.55
3:C:302:IMD:H5	5:F:462:HOH:O	2.06	0.55
1:A:97:LYS:HE2	5:A:419:HOH:O	2.06	0.55
1:H:9:ILE:HD12	1:H:10:GLY:H	1.72	0.55
1:B:228:ALA:O	1:B:232:MET:HG3	2.07	0.55
1:D:17:LEU:HD12	1:D:86:LEU:O	2.07	0.54
1:E:17:LEU:HD12	1:E:86:LEU:O	2.07	0.54
1:F:213:SER:OG	1:F:216:GLU:HG3	2.07	0.54
1:K:208:THR:HG23	1:K:210:GLU:HG3	1.90	0.54
1:L:30:LYS:HG2	5:L:525:HOH:O	2.08	0.53
1:L:213:SER:OG	1:L:216:GLU:HG3	2.09	0.53
1:I:185:LEU:HD23	1:I:198[B]:CYS:SG	2.48	0.53
1:E:33:LEU:HD22	1:E:57:ILE:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:553:HOH:O	3:K:302:IMD:H5	2.08	0.52
1:J:17:LEU:HD12	1:J:86:LEU:O	2.09	0.52
1:C:223:ASN:ND2	5:C:404:HOH:O	2.38	0.52
1:C:8:LYS:HD3	1:C:11:ASP:OD2	2.10	0.52
1:C:26:SER:O	1:C:30:LYS:HG2	2.09	0.52
1:F:87:ARG:NH1	5:F:408:HOH:O	2.40	0.52
1:L:17:LEU:HD12	1:L:86:LEU:O	2.09	0.52
1:D:135:LEU:O	1:D:139:GLN:HG2	2.10	0.51
1:E:1:MET:SD	5:E:623:HOH:O	2.60	0.51
1:I:169:LEU:HD23	1:K:121:LEU:HD23	1.90	0.51
1:B:185:LEU:HD23	1:B:198[B]:CYS:SG	2.50	0.51
1:E:185:LEU:HD23	1:E:198[B]:CYS:SG	2.51	0.51
1:I:195:LYS:NZ	5:I:406:HOH:O	2.43	0.51
1:E:83:LYS:NZ	5:E:408:HOH:O	2.33	0.51
3:G:302:IMD:H5	5:J:452:HOH:O	2.11	0.51
1:A:152:ASN:OD1	5:A:401:HOH:O	2.19	0.50
1:I:19:OCS:O	1:I:61:GLY:HA2	2.12	0.50
1:G:19:OCS:O	1:G:61:GLY:HA2	2.12	0.49
1:I:17:LEU:HD12	1:I:86:LEU:O	2.12	0.49
1:B:87:ARG:NH1	5:B:402:HOH:O	2.39	0.49
1:J:87:ARG:NH1	5:J:403:HOH:O	2.42	0.49
1:K:215:LYS:O	1:K:215:LYS:HD3	2.13	0.49
1:D:209:LYS:O	5:D:401:HOH:O	2.20	0.48
1:C:33:LEU:CD2	1:C:57:ILE:HD11	2.40	0.48
1:K:19:OCS:O	1:K:61:GLY:HA2	2.14	0.48
1:L:100:LEU:O	1:L:101:LYS:HG2	2.13	0.48
1:J:147:ASP:OD2	1:J:149:LYS:NZ	2.46	0.48
1:C:185:LEU:HD23	1:C:198[B]:CYS:SG	2.54	0.48
1:C:213:SER:OG	1:C:216:GLU:HG2	2.14	0.48
1:D:100:LEU:HD11	1:D:210:GLU:HB3	1.95	0.48
1:H:213:SER:HG	1:H:216:GLU:HG3	1.79	0.47
1:A:8:LYS:HB2	1:A:8:LYS:HE2	1.77	0.47
1:I:228:ALA:O	1:I:232:MET:HG3	2.15	0.47
1:H:19:OCS:O	1:H:61:GLY:HA2	2.14	0.46
1:L:30:LYS:HE3	5:L:525:HOH:O	2.14	0.46
1:F:213:SER:O	1:F:217:ARG:HG3	2.16	0.46
1:A:81:GLN:N	5:A:405:HOH:O	2.34	0.46
1:A:45:MET:HG2	1:A:72:TYR:CZ	2.51	0.46
1:A:19:OCS:O	1:A:61:GLY:HA2	2.16	0.45
1:H:121:LEU:CD2	1:J:169:LEU:HD23	2.46	0.45
1:B:45:MET:HG2	1:B:72:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:MET:HG2	1:G:72:TYR:CZ	2.51	0.45
1:A:17:LEU:HD12	1:A:86:LEU:O	2.15	0.45
1:E:19:OCS:O	1:E:61:GLY:HA2	2.17	0.45
1:B:19:OCS:O	1:B:61:GLY:HA2	2.16	0.45
1:G:169:LEU:HD23	1:L:121:LEU:HD23	1.99	0.45
1:H:30:LYS:HD2	5:H:542:HOH:O	2.16	0.44
1:J:19:OCS:O	1:J:61:GLY:HA2	2.18	0.44
1:G:30:LYS:HD3	5:G:551:HOH:O	2.17	0.44
1:L:100:LEU:HD11	1:L:210:GLU:HB3	2.00	0.44
1:C:17:LEU:HD12	1:C:86:LEU:O	2.18	0.44
1:F:195:LYS:HB3	1:F:195:LYS:HE3	1.87	0.44
1:H:215:LYS:HD3	1:H:219:GLU:OE2	2.18	0.43
1:C:228:ALA:HA	1:C:231:MET:HG2	1.99	0.43
1:A:195:LYS:HB3	1:A:195:LYS:HE3	1.85	0.43
1:B:15:GLN:NE2	1:B:232:MET:HB3	2.33	0.43
1:L:19:OCS:O	1:L:61:GLY:HA2	2.18	0.43
1:I:195:LYS:HB3	1:I:195:LYS:HE3	1.83	0.43
1:G:195:LYS:HB3	1:G:195:LYS:HE3	1.88	0.43
1:G:9:ILE:HD12	1:G:10:GLY:N	2.33	0.43
5:B:420:HOH:O	1:D:126:SER:HB2	2.17	0.43
1:A:42:VAL:HG12	1:A:43:ARG:HG3	2.01	0.43
1:C:121:LEU:HD21	1:E:169:LEU:HD23	2.01	0.42
1:B:28:ILE:HG12	1:B:225:ILE:HD13	2.02	0.42
1:C:1:MET:HG3	1:C:9:ILE:HD11	2.01	0.42
1:D:19:OCS:O	1:D:61:GLY:HA2	2.19	0.42
1:B:212:LEU:HD22	1:B:216:GLU:HB3	2.02	0.42
1:D:33:LEU:HD22	1:D:57:ILE:HG21	2.02	0.42
1:H:17:LEU:HD12	1:H:86:LEU:O	2.19	0.42
1:G:17:LEU:HD12	1:G:86:LEU:O	2.20	0.42
1:A:121:LEU:CD2	1:F:169:LEU:HD23	2.50	0.42
1:D:23:LEU:HD23	1:D:23:LEU:HA	1.88	0.42
1:H:87:ARG:NH1	5:H:408:HOH:O	2.52	0.42
1:B:114:LYS:HB2	1:E:114:LYS:HB2	2.02	0.42
1:C:15:GLN:NE2	1:C:57:ILE:HG22	2.34	0.42
1:D:133:LEU:HD23	1:D:133:LEU:HA	1.92	0.41
1:F:33:LEU:CD2	1:F:57:ILE:HD11	2.46	0.41
1:I:8:LYS:HE3	1:I:8:LYS:HB2	1.84	0.41
1:I:42:VAL:HG12	1:I:43:ARG:HG3	2.02	0.41
1:B:17:LEU:HD12	1:B:86:LEU:O	2.20	0.41
1:B:227:LEU:O	1:B:231:MET:HG3	2.21	0.41
1:G:9:ILE:HG22	5:G:557:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:45:MET:HG2	1:H:72:TYR:CZ	2.55	0.41
1:F:57:ILE:HD12	1:F:57:ILE:O	2.20	0.41
1:J:45:MET:HG2	1:J:72:TYR:CZ	2.56	0.41
1:F:19:OCS:O	1:F:61:GLY:HA2	2.21	0.41
1:I:8:LYS:HE2	1:I:11:ASP:OD1	2.21	0.41
1:A:28:ILE:HG12	1:A:225:ILE:HD13	2.03	0.40
1:H:169:LEU:HD23	1:J:121:LEU:HD21	2.03	0.40
1:A:135:LEU:HD13	1:F:135:LEU:HD13	2.03	0.40
1:J:33:LEU:HD22	1:J:57:ILE:HG21	2.02	0.40
1:D:42:VAL:HG12	1:D:43:ARG:HG3	2.03	0.40
1:D:195:LYS:HB3	1:D:195:LYS:HE3	1.87	0.40
1:K:205:HIS:CG	1:K:208:THR:HG22	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:606:HOH:O	5:B:566:HOH:O[1_545]	2.17	0.03

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	232/233 (100%)	227 (98%)	5 (2%)	0	100	100
1	B	232/233 (100%)	225 (97%)	7 (3%)	0	100	100
1	C	233/233 (100%)	227 (97%)	6 (3%)	0	100	100
1	D	233/233 (100%)	225 (97%)	8 (3%)	0	100	100
1	E	232/233 (100%)	225 (97%)	7 (3%)	0	100	100
1	F	233/233 (100%)	225 (97%)	8 (3%)	0	100	100
1	G	233/233 (100%)	228 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	233/233 (100%)	226 (97%)	7 (3%)	0	100	100
1	I	232/233 (100%)	227 (98%)	5 (2%)	0	100	100
1	J	232/233 (100%)	224 (97%)	8 (3%)	0	100	100
1	K	233/233 (100%)	227 (97%)	6 (3%)	0	100	100
1	L	233/233 (100%)	226 (97%)	7 (3%)	0	100	100
All	All	2791/2796 (100%)	2712 (97%)	79 (3%)	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	197/195 (101%)	196 (100%)	1 (0%)	88	78
1	B	197/195 (101%)	195 (99%)	2 (1%)	76	57
1	C	198/195 (102%)	196 (99%)	2 (1%)	76	57
1	D	198/195 (102%)	196 (99%)	2 (1%)	76	57
1	E	197/195 (101%)	195 (99%)	2 (1%)	76	57
1	F	198/195 (102%)	194 (98%)	4 (2%)	55	25
1	G	198/195 (102%)	195 (98%)	3 (2%)	65	39
1	H	198/195 (102%)	194 (98%)	4 (2%)	55	25
1	I	197/195 (101%)	196 (100%)	1 (0%)	88	78
1	J	197/195 (101%)	196 (100%)	1 (0%)	88	78
1	K	198/195 (102%)	196 (99%)	2 (1%)	76	57
1	L	198/195 (102%)	195 (98%)	3 (2%)	65	39
All	All	2371/2340 (101%)	2344 (99%)	27 (1%)	71	53

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	GLU
1	B	179	GLU
1	B	215	LYS
1	C	179	GLU
1	C	209	LYS
1	D	44	ASN
1	D	179	GLU
1	E	44	ASN
1	E	179	GLU
1	F	1	MET
1	F	44	ASN
1	F	142	LYS
1	F	179	GLU
1	G	8	LYS
1	G	101	LYS
1	G	179	GLU
1	H	1	MET
1	H	37	LYS
1	H	179	GLU
1	H	215	LYS
1	I	179	GLU
1	J	179	GLU
1	K	44	ASN
1	K	179	GLU
1	L	2	THR
1	L	44	ASN
1	L	179	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	15	GLN
1	E	81	GLN
1	E	139	GLN
1	G	81	GLN
1	H	223	ASN
1	I	223	ASN
1	K	139	GLN
1	K	223	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)

12 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	OCS	E	19	1	7,8,9	1.13	0	6,11,13	1.90	1 (16%)
1	OCS	J	19	1	7,8,9	0.96	0	6,11,13	1.85	2 (33%)
1	OCS	B	19	1	7,8,9	0.89	0	6,11,13	1.58	2 (33%)
1	OCS	C	19	1	7,8,9	0.95	0	6,11,13	1.78	2 (33%)
1	OCS	H	19	1	7,8,9	1.11	0	6,11,13	1.68	2 (33%)
1	OCS	D	19	1	7,8,9	0.86	0	6,11,13	1.54	2 (33%)
1	OCS	I	19	1	7,8,9	0.91	0	6,11,13	1.53	2 (33%)
1	OCS	A	19	1	7,8,9	0.91	0	6,11,13	1.80	2 (33%)
1	OCS	F	19	1	7,8,9	0.91	0	6,11,13	1.89	2 (33%)
1	OCS	G	19	1	7,8,9	0.89	0	6,11,13	1.66	1 (16%)
1	OCS	L	19	1	7,8,9	0.94	0	6,11,13	1.71	2 (33%)
1	OCS	K	19	1	7,8,9	0.91	0	6,11,13	1.63	2 (33%)

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
1	OCS	E	19	1	-	1/4/7/9	-
1	OCS	J	19	1	-	1/4/7/9	-
1	OCS	B	19	1	-	1/4/7/9	-
1	OCS	C	19	1	-	1/4/7/9	-
1	OCS	H	19	1	-	1/4/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OCS	D	19	1	-	1/4/7/9	-
1	OCS	I	19	1	-	1/4/7/9	-
1	OCS	A	19	1	-	1/4/7/9	-
1	OCS	F	19	1	-	1/4/7/9	-
1	OCS	G	19	1	-	1/4/7/9	-
1	OCS	L	19	1	-	1/4/7/9	-
1	OCS	K	19	1	-	1/4/7/9	-

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	19	OCS	OD2-SG-CB	3.96	112.05	105.74
1	J	19	OCS	OD1-SG-CB	3.50	111.10	106.94
1	F	19	OCS	OD2-SG-CB	3.41	111.17	105.74
1	A	19	OCS	OD1-SG-CB	3.38	110.95	106.94
1	C	19	OCS	OD2-SG-CB	3.03	110.58	105.74
1	L	19	OCS	OD2-SG-CB	3.02	110.55	105.74
1	G	19	OCS	OD2-SG-CB	2.98	110.49	105.74
1	K	19	OCS	OD1-SG-CB	2.79	110.26	106.94
1	I	19	OCS	OD2-SG-CB	2.76	110.13	105.74
1	H	19	OCS	OD2-SG-CB	2.73	110.09	105.74
1	H	19	OCS	OD1-SG-CB	2.64	110.08	106.94
1	F	19	OCS	OD1-SG-CB	2.62	110.06	106.94
1	C	19	OCS	OD1-SG-CB	2.61	110.04	106.94
1	D	19	OCS	OD1-SG-CB	2.58	110.00	106.94
1	B	19	OCS	OD1-SG-CB	2.50	109.91	106.94
1	B	19	OCS	OD2-SG-CB	2.49	109.72	105.74
1	J	19	OCS	OD2-SG-CB	2.47	109.67	105.74
1	L	19	OCS	OD1-SG-CB	2.43	109.83	106.94
1	A	19	OCS	OD2-SG-CB	2.38	109.54	105.74
1	K	19	OCS	OD2-SG-CB	2.37	109.52	105.74
1	D	19	OCS	OD2-SG-CB	2.31	109.42	105.74
1	I	19	OCS	OD1-SG-CB	2.03	109.35	106.94

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	19	OCS	N-CA-CB-SG
1	B	19	OCS	N-CA-CB-SG

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Mol	Chain	Res	Type	Atoms
1	C	19	OCS	N-CA-CB-SG
1	D	19	OCS	N-CA-CB-SG
1	E	19	OCS	N-CA-CB-SG
1	F	19	OCS	N-CA-CB-SG
1	G	19	OCS	N-CA-CB-SG
1	H	19	OCS	N-CA-CB-SG
1	I	19	OCS	N-CA-CB-SG
1	J	19	OCS	N-CA-CB-SG
1	K	19	OCS	N-CA-CB-SG
1	L	19	OCS	N-CA-CB-SG

There are no ring outliers.

11 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	19	OCS	1	0
1	J	19	OCS	1	0
1	B	19	OCS	1	0
1	H	19	OCS	1	0
1	D	19	OCS	1	0
1	I	19	OCS	1	0
1	A	19	OCS	1	0
1	F	19	OCS	1	0
1	G	19	OCS	1	0
1	L	19	OCS	1	0
1	K	19	OCS	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 12 are monoatomic - leaving 25 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	06K	E	301	-	10,12,12	1.17	1 (10%)	8,17,17	4.54	6 (75%)
3	IMD	H	302	-	3,5,5	0.40	0	4,5,5	0.74	0
3	IMD	G	302	-	3,5,5	0.50	0	4,5,5	0.69	0
2	06K	C	301	-	10,12,12	1.30	2 (20%)	8,17,17	4.39	5 (62%)
2	06K	H	301	-	10,12,12	1.25	1 (10%)	8,17,17	4.31	5 (62%)
3	IMD	E	303	-	3,5,5	0.43	0	4,5,5	0.57	0
2	06K	D	301	-	10,12,12	1.14	1 (10%)	8,17,17	4.05	6 (75%)
2	06K	J	301	-	10,12,12	1.07	0	8,17,17	4.55	6 (75%)
3	IMD	L	302	-	3,5,5	0.37	0	4,5,5	0.73	0
2	06K	A	301	-	10,12,12	1.09	1 (10%)	8,17,17	3.97	5 (62%)
2	06K	I	301	-	10,12,12	1.06	1 (10%)	8,17,17	4.01	5 (62%)
3	IMD	B	302	-	3,5,5	0.43	0	4,5,5	0.73	0
3	IMD	C	302	-	3,5,5	0.41	0	4,5,5	0.74	0
3	IMD	E	302	-	3,5,5	0.42	0	4,5,5	0.67	0
2	06K	F	301	-	10,12,12	1.35	1 (10%)	8,17,17	4.22	6 (75%)
3	IMD	D	302	-	3,5,5	0.37	0	4,5,5	0.70	0
2	06K	B	301	-	10,12,12	1.21	1 (10%)	8,17,17	4.14	5 (62%)
2	06K	K	301	-	10,12,12	1.12	1 (10%)	8,17,17	4.25	5 (62%)
3	IMD	I	302	-	3,5,5	0.41	0	4,5,5	0.69	0
3	IMD	K	302	-	3,5,5	0.37	0	4,5,5	0.66	0
2	06K	G	301	-	10,12,12	0.94	0	8,17,17	4.11	6 (75%)
3	IMD	J	302	-	3,5,5	0.44	0	4,5,5	0.65	0
3	IMD	A	302	-	3,5,5	0.41	0	4,5,5	0.72	0
2	06K	L	301	-	10,12,12	1.20	1 (10%)	8,17,17	4.76	5 (62%)
3	IMD	F	302	-	3,5,5	0.41	0	4,5,5	0.72	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
2	06K	E	301	-	-	-	0/2/2/2
3	IMD	H	302	-	-	-	0/1/1/1
3	IMD	G	302	-	-	-	0/1/1/1
2	06K	C	301	-	-	-	0/2/2/2
2	06K	H	301	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IMD	E	303	-	-	-	0/1/1/1
2	06K	D	301	-	-	-	0/2/2/2
2	06K	J	301	-	-	-	0/2/2/2
3	IMD	L	302	-	-	-	0/1/1/1
2	06K	A	301	-	-	-	0/2/2/2
2	06K	I	301	-	-	-	0/2/2/2
3	IMD	B	302	-	-	-	0/1/1/1
3	IMD	C	302	-	-	-	0/1/1/1
3	IMD	E	302	-	-	-	0/1/1/1
2	06K	F	301	-	-	-	0/2/2/2
3	IMD	D	302	-	-	-	0/1/1/1
2	06K	B	301	-	-	-	0/2/2/2
2	06K	K	301	-	-	-	0/2/2/2
3	IMD	I	302	-	-	-	0/1/1/1
3	IMD	K	302	-	-	-	0/1/1/1
2	06K	G	301	-	-	-	0/2/2/2
3	IMD	J	302	-	-	-	0/1/1/1
3	IMD	A	302	-	-	-	0/1/1/1
2	06K	L	301	-	-	-	0/2/2/2
3	IMD	F	302	-	-	-	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	06K	C2-N3	3.45	1.33	1.30
2	C	301	06K	C2-N3	2.65	1.32	1.30
2	L	301	06K	C2-N3	2.60	1.32	1.30
2	E	301	06K	C2-N3	2.55	1.32	1.30
2	H	301	06K	C2-N3	2.45	1.32	1.30
2	B	301	06K	C2-N3	2.40	1.32	1.30
2	D	301	06K	C2-N3	2.40	1.32	1.30
2	A	301	06K	C2-N3	2.40	1.32	1.30
2	K	301	06K	C2-N3	2.13	1.32	1.30
2	C	301	06K	C6-C5	-2.07	1.41	1.43
2	I	301	06K	C2-N3	2.04	1.31	1.30

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	301	06K	C2-N3-C4	8.20	120.59	114.09
2	L	301	06K	N3-C2-N1	-8.07	122.49	130.62
2	E	301	06K	N3-C2-N1	-7.70	122.86	130.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	301	06K	C2-N3-C4	7.48	120.01	114.09
2	J	301	06K	N3-C2-N1	-7.46	123.11	130.62
2	C	301	06K	N3-C2-N1	-7.45	123.11	130.62
2	K	301	06K	C2-N3-C4	7.45	119.99	114.09
2	L	301	06K	C2-N3-C4	7.43	119.97	114.09
2	H	301	06K	N3-C2-N1	-7.30	123.27	130.62
2	F	301	06K	C2-N3-C4	7.13	119.73	114.09
2	C	301	06K	C2-N3-C4	7.12	119.73	114.09
2	E	301	06K	C2-N3-C4	7.09	119.71	114.09
2	K	301	06K	N3-C2-N1	-7.06	123.50	130.62
2	B	301	06K	C2-N3-C4	7.00	119.63	114.09
2	B	301	06K	N3-C2-N1	-6.97	123.60	130.62
2	F	301	06K	N3-C2-N1	-6.79	123.78	130.62
2	G	301	06K	N3-C2-N1	-6.66	123.91	130.62
2	I	301	06K	C2-N3-C4	6.65	119.36	114.09
2	H	301	06K	C2-N3-C4	6.64	119.35	114.09
2	I	301	06K	N3-C2-N1	-6.55	124.02	130.62
2	D	301	06K	N3-C2-N1	-6.35	124.22	130.62
2	A	301	06K	N3-C2-N1	-6.33	124.25	130.62
2	D	301	06K	C2-N3-C4	6.31	119.09	114.09
2	A	301	06K	C2-N3-C4	6.27	119.05	114.09
2	L	301	06K	CL1-C2-N3	5.67	120.54	115.70
2	A	301	06K	CL1-C2-N3	5.09	120.04	115.70
2	F	301	06K	CL1-C2-N3	5.02	119.99	115.70
2	D	301	06K	CL1-C2-N3	5.00	119.97	115.70
2	H	301	06K	CL1-C2-N3	4.77	119.77	115.70
2	I	301	06K	CL1-C2-N3	4.67	119.69	115.70
2	E	301	06K	CL1-C2-N3	4.51	119.55	115.70
2	C	301	06K	CL1-C2-N3	4.22	119.30	115.70
2	B	301	06K	CL1-C2-N3	4.11	119.21	115.70
2	E	301	06K	C6-N1-C2	3.99	120.95	115.34
2	L	301	06K	C6-N1-C2	3.97	120.92	115.34
2	J	301	06K	CL1-C2-N3	3.95	119.07	115.70
2	C	301	06K	CL2-C6-N1	3.62	120.68	114.39
2	H	301	06K	C6-N1-C2	3.49	120.24	115.34
2	H	301	06K	CL2-C6-N1	3.47	120.42	114.39
2	D	301	06K	CL2-C6-N1	3.41	120.32	114.39
2	K	301	06K	CL2-C6-N1	3.37	120.24	114.39
2	K	301	06K	CL1-C2-N3	3.35	118.56	115.70
2	E	301	06K	CL2-C6-N1	3.29	120.11	114.39
2	B	301	06K	CL2-C6-N1	3.19	119.93	114.39
2	C	301	06K	C6-N1-C2	3.16	119.78	115.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	301	06K	C6-N1-C2	3.12	119.73	115.34
2	A	301	06K	CL2-C6-N1	3.07	119.72	114.39
2	G	301	06K	CL2-C6-N1	3.06	119.71	114.39
2	D	301	06K	C6-N1-C2	3.05	119.63	115.34
2	I	301	06K	C6-N1-C2	3.00	119.56	115.34
2	A	301	06K	C6-N1-C2	2.92	119.45	115.34
2	K	301	06K	C6-N1-C2	2.88	119.39	115.34
2	G	301	06K	C6-N1-C2	2.87	119.37	115.34
2	L	301	06K	CL2-C6-N1	2.82	119.29	114.39
2	F	301	06K	C6-N1-C2	2.82	119.30	115.34
2	B	301	06K	C6-N1-C2	2.81	119.28	115.34
2	F	301	06K	CL2-C6-N1	2.74	119.16	114.39
2	G	301	06K	C4-C5-N7	-2.65	106.63	109.40
2	J	301	06K	C4-C5-N7	-2.65	106.64	109.40
2	J	301	06K	CL2-C6-N1	2.58	118.87	114.39
2	G	301	06K	CL1-C2-N1	2.55	118.79	115.15
2	I	301	06K	CL2-C6-N1	2.51	118.75	114.39
2	E	301	06K	C4-C5-N7	-2.30	107.01	109.40
2	D	301	06K	C4-C5-N7	-2.15	107.16	109.40
2	F	301	06K	C4-C5-N7	-2.09	107.23	109.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

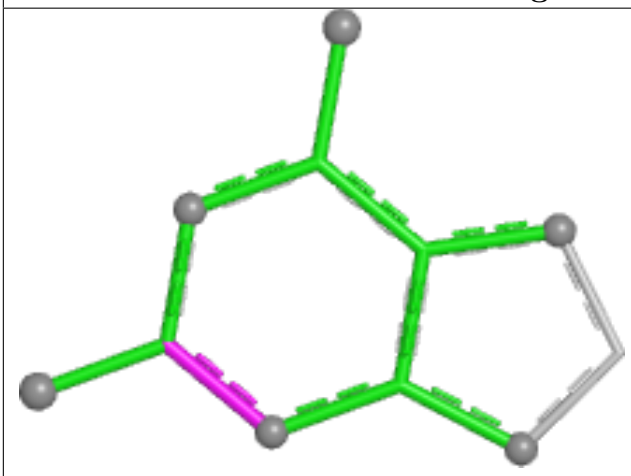
12 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	302	IMD	1	0
3	G	302	IMD	1	0
3	L	302	IMD	1	0
3	B	302	IMD	1	0
3	C	302	IMD	1	0
3	E	302	IMD	1	0
3	D	302	IMD	1	0
3	I	302	IMD	1	0
3	K	302	IMD	1	0
3	J	302	IMD	1	0
3	A	302	IMD	1	0
3	F	302	IMD	1	0

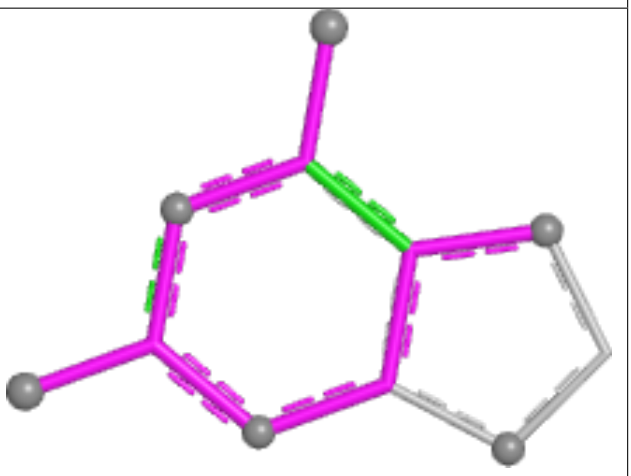
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 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.

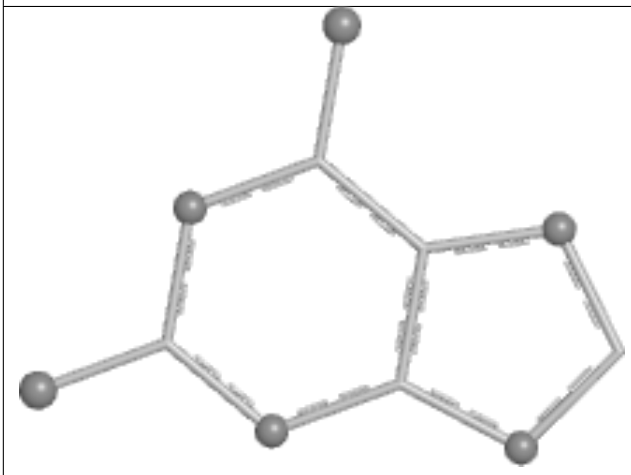
Ligand 06K E 301



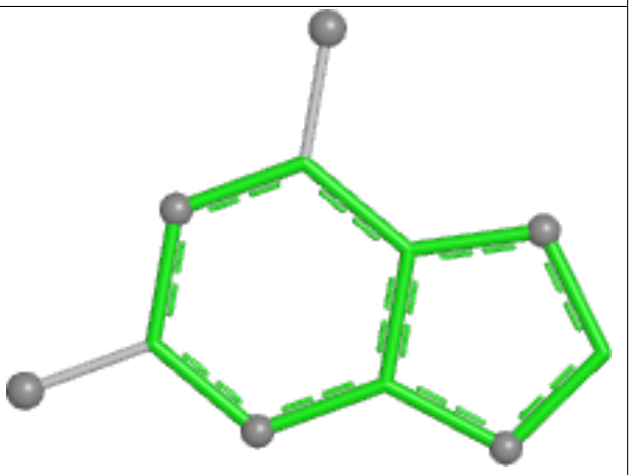
Bond lengths



Bond angles

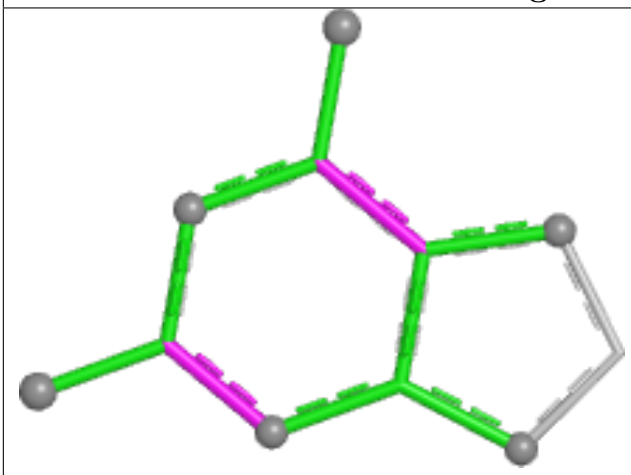


Torsions



Rings

Ligand 06K C 301



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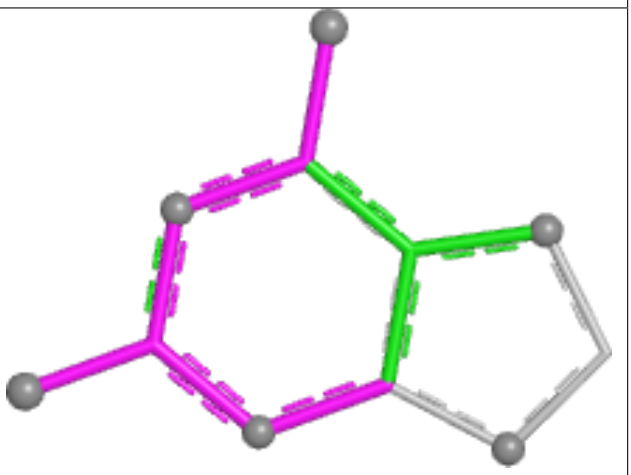
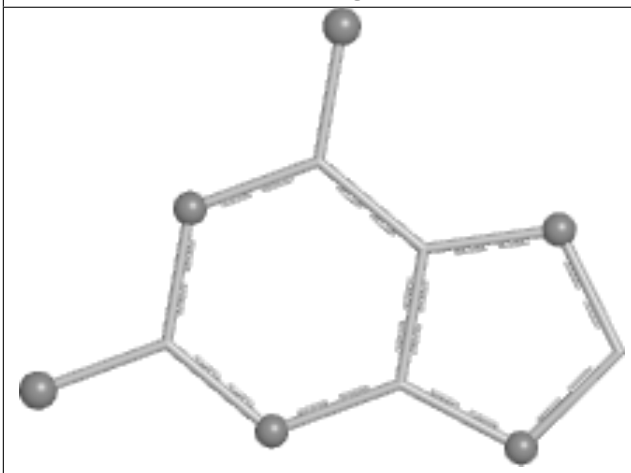


Bond angles



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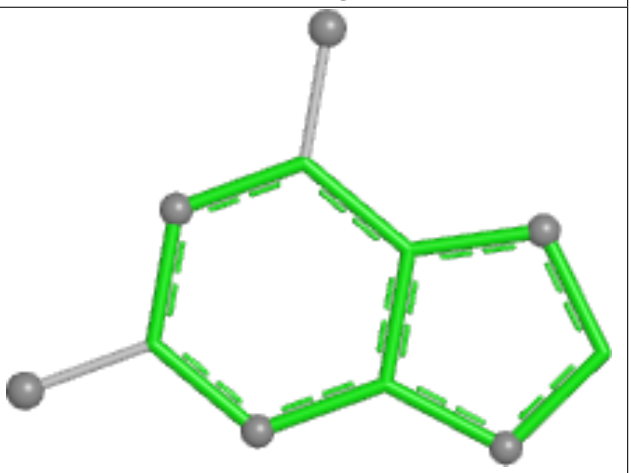
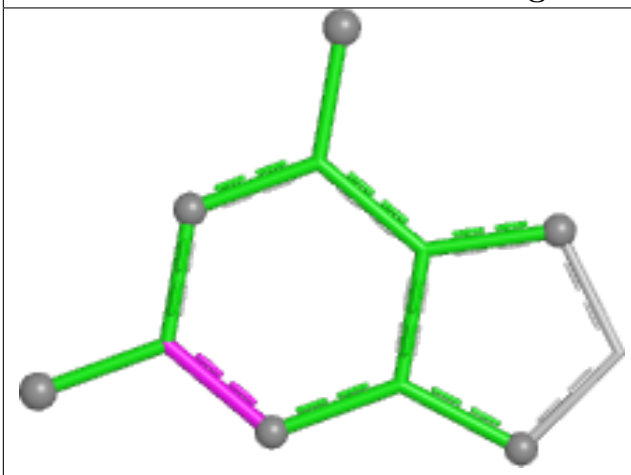


Rings

Ligand 06K H 301



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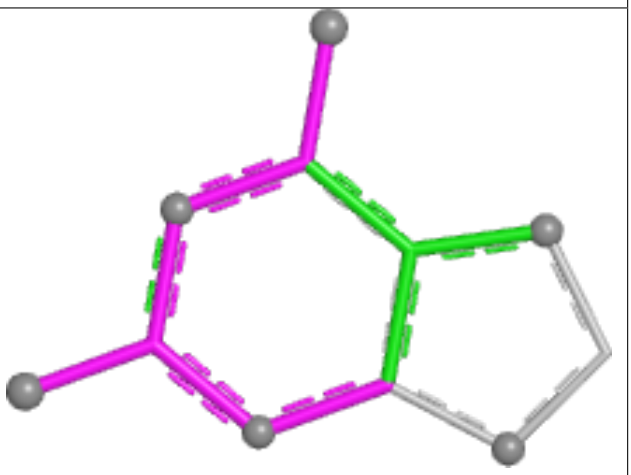
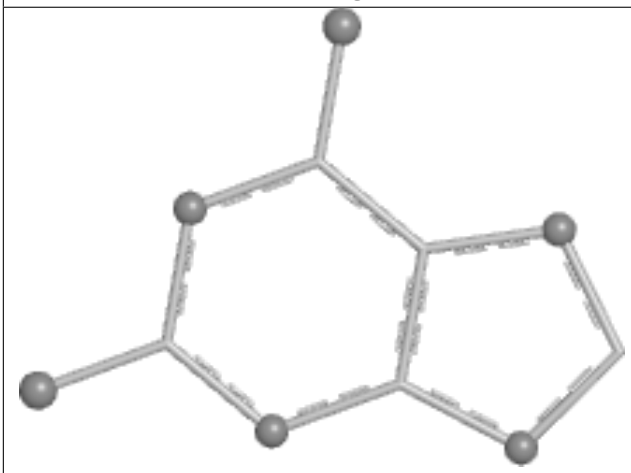


Bond angles



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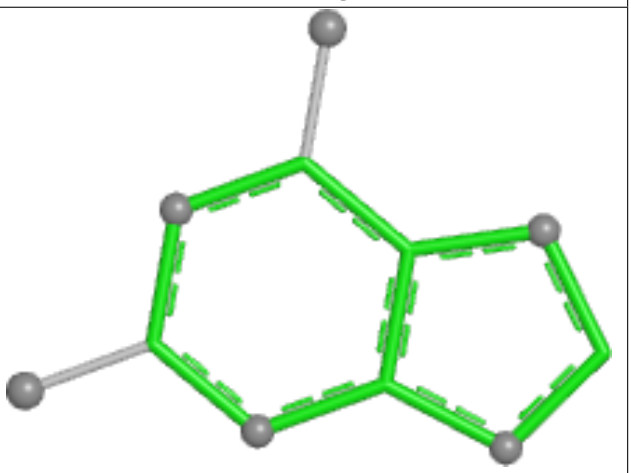
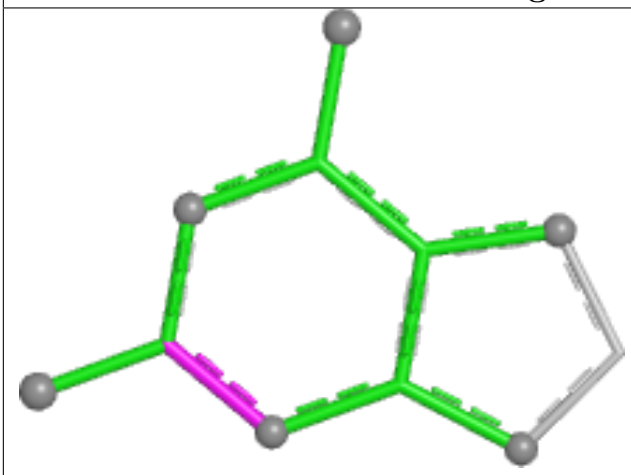


Rings

Ligand 06K D 301



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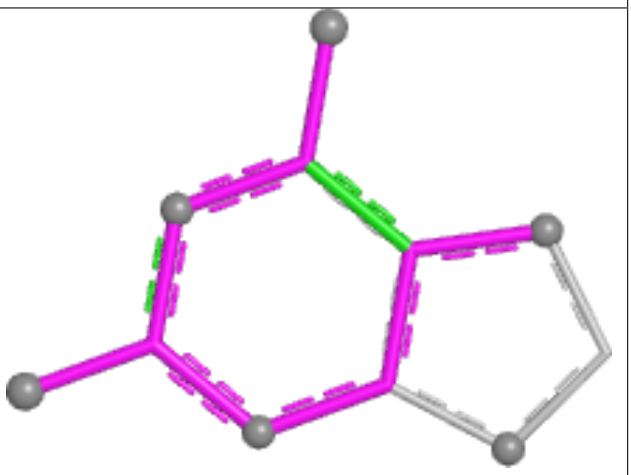
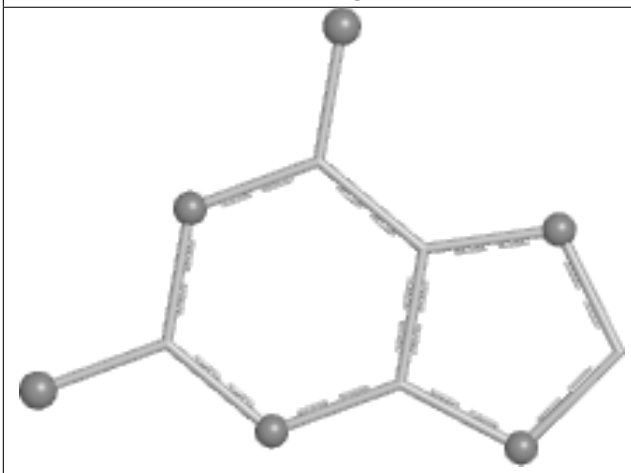


Bond angles



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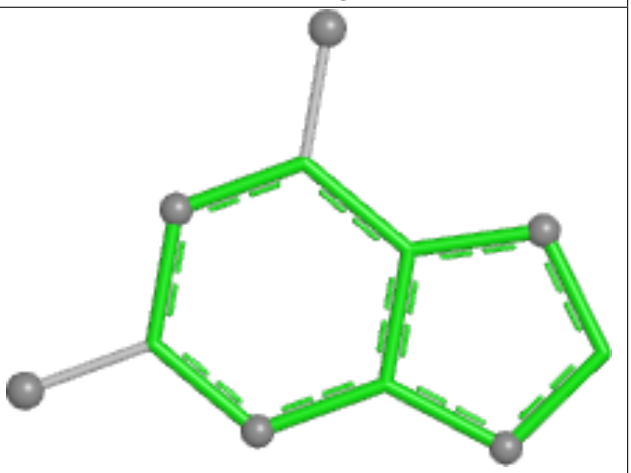
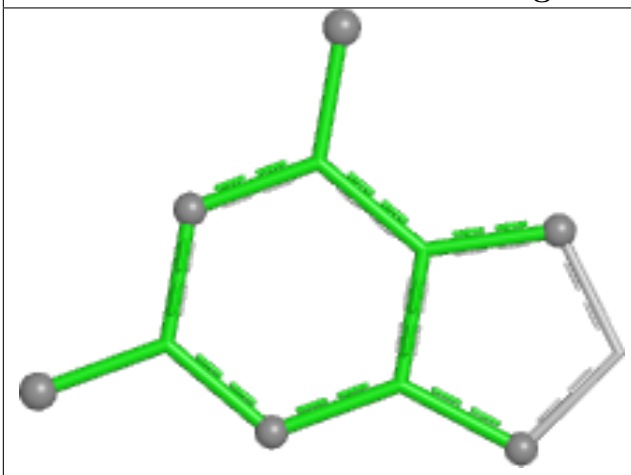
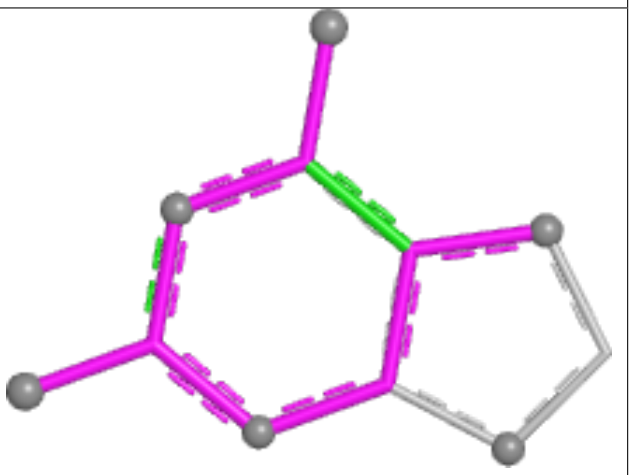


Rings

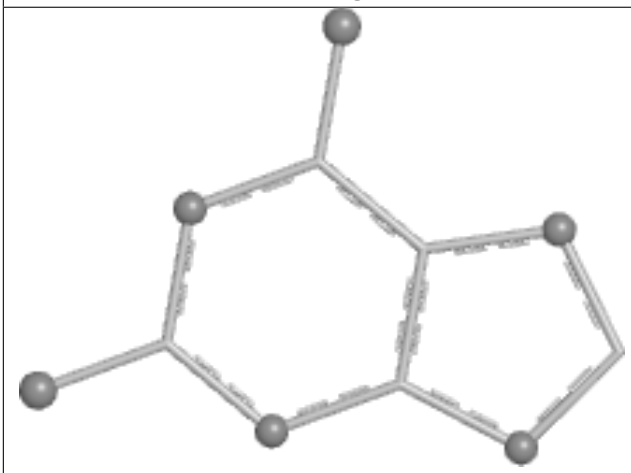
Ligand 06K J 301



Bond lengths



Bond angles



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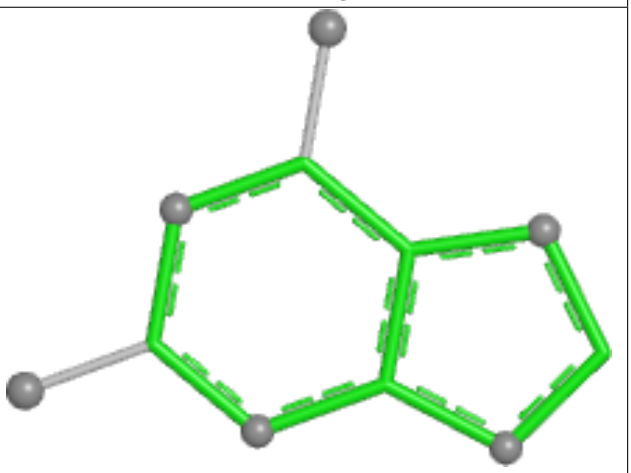
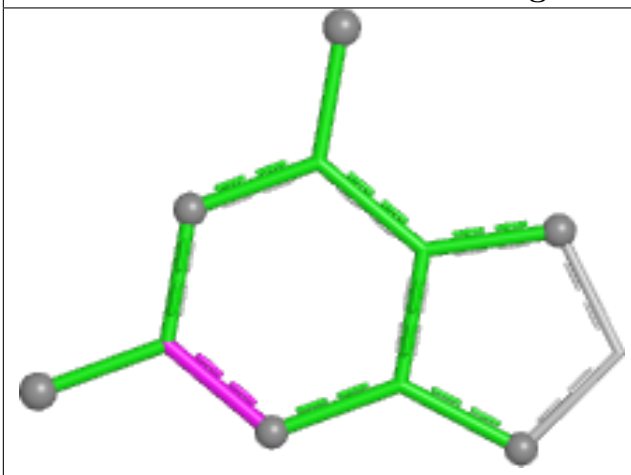
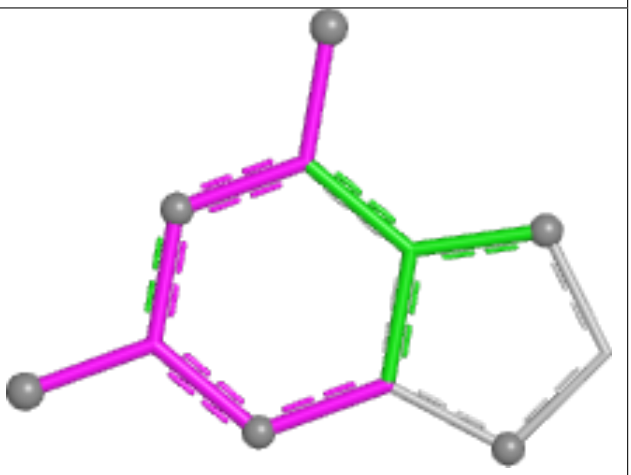


Rings

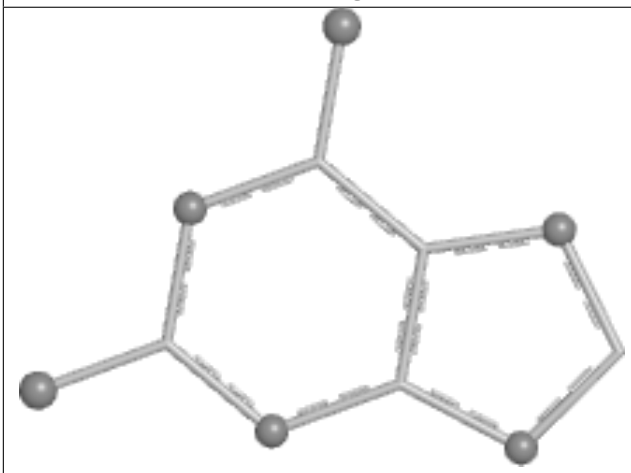
Ligand 06K A 301



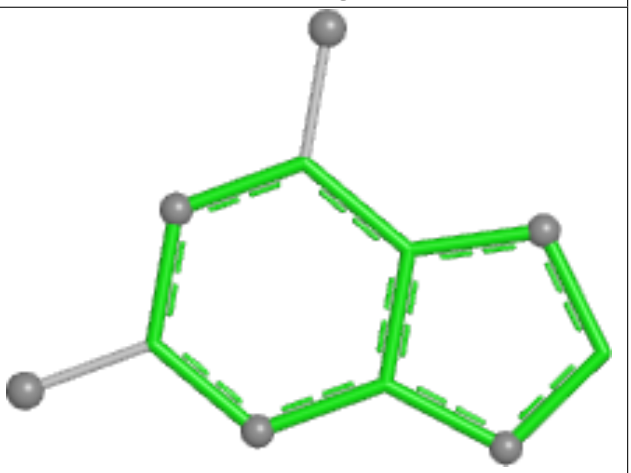
Bond lengths



Bond angles

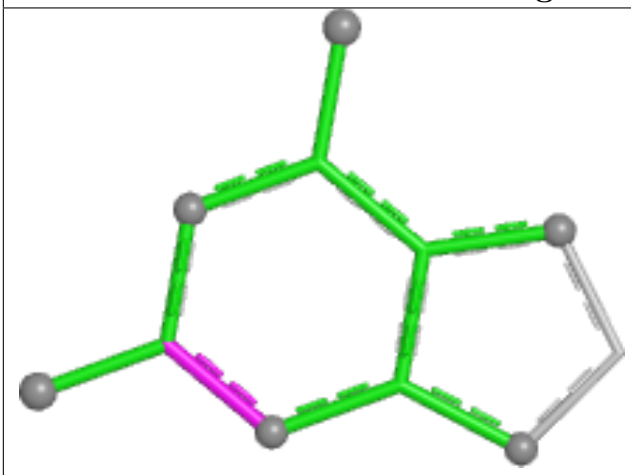


Torsions

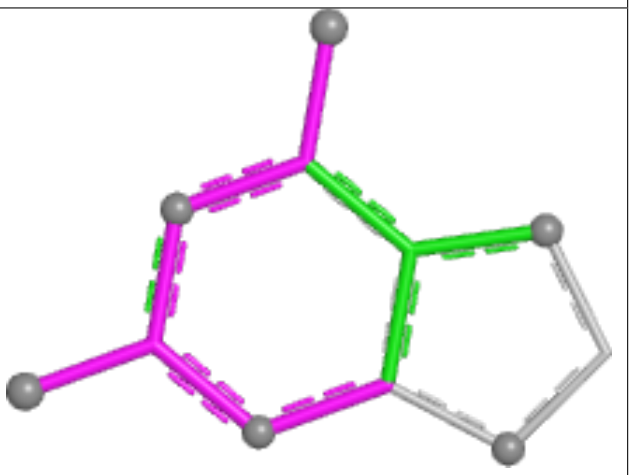


Rings

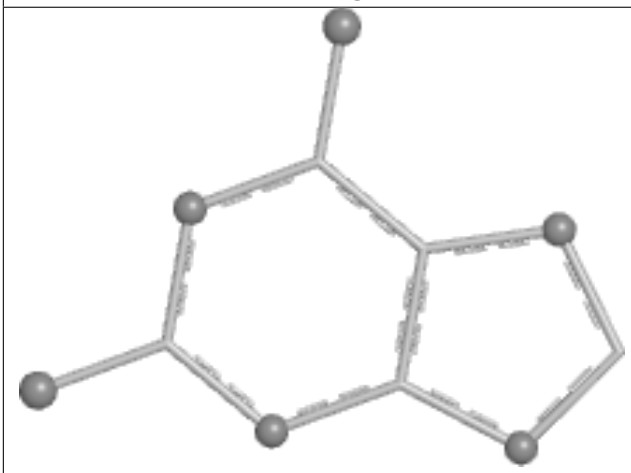
Ligand 06K I 301



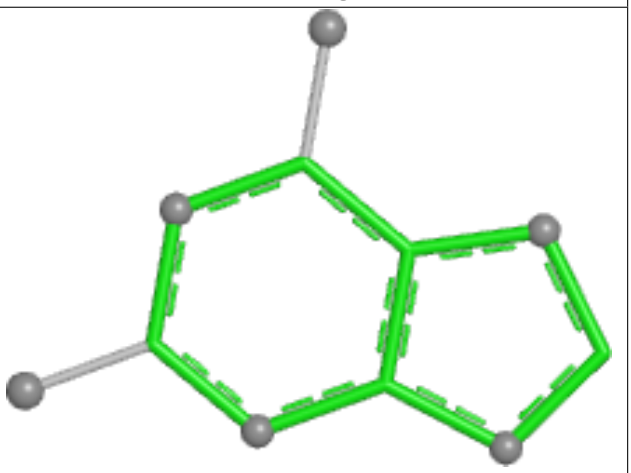
Bond lengths



Bond angles

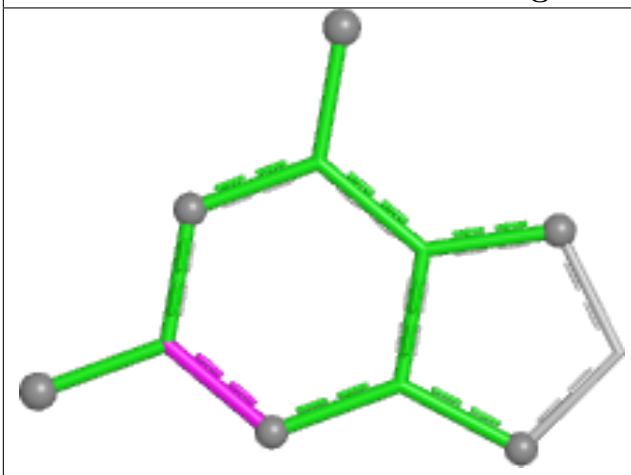


Torsions

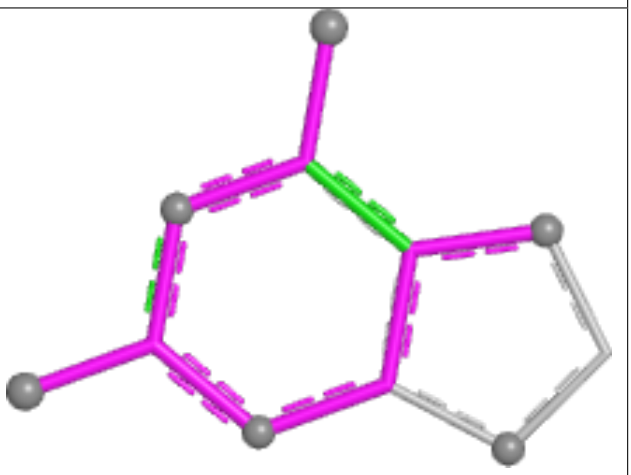


Rings

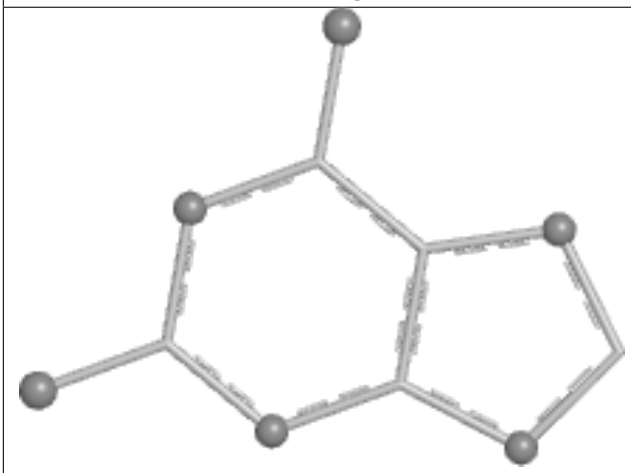
Ligand 06K F 301



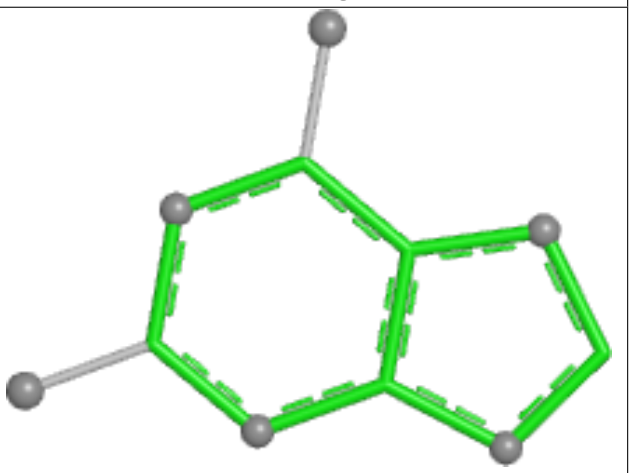
Bond lengths



Bond angles

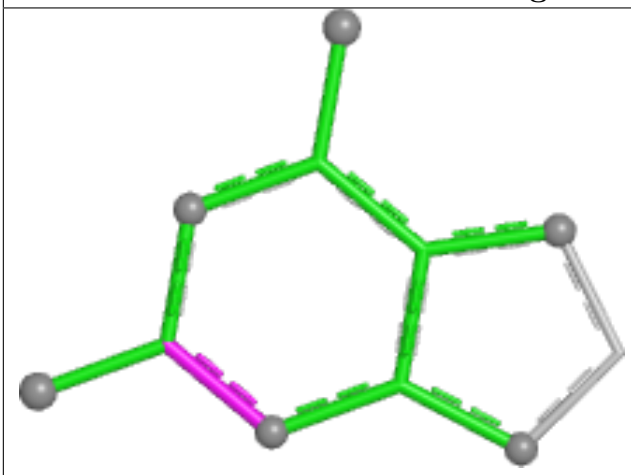


Torsions

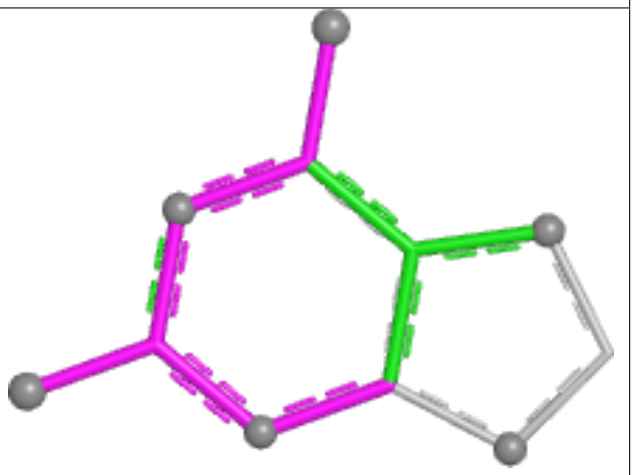


Rings

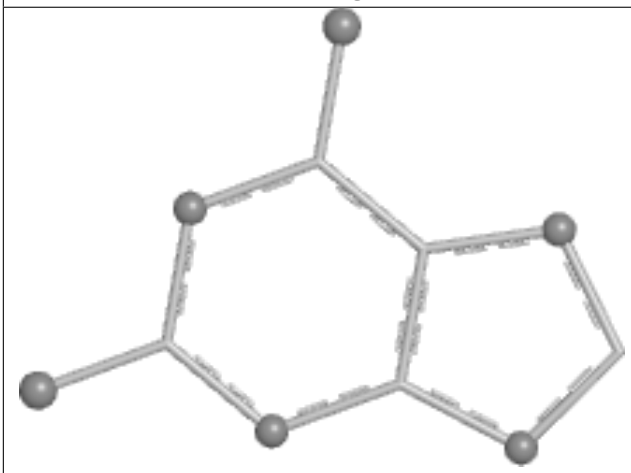
Ligand 06K B 301



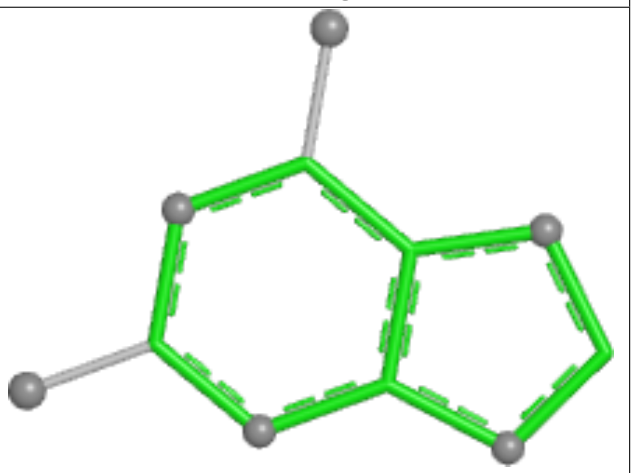
Bond lengths



Bond angles

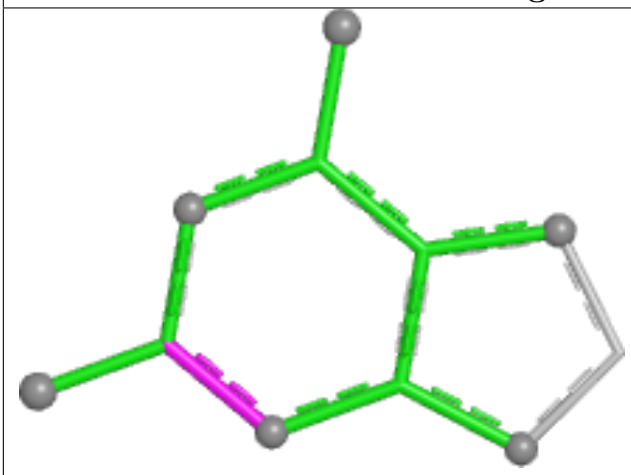


Torsions

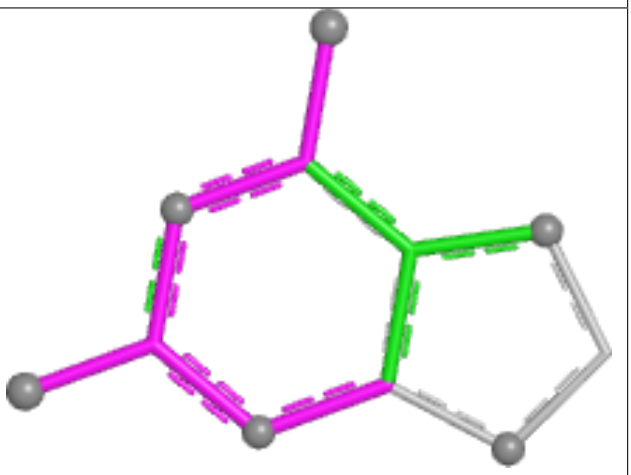


Rings

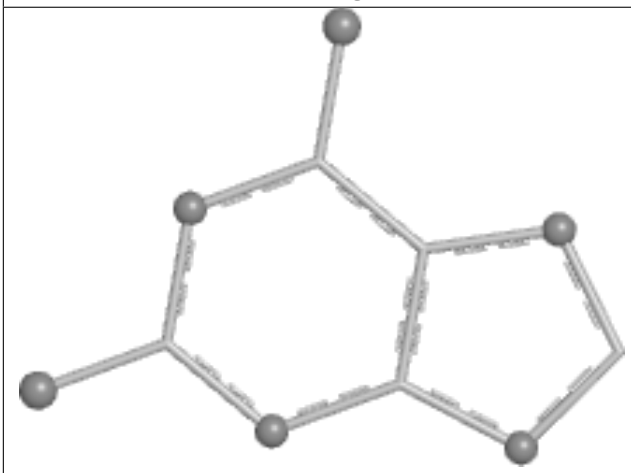
Ligand 06K K 301



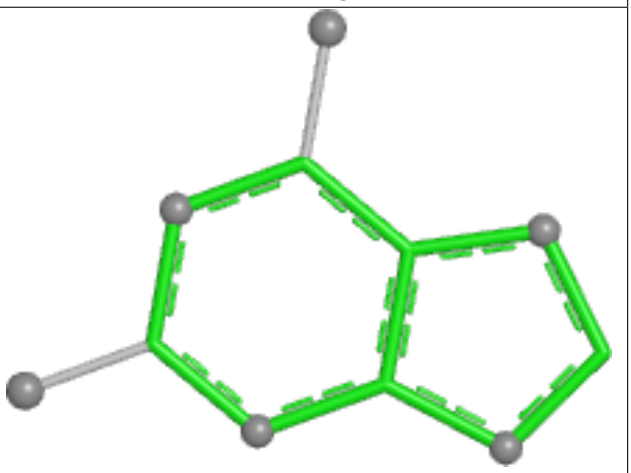
Bond lengths



Bond angles

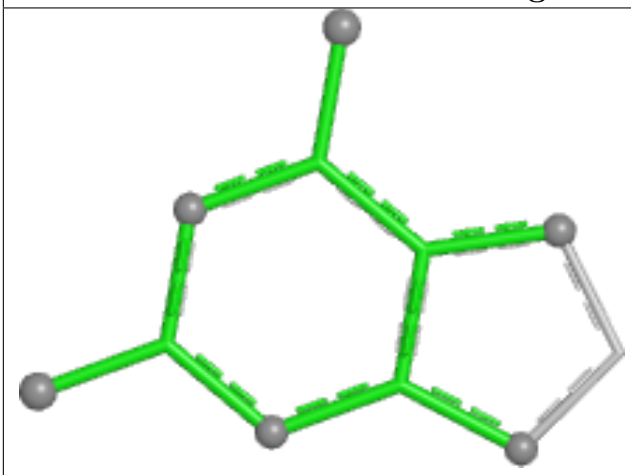


Torsions

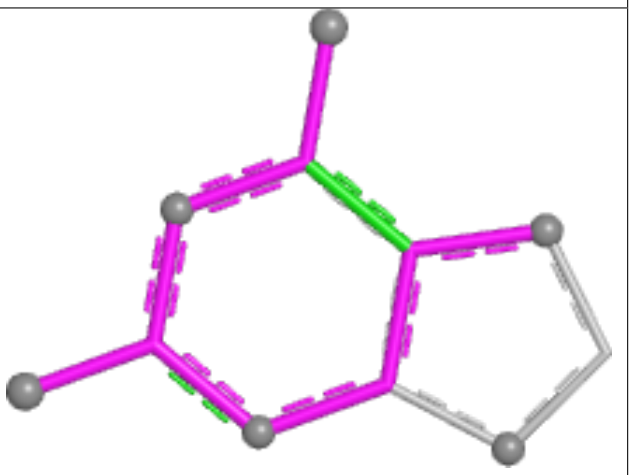


Rings

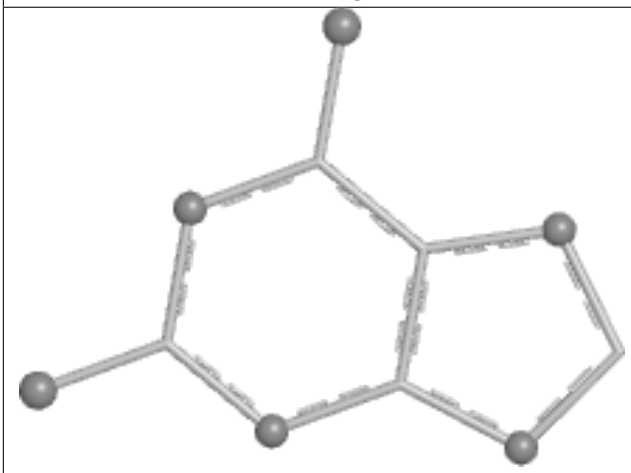
Ligand 06K G 301



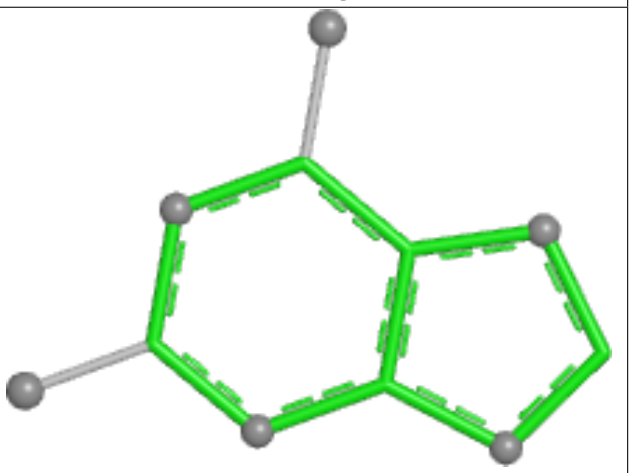
Bond lengths



Bond angles

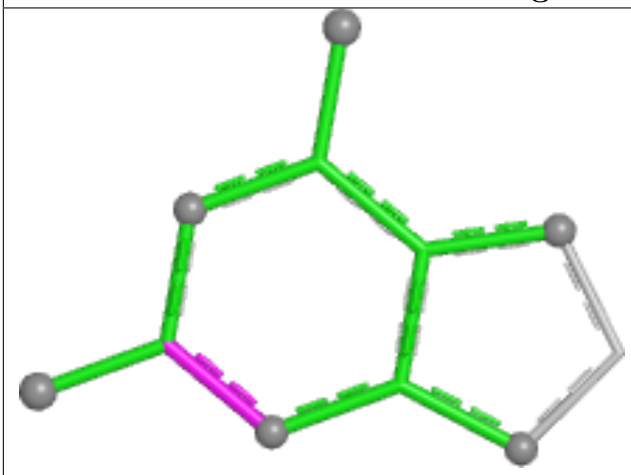


Torsions

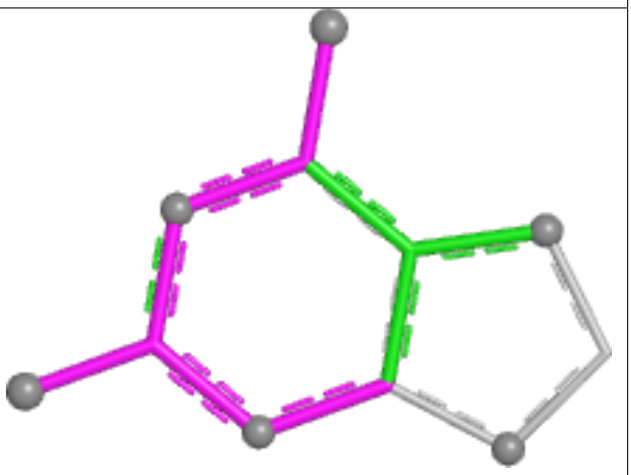


Rings

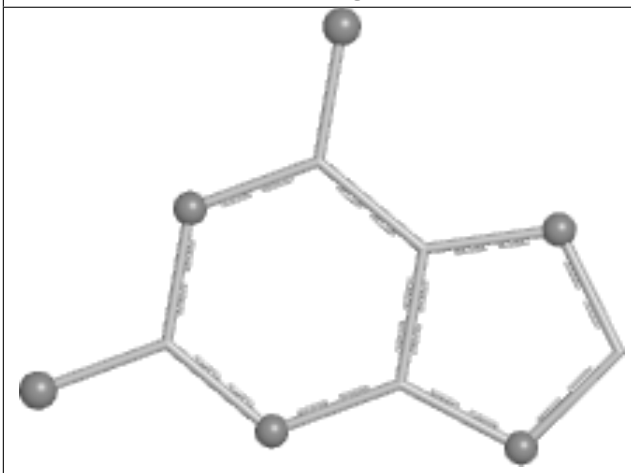
Ligand 06K L 301



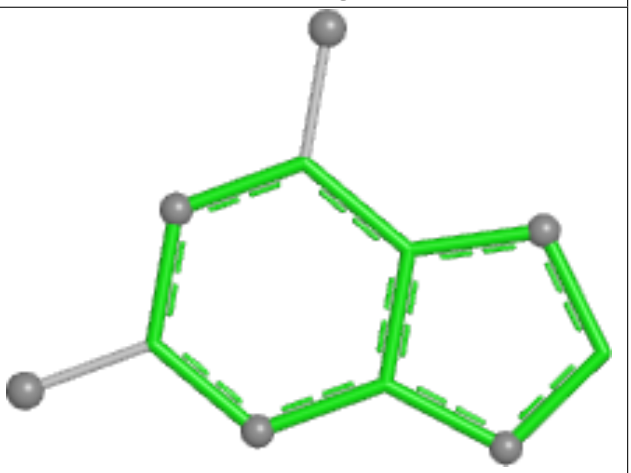
Bond lengths



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	232/233 (99%)	0.07	9 (3%)	39	44	10, 16, 30, 41	0
1	B	232/233 (99%)	-0.01	4 (1%)	70	75	9, 15, 29, 39	0
1	C	232/233 (99%)	-0.04	3 (1%)	77	81	9, 15, 30, 40	0
1	D	232/233 (99%)	0.21	5 (2%)	62	67	9, 16, 32, 45	0
1	E	232/233 (99%)	0.06	4 (1%)	70	75	9, 15, 29, 42	0
1	F	232/233 (99%)	0.19	10 (4%)	35	39	9, 17, 37, 49	0
1	G	232/233 (99%)	-0.07	2 (0%)	84	87	10, 16, 29, 43	0
1	H	232/233 (99%)	0.04	6 (2%)	56	61	10, 16, 29, 39	0
1	I	232/233 (99%)	0.02	5 (2%)	62	67	10, 16, 31, 43	0
1	J	232/233 (99%)	0.10	3 (1%)	77	81	9, 15, 30, 41	0
1	K	232/233 (99%)	0.09	8 (3%)	45	49	9, 16, 35, 48	0
1	L	232/233 (99%)	0.14	10 (4%)	35	39	9, 17, 37, 51	0
All	All	2784/2796 (99%)	0.07	69 (2%)	57	62	9, 16, 31, 51	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1	MET	4.8
1	H	9	ILE	4.7
1	F	1	MET	4.2
1	I	9	ILE	4.2
1	C	9	ILE	4.1
1	A	9	ILE	4.1
1	G	9	ILE	3.9
1	D	219	GLU	3.9
1	A	1	MET	3.8
1	B	218	VAL	3.7
1	L	215	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	K	215	LYS	3.5
1	F	215	LYS	3.4
1	I	214	PRO	3.4
1	F	214	PRO	3.4
1	J	233	SER	3.4
1	K	208	THR	3.3
1	J	214	PRO	3.3
1	K	1	MET	3.2
1	D	215	LYS	3.2
1	F	210	GLU	3.1
1	B	9	ILE	3.1
1	E	1	MET	3.1
1	B	214	PRO	3.1
1	L	1	MET	3.0
1	I	215	LYS	3.0
1	I	213	SER	2.8
1	A	207	ILE	2.6
1	D	210	GLU	2.6
1	K	209	LYS	2.6
1	F	233	SER	2.6
1	A	215	LYS	2.6
1	A	210	GLU	2.5
1	D	1	MET	2.5
1	B	215	LYS	2.5
1	L	219	GLU	2.4
1	E	214	PRO	2.4
1	L	218	VAL	2.4
1	A	208	THR	2.4
1	F	212	LEU	2.4
1	L	233	SER	2.4
1	F	57	ILE	2.4
1	J	1	MET	2.4
1	K	214	PRO	2.3
1	E	9	ILE	2.3
1	H	215	LYS	2.3
1	F	208	THR	2.3
1	K	213	SER	2.3
1	L	210	GLU	2.2
1	H	214	PRO	2.2
1	C	1	MET	2.2
1	A	219	GLU	2.2
1	H	208	THR	2.2

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Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	9	ILE	2.2
1	A	121	LEU	2.1
1	C	215	LYS	2.1
1	K	207	ILE	2.1
1	L	9	ILE	2.1
1	L	214	PRO	2.1
1	H	1	MET	2.1
1	L	213	SER	2.0
1	H	210	GLU	2.0
1	I	57	ILE	2.0
1	A	218	VAL	2.0
1	E	233	SER	2.0
1	F	99	GLY	2.0
1	K	210	GLU	2.0
1	L	57	ILE	2.0
1	F	223	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	OCS	A	19	9/10	0.92	0.12	12,14,28,28	0
1	OCS	H	19	9/10	0.92	0.12	12,14,27,28	0
1	OCS	E	19	9/10	0.94	0.10	11,14,27,27	0
1	OCS	J	19	9/10	0.94	0.11	13,14,27,28	0
1	OCS	D	19	9/10	0.95	0.10	12,15,25,25	0
1	OCS	I	19	9/10	0.95	0.09	13,14,26,26	0
1	OCS	C	19	9/10	0.95	0.10	12,14,23,24	0
1	OCS	K	19	9/10	0.95	0.10	13,15,24,25	0
1	OCS	L	19	9/10	0.95	0.11	13,15,23,25	0
1	OCS	G	19	9/10	0.96	0.09	13,15,25,26	0
1	OCS	F	19	9/10	0.96	0.09	12,14,26,26	0
1	OCS	B	19	9/10	0.97	0.08	11,14,23,27	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

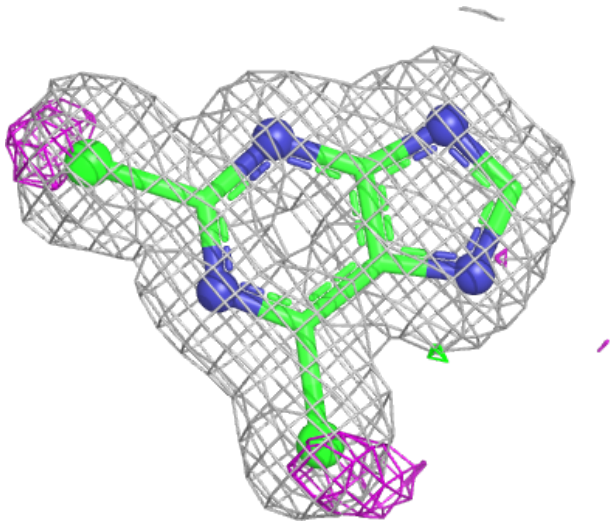
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

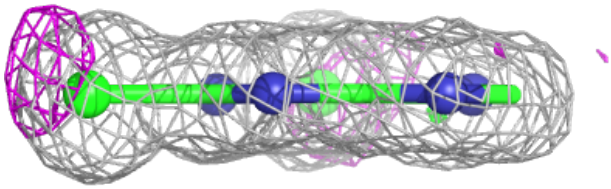
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	IMD	C	302	5/5	0.94	0.08	17,19,22,24	0
3	IMD	E	303	5/5	0.94	0.12	29,30,33,34	0
2	06K	F	301	11/11	0.95	0.08	13,16,25,25	0
3	IMD	E	302	5/5	0.95	0.09	16,17,20,21	0
3	IMD	A	302	5/5	0.95	0.10	17,17,19,23	0
3	IMD	F	302	5/5	0.95	0.09	17,17,19,23	0
3	IMD	L	302	5/5	0.95	0.08	17,18,21,23	0
2	06K	L	301	11/11	0.96	0.07	15,17,24,25	0
2	06K	J	301	11/11	0.96	0.08	12,16,23,25	0
3	IMD	B	302	5/5	0.96	0.08	19,20,22,23	0
3	IMD	H	302	5/5	0.96	0.07	14,16,20,22	0
3	IMD	I	302	5/5	0.96	0.08	16,18,19,25	0
2	06K	K	301	11/11	0.96	0.07	12,14,21,23	0
2	06K	A	301	11/11	0.97	0.06	12,15,21,22	0
2	06K	G	301	11/11	0.97	0.06	11,13,19,21	0
3	IMD	D	302	5/5	0.97	0.09	17,18,22,25	0
2	06K	H	301	11/11	0.97	0.06	11,14,20,21	0
2	06K	I	301	11/11	0.97	0.07	12,14,20,21	0
2	06K	B	301	11/11	0.97	0.06	11,13,20,21	0
3	IMD	G	302	5/5	0.97	0.07	18,18,23,24	0
2	06K	C	301	11/11	0.97	0.06	12,13,18,23	0
2	06K	D	301	11/11	0.97	0.07	11,16,21,23	0
3	IMD	J	302	5/5	0.97	0.06	16,18,21,23	0
3	IMD	K	302	5/5	0.97	0.07	18,20,21,24	0
2	06K	E	301	11/11	0.97	0.06	14,17,23,23	0
4	MG	A	303	1/1	0.98	0.14	17,17,17,17	0
4	MG	B	303	1/1	0.99	0.13	17,17,17,17	0
4	MG	D	303	1/1	0.99	0.10	21,21,21,21	0
4	MG	E	304	1/1	0.99	0.06	23,23,23,23	0
4	MG	F	303	1/1	0.99	0.09	22,22,22,22	0
4	MG	G	303	1/1	0.99	0.10	15,15,15,15	0
4	MG	H	303	1/1	0.99	0.09	17,17,17,17	0
4	MG	J	303	1/1	0.99	0.07	26,26,26,26	0
4	MG	K	303	1/1	0.99	0.11	19,19,19,19	0
4	MG	L	303	1/1	0.99	0.08	21,21,21,21	0
4	MG	I	303	1/1	1.00	0.12	17,17,17,17	0
4	MG	C	303	1/1	1.00	0.12	17,17,17,17	0

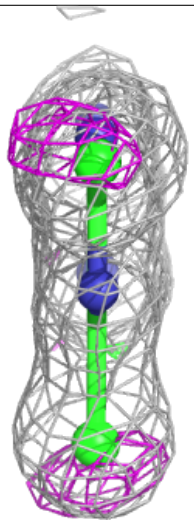
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 06K 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)

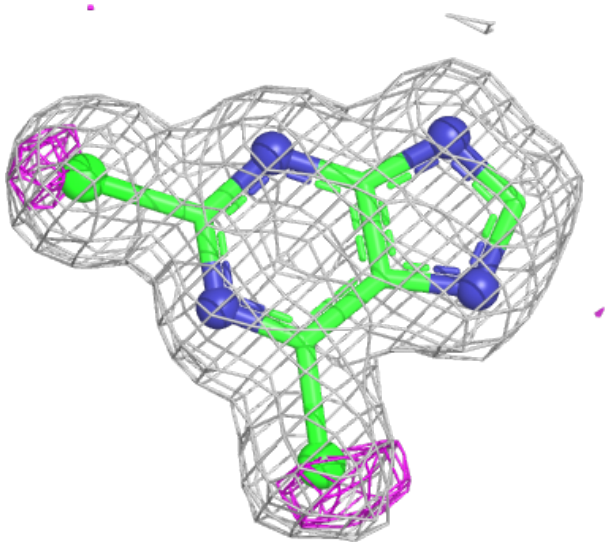


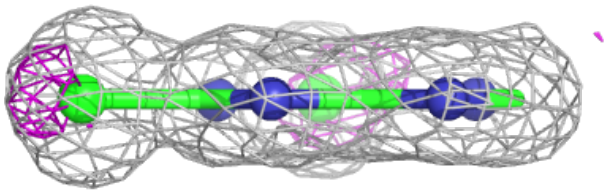


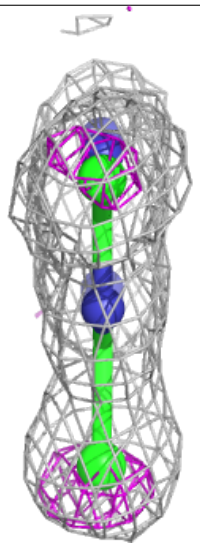


Electron density around 06K L 301:

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

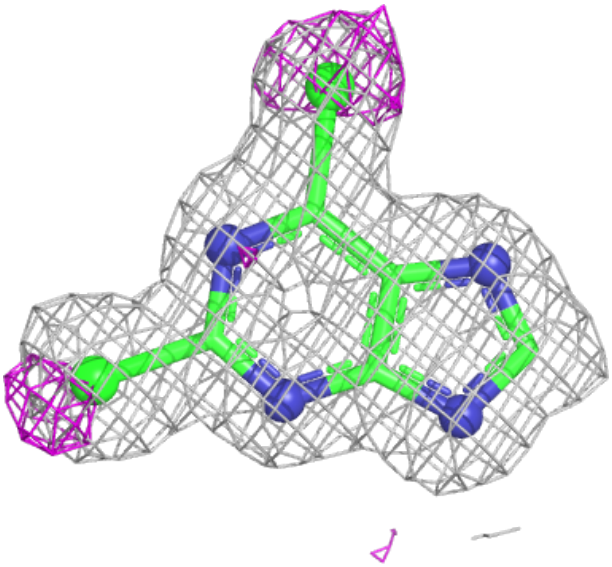


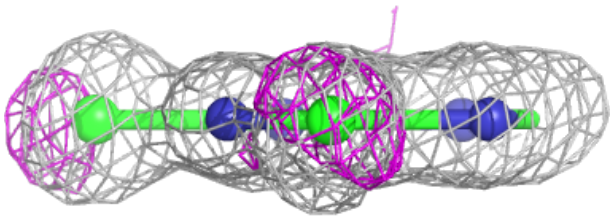


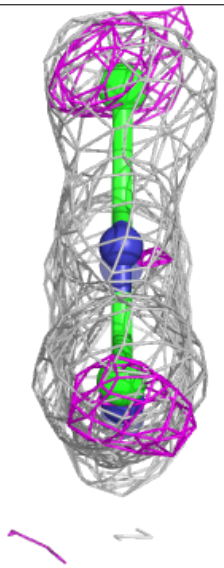


Electron density around 06K J 301:

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

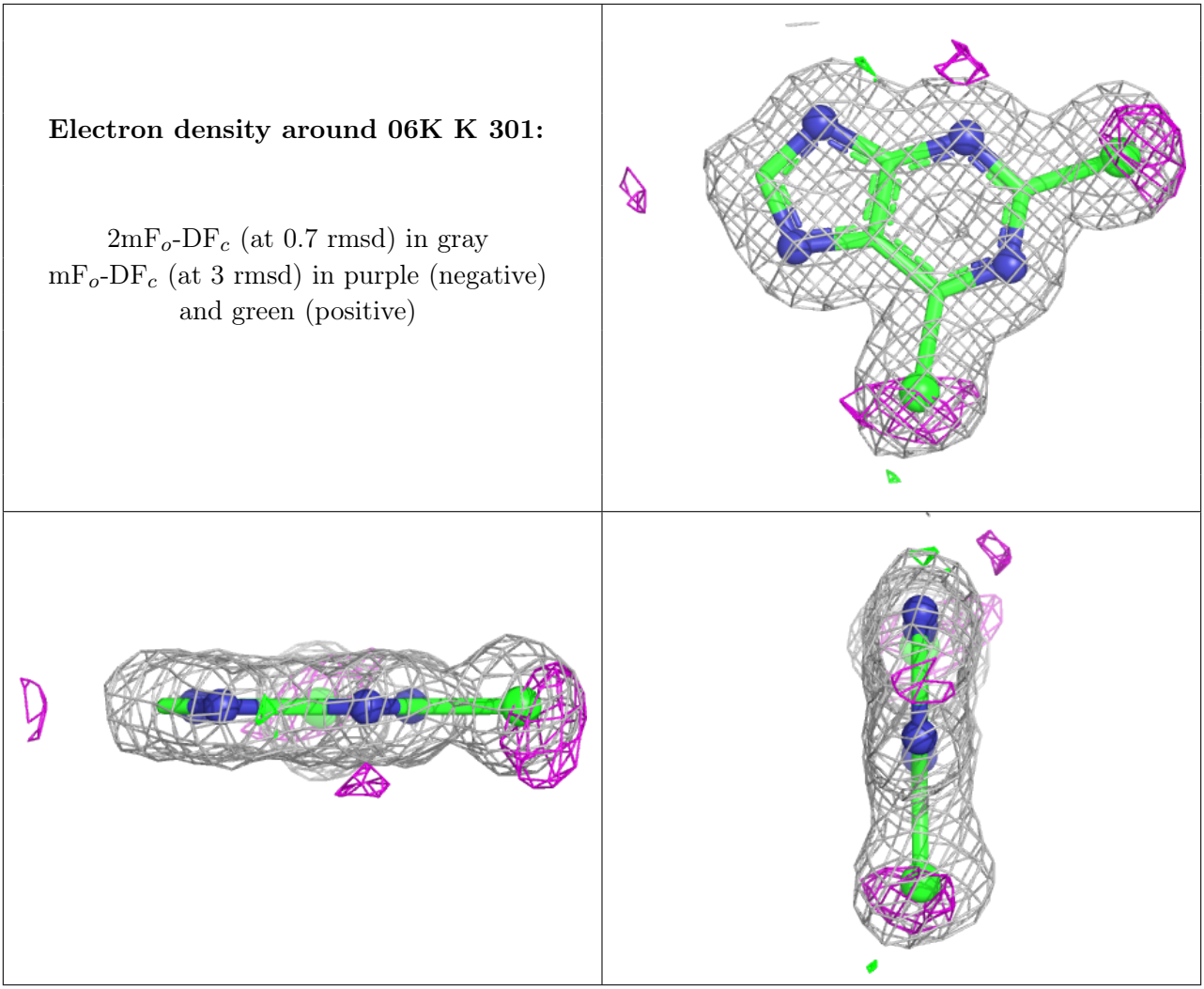






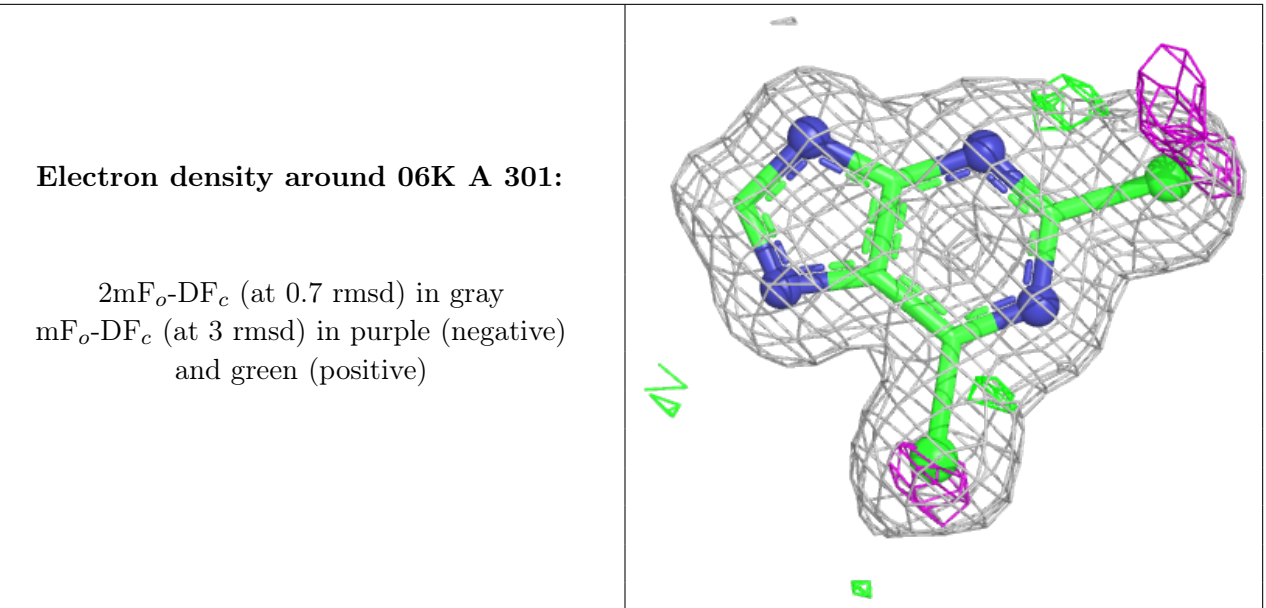
Electron density around 06K K 301:

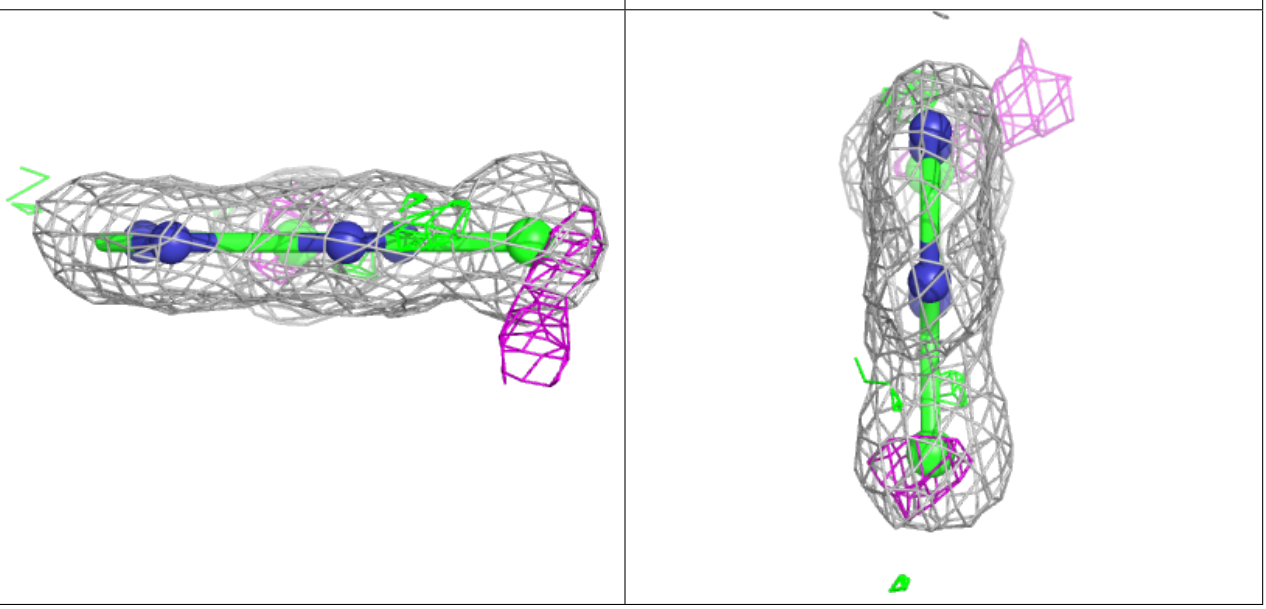
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 06K A 301:

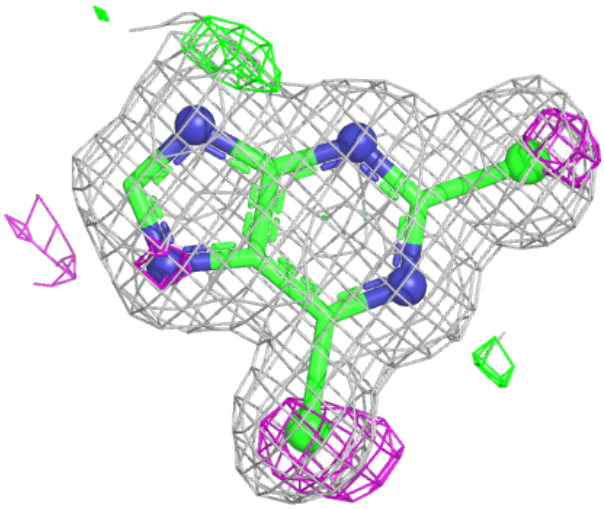
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

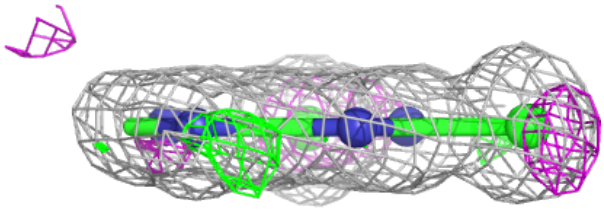


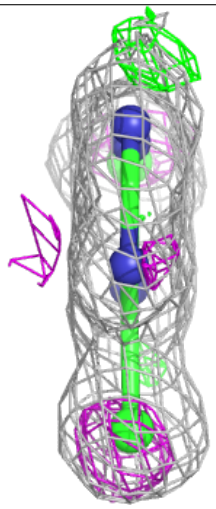


Electron density around 06K G 301:

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

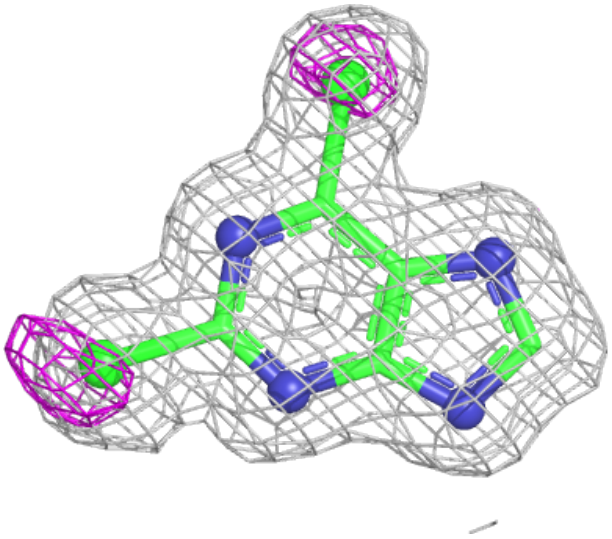


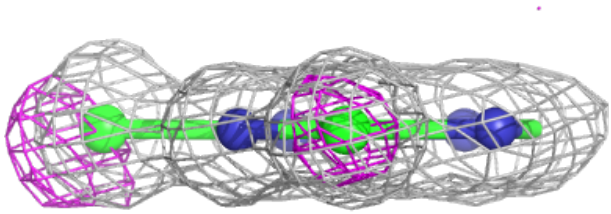


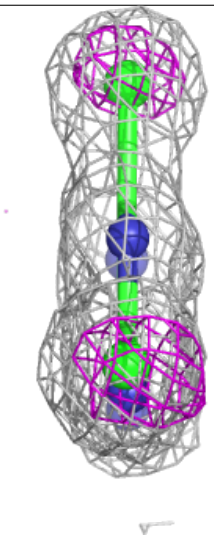


Electron density around 06K H 301:

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

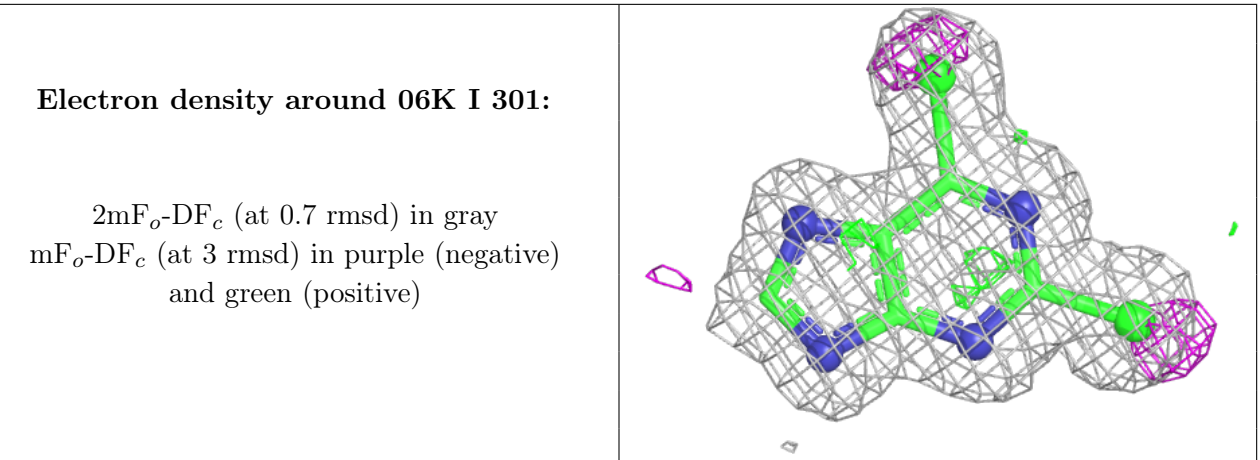


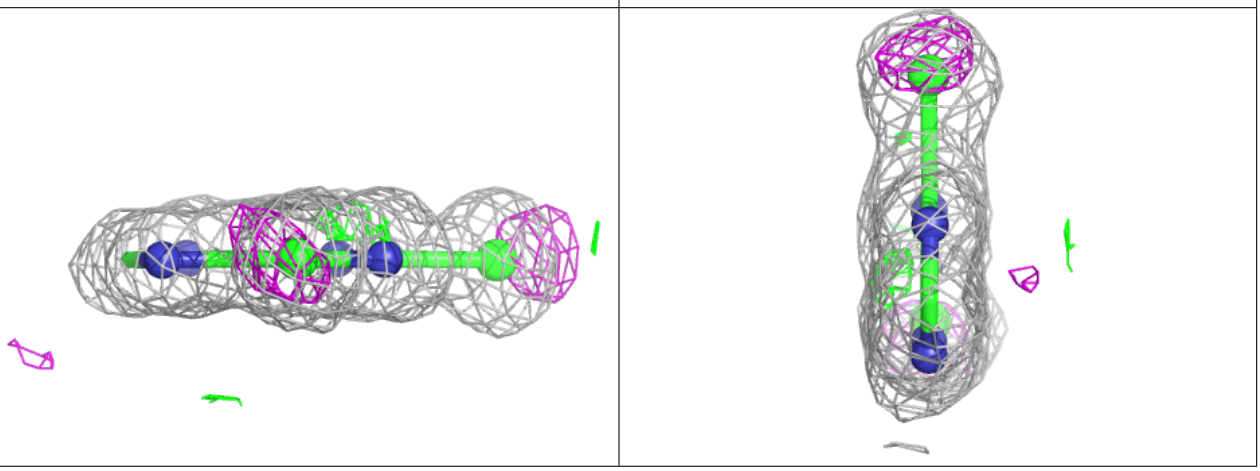




Electron density around 06K I 301:

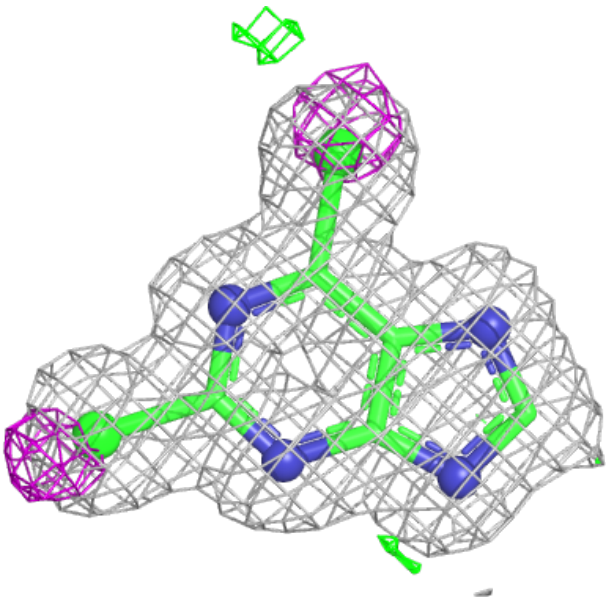
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

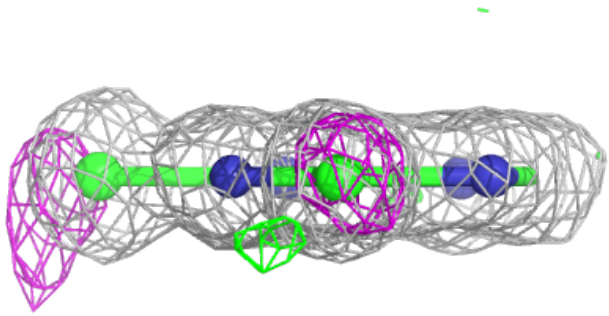


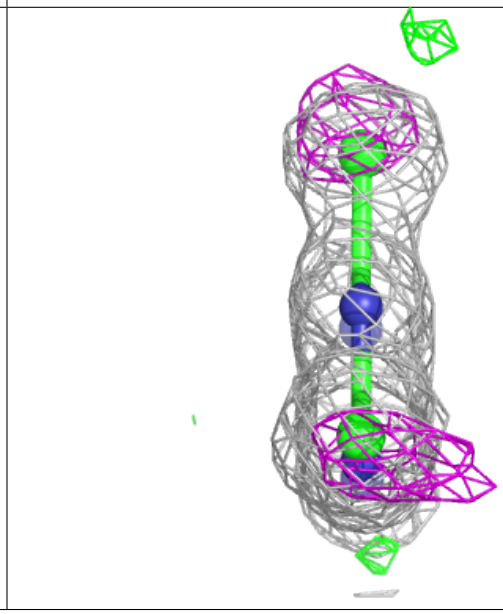


Electron density around 06K B 301:

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

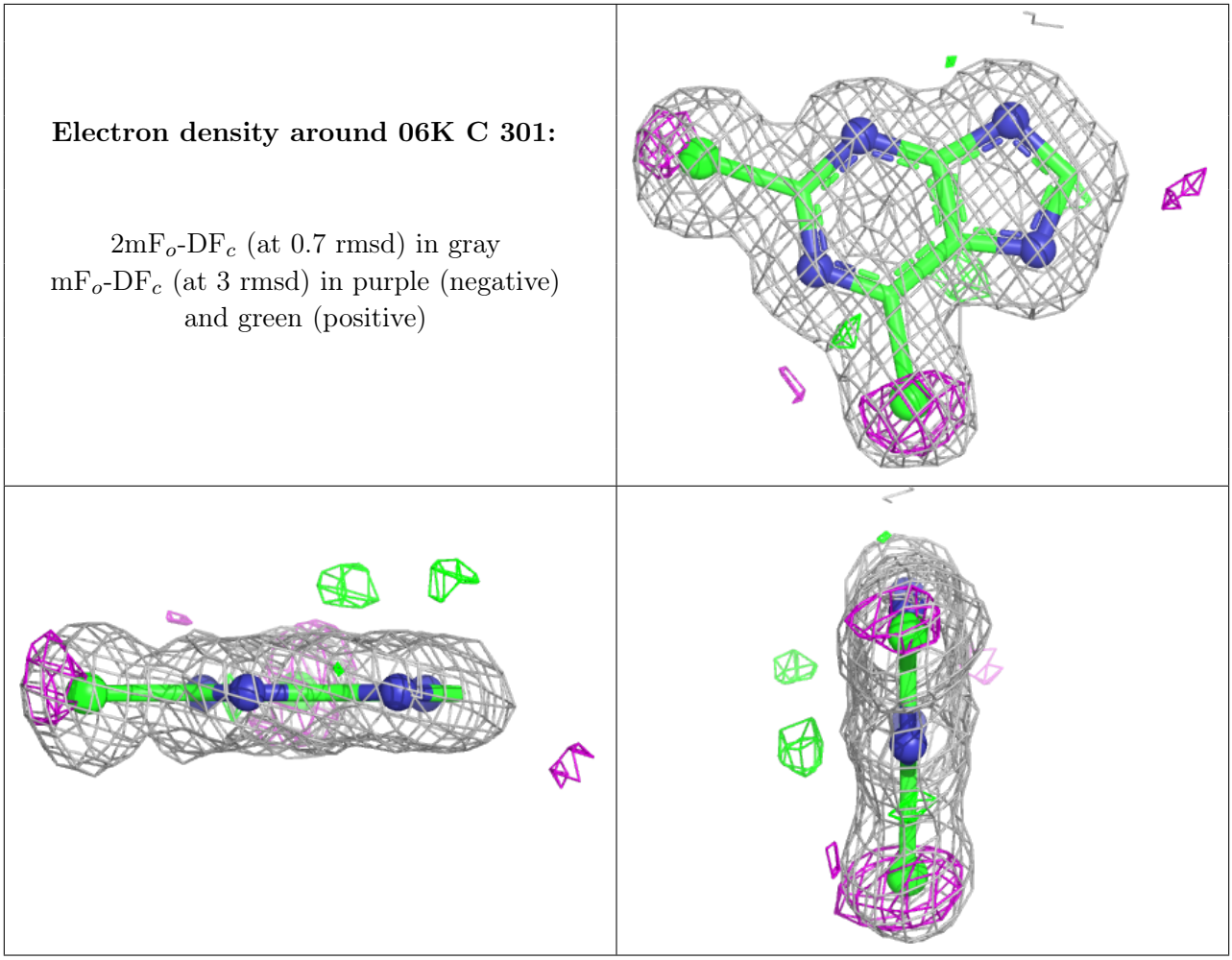






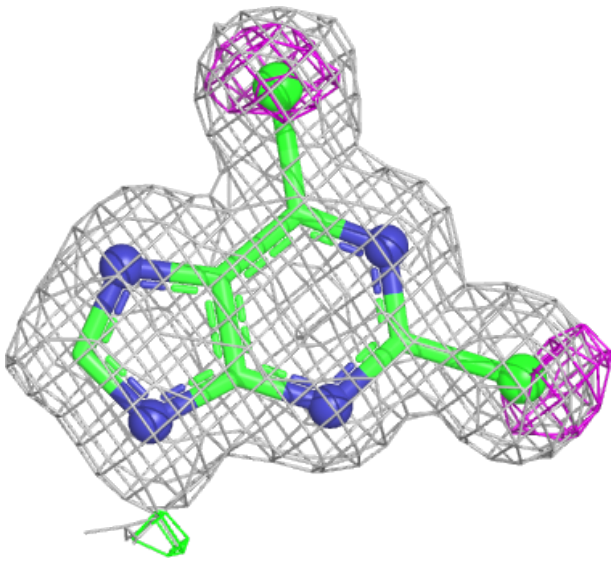
Electron density around 06K C 301:

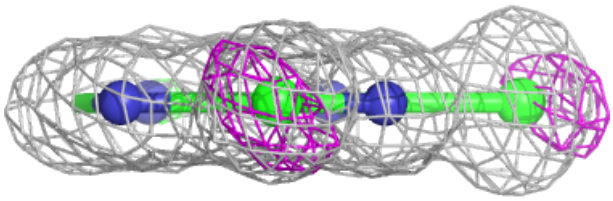
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

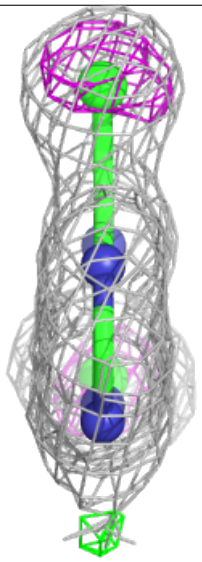


Electron density around 06K D 301:

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

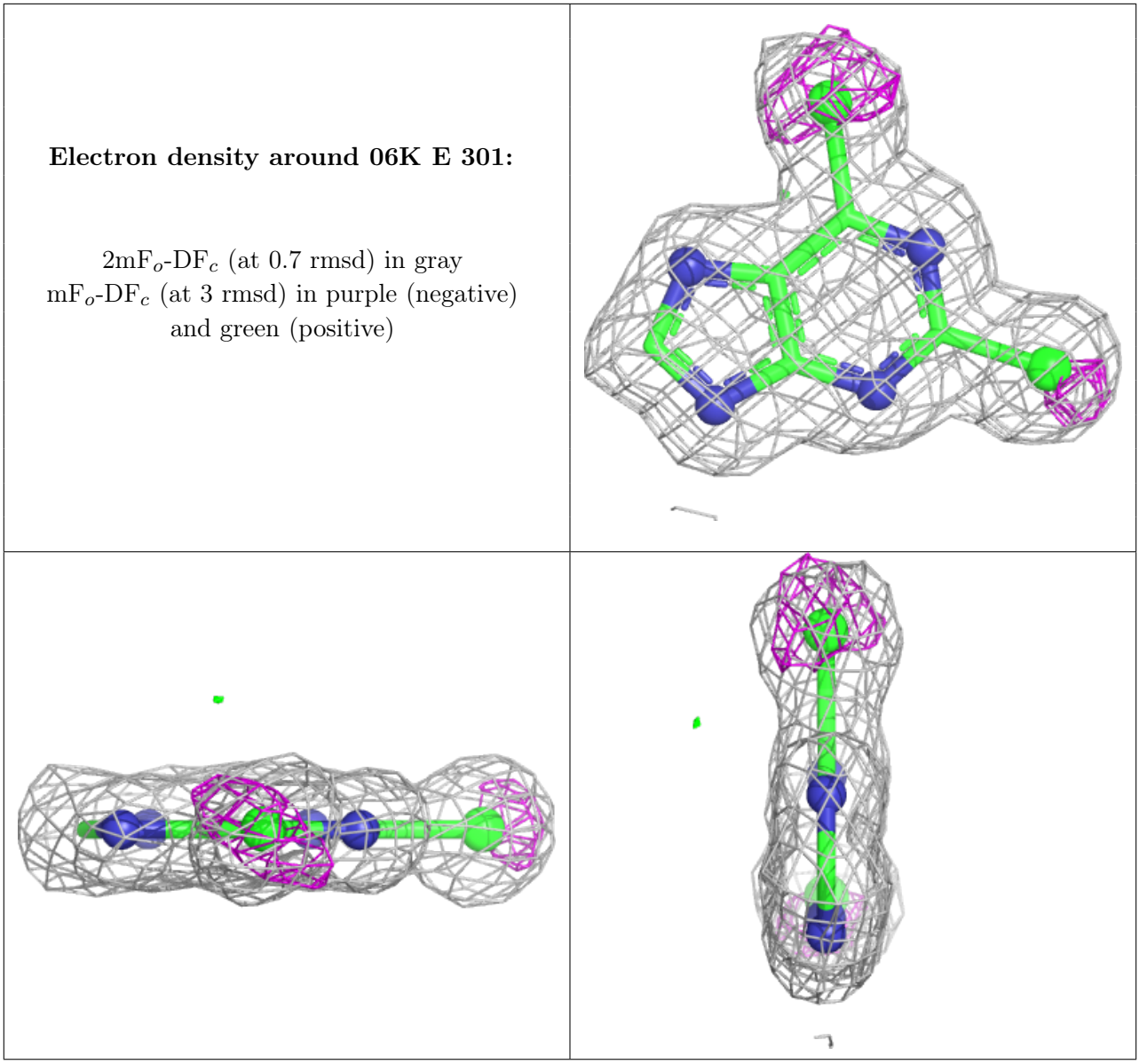






Electron density around 06K E 301:

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



6.5 Other polymers

There are no such residues in this entry.