



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 18, 2025 – 04:51 PM JST

PDB ID : 9LQF / pdb_00009lqf
Title : Crystal structure of SAM lyase in complex with SAH-AMP
Authors : Duan, B.; Zhao, B.
Deposited on : 2025-01-28
Resolution : 1.59 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

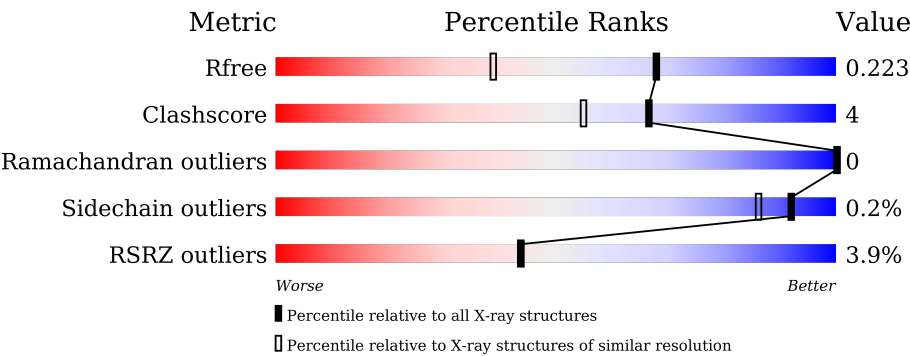
MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

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 1.59 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}	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	125	<div><div>10%</div><div><div></div><div>86%</div><div>11%</div><div>..</div></div></div>
1	B	125	<div><div>2%</div><div><div></div><div>90%</div><div>10%</div></div></div>
1	C	125	<div><div>5%</div><div><div></div><div>88%</div><div>10%</div><div>.</div></div></div>
1	D	125	<div><div>4%</div><div><div></div><div>85%</div><div>13%</div><div>.</div></div></div>
1	E	125	<div><div>2%</div><div><div></div><div>98%</div><div>..</div></div></div>
1	F	125	<div><div>2%</div><div><div></div><div>90%</div><div>9%</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	125	<div><div style="width: 7%;">7%</div><div style="width: 90%;"></div><div style="width: 9%; background-color: #ffff00;">9%</div><div style="width: 4%; background-color: #cccccc;"></div></div>
1	H	125	<div><div style="width: 3%;">3%</div><div style="width: 92%;"></div><div style="width: 6%; background-color: #ffff00;">6%</div><div style="width: 9%; background-color: #cccccc;"></div></div>
1	I	125	<div><div style="width: 1%;">1%</div><div style="width: 90%;"></div><div style="width: 9%; background-color: #ffff00;">9%</div><div style="width: 10%; background-color: #cccccc;"></div></div>
1	J	125	<div><div style="width: 4%;">4%</div><div style="width: 87%;"></div><div style="width: 13%; background-color: #ffff00;">13%</div></div>
1	K	125	<div><div style="width: 2%;">2%</div><div style="width: 92%;"></div><div style="width: 6%; background-color: #ffff00;">6%</div><div style="width: 10%; background-color: #cccccc;"></div></div>
1	L	125	<div><div style="width: 6%;">6%</div><div style="width: 89%;"></div><div style="width: 9%; background-color: #ffff00;">9%</div><div style="width: 5%; background-color: #cccccc;"></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13896 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 SAM lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	0	1	0
			1001	639	160	199	3			
1	D	122	Total	C	N	O	S	0	1	0
			994	635	159	197	3			
1	E	124	Total	C	N	O	S	0	1	0
			1006	642	161	199	4			
1	B	125	Total	C	N	O	S	0	0	0
			1006	642	161	199	4			
1	C	123	Total	C	N	O	S	0	0	0
			992	634	159	196	3			
1	F	123	Total	C	N	O	S	0	1	0
			998	637	160	198	3			
1	G	123	Total	C	N	O	S	0	1	0
			998	637	160	198	3			
1	H	122	Total	C	N	O	S	0	0	0
			988	632	158	195	3			
1	I	123	Total	C	N	O	S	0	0	0
			992	634	159	196	3			
1	J	125	Total	C	N	O	S	0	1	0
			1012	645	162	201	4			
1	K	123	Total	C	N	O	S	0	0	0
			992	634	159	196	3			
1	L	122	Total	C	N	O	S	0	1	0
			997	638	160	196	3			

There are 12 discrepancies between the modelled and reference sequences:

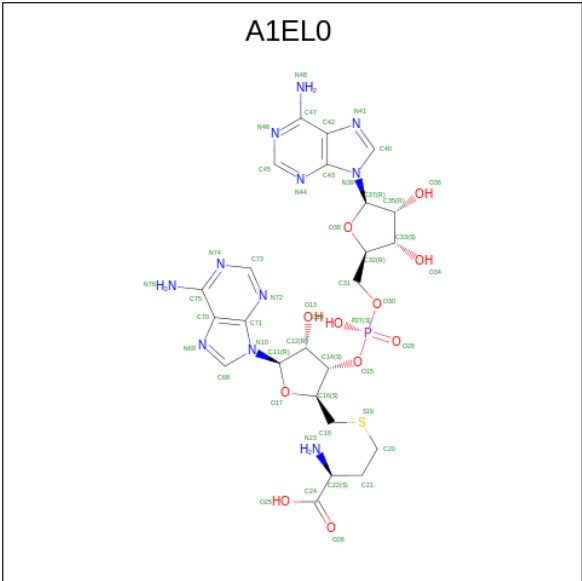
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A5I3U9
D	0	SER	-	expression tag	UNP A5I3U9
E	0	SER	-	expression tag	UNP A5I3U9
B	0	SER	-	expression tag	UNP A5I3U9
C	0	SER	-	expression tag	UNP A5I3U9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	SER	-	expression tag	UNP A5I3U9
G	0	SER	-	expression tag	UNP A5I3U9
H	0	SER	-	expression tag	UNP A5I3U9
I	0	SER	-	expression tag	UNP A5I3U9
J	0	SER	-	expression tag	UNP A5I3U9
K	0	SER	-	expression tag	UNP A5I3U9
L	0	SER	-	expression tag	UNP A5I3U9

- Molecule 2 is (2 {S})-4-(((2 {S}),3 {S}),4 {R}),5 {R})-5-(6-aminopurin-9-yl)-3-(((2 {R}),3 {S}),4 {R}),5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-4-oxidanyl-oxolan-2-yl]methylsulfanyl]-2-azanyl-butanoic acid (CCD ID: A1EL0) (formula: C₂₄H₃₂N₁₁O₁₁PS) (labeled as "Ligand of Interest" by depositor).



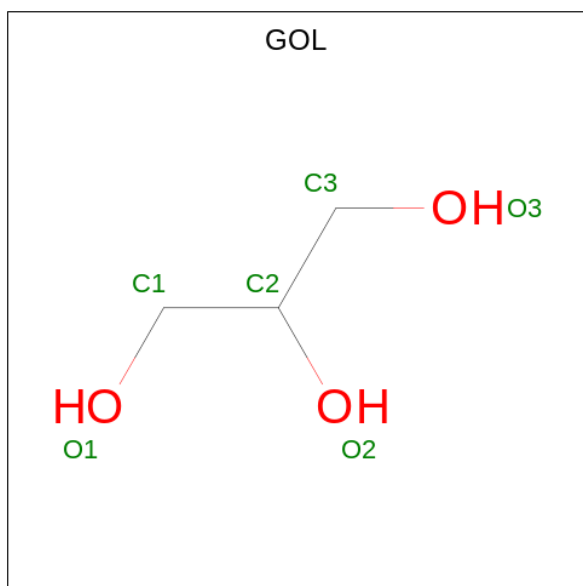
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	24	11	11	1	1		
2	D	1	Total	C	N	O	P	S	0	0
			48	24	11	11	1	1		
2	E	1	Total	C	N	O	P	S	0	0
			48	24	11	11	1	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	24	11	11	1	1		
2	C	1	Total	C	N	O	P	S	0	0
			48	24	11	11	1	1		
2	F	1	Total	C	N	O	P	S	0	0
			48	24	11	11	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	N	O	P	S	
			48	24	11	11	1	1	0
2	H	1	Total	C	N	O	P	S	
			48	24	11	11	1	1	0
2	I	1	Total	C	N	O	P	S	
			48	24	11	11	1	1	0
2	J	1	Total	C	N	O	P	S	
			48	24	11	11	1	1	0
2	K	1	Total	C	N	O	P	S	
			48	24	11	11	1	1	0
2	L	1	Total	C	N	O	P	S	
			48	24	11	11	1	1	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		

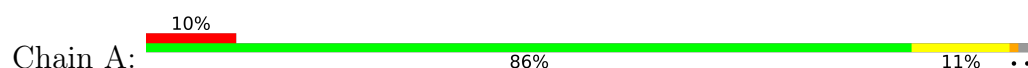
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	88	Total	O	0	0
			88	88		
4	D	105	Total	O	0	0
			105	105		
4	E	112	Total	O	0	0
			112	112		
4	B	129	Total	O	0	0
			129	129		
4	C	114	Total	O	0	0
			114	114		
4	F	131	Total	O	0	0
			131	131		
4	G	91	Total	O	0	0
			91	91		
4	H	86	Total	O	0	0
			86	86		
4	I	109	Total	O	0	0
			109	109		
4	J	111	Total	O	0	0
			111	111		
4	K	100	Total	O	0	0
			100	100		
4	L	114	Total	O	0	0
			114	114		

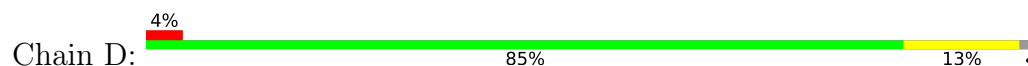
3 Residue-property plots [i](#)

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: SAM lyase



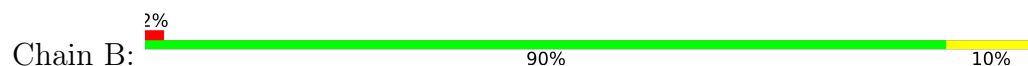
- Molecule 1: SAM lyase



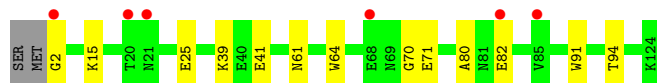
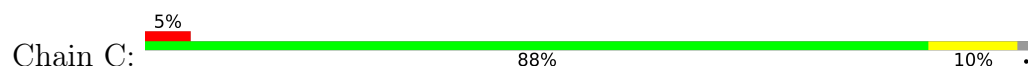
- Molecule 1: SAM lyase



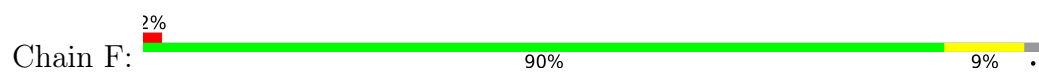
- Molecule 1: SAM lyase



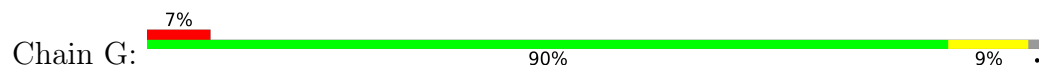
- Molecule 1: SAM lyase



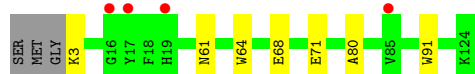
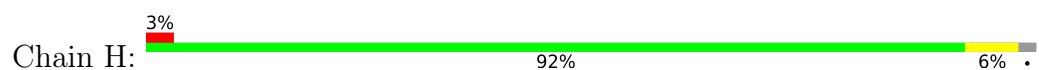
- Molecule 1: SAM lyase



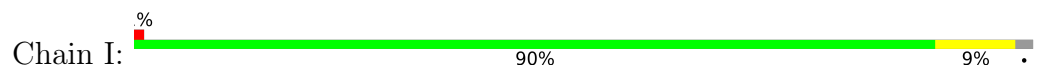
- Molecule 1: SAM lyase



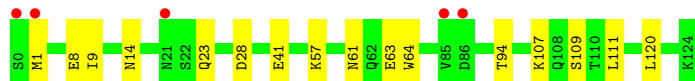
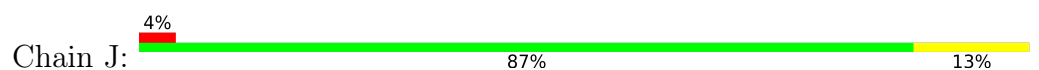
- Molecule 1: SAM lyase



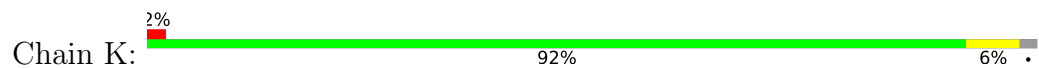
- Molecule 1: SAM lyase



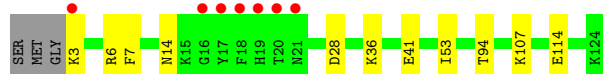
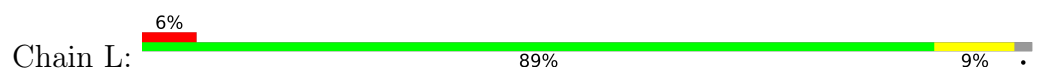
- Molecule 1: SAM lyase



- Molecule 1: SAM lyase



- Molecule 1: SAM lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.94Å 109.93Å 94.22Å 90.00° 111.07° 90.00°	Depositor
Resolution (Å)	45.57 – 1.59 45.57 – 1.59	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.57-1.59) 98.5 (45.57-1.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.59Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, R_{free}	0.186 , 0.223 0.186 , 0.223	Depositor DCC
R_{free} test set	9792 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13896	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7013e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, A1EL0

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	0.29	0/1020	0.48	0/1375
1	B	0.30	0/1025	0.50	0/1381
1	C	0.29	0/1011	0.50	1/1363 (0.1%)
1	D	0.24	0/1013	0.43	0/1366
1	E	0.25	0/1025	0.45	0/1381
1	F	0.29	0/1017	0.46	0/1371
1	G	0.26	0/1017	0.45	0/1371
1	H	0.24	0/1007	0.44	0/1358
1	I	0.25	0/1011	0.48	0/1363
1	J	0.32	0/1031	0.51	0/1389
1	K	0.26	0/1011	0.44	0/1363
1	L	0.25	0/1016	0.44	0/1369
All	All	0.27	0/12204	0.47	1/16450 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	GLY	N-CA-C	5.53	117.20	111.95

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	6	ARG	Sidechain

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	1001	0	982	10	0
1	B	1006	0	994	9	1
1	C	992	0	977	11	0
1	D	994	0	978	12	0
1	E	1006	0	993	1	0
1	F	998	0	981	10	0
1	G	998	0	981	7	0
1	H	988	0	974	5	0
1	I	992	0	977	7	0
1	J	1012	0	998	12	0
1	K	992	0	977	6	0
1	L	997	0	985	9	0
2	A	48	0	0	0	0
2	B	48	0	0	0	0
2	C	48	0	0	2	0
2	D	48	0	0	2	0
2	E	48	0	0	0	0
2	F	48	0	0	1	0
2	G	48	0	0	0	0
2	H	48	0	0	1	0
2	I	48	0	0	0	0
2	J	48	0	0	1	0
2	K	48	0	0	0	0
2	L	48	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
3	G	6	0	8	0	0
3	H	6	0	8	0	0
3	J	6	0	8	0	0
3	K	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	88	0	0	0	0
4	B	129	0	0	3	2
4	C	114	0	0	4	1
4	D	105	0	0	4	3
4	E	112	0	0	0	0
4	F	131	0	0	5	2
4	G	91	0	0	0	1
4	H	86	0	0	2	2
4	I	109	0	0	1	0
4	J	111	0	0	1	0
4	K	100	0	0	1	0
4	L	114	0	0	2	0
All	All	13896	0	11869	89	6

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 4.

All (89) 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:3:LYS:N	4:H:301:HOH:O	2.14	0.80
1:D:46:ASN:OD1	4:D:301:HOH:O	1.99	0.79
1:D:23:GLN:NE2	4:D:302:HOH:O	2.12	0.71
1:F:63:GLU:OE2	4:F:401:HOH:O	2.09	0.69
1:F:2:GLY:N	4:F:405:HOH:O	2.25	0.68
1:J:8:GLU:CD	1:L:6:ARG:HH22	2.01	0.68
1:F:43:GLU:O	4:F:402:HOH:O	2.12	0.67
1:D:93:ASP:O	1:D:97:LYS:HG2	1.95	0.67
1:A:28:ASP:OD1	1:D:57:LYS:NZ	2.26	0.67
1:C:25:GLU:OE1	4:C:301:HOH:O	2.13	0.66
1:K:25:GLU:OE2	4:K:301:HOH:O	2.12	0.66
1:B:23:GLN:NE2	4:B:302:HOH:O	2.22	0.64
1:G:15:LYS:HE3	1:G:21:ASN:HA	1.82	0.61
1:I:83:GLU:OE2	1:I:124:LYS:NZ	2.27	0.60
1:B:62:GLN:NE2	4:B:303:HOH:O	2.22	0.60
1:C:71:GLU:HG2	2:C:201:A1EL0:O26	2.02	0.60
1:K:53:ILE:HG23	1:K:74:VAL:HG13	1.85	0.58
1:G:8:GLU:CD	1:I:6:ARG:HH22	2.10	0.57
2:C:201:A1EL0:S19	2:C:201:A1EL0:N23	2.77	0.56
1:C:39:LYS:NZ	1:F:61:ASN:HD21	2.03	0.56
1:J:1:MET:HA	1:J:120:LEU:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:GLU:OE2	2:D:201:A1EL0:N23	2.42	0.52
1:C:2:GLY:N	4:C:307:HOH:O	2.43	0.52
1:A:15:LYS:HG2	1:A:20:THR:HG23	1.91	0.52
1:D:3:LYS:N	4:D:309:HOH:O	2.44	0.51
1:F:61:ASN:HB3	1:F:64:TRP:CD2	2.46	0.51
1:G:15:LYS:NZ	1:G:20:THR:O	2.34	0.51
1:I:39:LYS:O	1:I:43:GLU:HG3	2.11	0.51
1:H:68:GLU:OE2	4:H:302:HOH:O	2.19	0.50
1:J:61:ASN:HB3	1:J:64:TRP:CD2	2.46	0.50
1:G:100:LYS:HE2	1:I:123:PHE:CE1	2.47	0.50
1:C:39:LYS:HZ3	1:F:61:ASN:HD21	1.58	0.50
1:D:72:GLU:OE2	4:D:303:HOH:O	2.20	0.50
1:L:3[A]:LYS:N	4:L:303:HOH:O	2.44	0.50
1:C:82:GLU:HG2	4:C:387:HOH:O	2.12	0.50
1:C:15:LYS:HZ3	1:C:15:LYS:H	1.60	0.49
1:H:71:GLU:OE2	2:H:201:A1EL0:N23	2.46	0.49
1:B:14:ASN:ND2	1:B:107:LYS:HB2	2.28	0.49
1:K:53:ILE:HG23	1:K:74:VAL:CG1	2.43	0.48
1:A:53:ILE:HG23	1:A:74:VAL:HG13	1.95	0.48
1:D:109[A]:SER:OG	2:D:201:A1EL0:O26	2.25	0.48
1:K:41:GLU:HG2	1:K:94:THR:HG23	1.96	0.48
1:A:14:ASN:ND2	1:A:107:LYS:HB2	2.28	0.48
1:A:15:LYS:HZ2	1:A:20:THR:HG23	1.79	0.48
1:I:2:GLY:N	4:I:307:HOH:O	2.47	0.47
1:K:61:ASN:HB3	1:K:64:TRP:CD2	2.50	0.47
1:C:41:GLU:HG2	1:C:94:THR:HG23	1.98	0.46
1:C:61:ASN:HB3	1:C:64:TRP:CD2	2.51	0.46
1:A:41:GLU:HG2	1:A:94:THR:HG23	1.98	0.46
1:F:57:LYS:HD2	4:F:415:HOH:O	2.15	0.46
1:L:41:GLU:HG2	1:L:94:THR:HG23	1.98	0.46
1:H:61:ASN:HB3	1:H:64:TRP:CD2	2.51	0.45
1:I:7:PHE:HA	1:I:114:GLU:O	2.16	0.45
1:B:57:LYS:NZ	1:F:28:ASP:OD1	2.49	0.45
1:L:14:ASN:ND2	1:L:107:LYS:HB2	2.31	0.45
1:F:80:ALA:HB2	1:F:91:TRP:CD2	2.51	0.45
1:G:30:VAL:HG11	1:G:74:VAL:HG21	1.98	0.45
1:C:71:GLU:OE1	4:C:302:HOH:O	2.21	0.44
1:G:80:ALA:HB2	1:G:91:TRP:CD2	2.51	0.44
1:J:109[B]:SER:OG	2:J:201:A1EL0:O25	2.29	0.44
1:G:61:ASN:HB3	1:G:64:TRP:CD2	2.53	0.44
1:A:14:ASN:HD22	1:A:107:LYS:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ALA:HB2	1:C:91:TRP:CD2	2.53	0.44
1:B:87:ASP:OD1	4:B:301:HOH:O	2.21	0.43
1:H:80:ALA:HB2	1:H:91:TRP:CD2	2.54	0.43
1:J:28:ASP:OD1	1:K:57:LYS:NZ	2.45	0.43
1:D:8:GLU:HG3	1:D:77:THR:HG22	1.99	0.43
1:J:14:ASN:HD22	1:J:107:LYS:HB2	1.84	0.43
1:B:14:ASN:HD22	1:B:107:LYS:HB2	1.84	0.43
1:J:23:GLN:NE2	4:J:305:HOH:O	2.48	0.43
1:D:41:GLU:HG2	1:D:94:THR:HG23	2.00	0.42
1:B:41:GLU:HG2	1:B:94:THR:HG23	2.01	0.42
1:J:57:LYS:O	1:L:53:ILE:HG12	2.19	0.42
1:A:32:GLY:O	1:A:36:LYS:HE2	2.18	0.42
1:I:27:LEU:HD22	1:I:53:ILE:HG13	2.00	0.42
1:B:61:ASN:HB3	1:B:64:TRP:CD2	2.55	0.42
1:J:41:GLU:HG2	1:J:94:THR:HG23	2.02	0.42
1:L:36:LYS:HD3	1:L:36:LYS:HA	1.82	0.42
1:A:61:ASN:HB3	1:A:64:TRP:CD2	2.54	0.42
1:J:9:ILE:HG23	1:J:111:LEU:HD21	2.02	0.41
1:A:80:ALA:HB2	1:A:91:TRP:CD2	2.55	0.41
1:B:61:ASN:HD21	1:F:39:LYS:NZ	2.19	0.41
1:J:57:LYS:NZ	1:L:28:ASP:OD1	2.33	0.41
1:J:61:ASN:OD1	1:J:63:GLU:HG3	2.21	0.41
1:L:107:LYS:NZ	4:L:306:HOH:O	2.47	0.41
1:L:7:PHE:HA	1:L:114:GLU:O	2.21	0.41
1:D:36:LYS:HE2	1:D:36:LYS:HB3	1.95	0.41
1:D:53:ILE:HG12	1:E:57:LYS:O	2.21	0.40
2:F:302:A1EL0:O34	4:F:403:HOH:O	2.22	0.40

All (6) 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)
4:F:402:HOH:O	4:H:306:HOH:O[2_444]	1.91	0.29
4:D:301:HOH:O	4:B:391:HOH:O[2_444]	2.00	0.20
4:C:316:HOH:O	4:G:302:HOH:O[2_443]	2.00	0.20
4:F:402:HOH:O	4:H:325:HOH:O[2_444]	2.07	0.13
4:D:301:HOH:O	4:B:339:HOH:O[2_444]	2.09	0.11
1:B:43:GLU:O	4:D:301:HOH:O[2_454]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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	122/125 (98%)	119 (98%)	3 (2%)	0	100	100
1	B	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
1	C	121/125 (97%)	119 (98%)	2 (2%)	0	100	100
1	D	121/125 (97%)	120 (99%)	1 (1%)	0	100	100
1	E	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	F	122/125 (98%)	121 (99%)	1 (1%)	0	100	100
1	G	122/125 (98%)	120 (98%)	2 (2%)	0	100	100
1	H	120/125 (96%)	119 (99%)	1 (1%)	0	100	100
1	I	121/125 (97%)	119 (98%)	2 (2%)	0	100	100
1	J	124/125 (99%)	123 (99%)	1 (1%)	0	100	100
1	K	121/125 (97%)	118 (98%)	3 (2%)	0	100	100
1	L	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
All	All	1460/1500 (97%)	1439 (99%)	21 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	112/113 (99%)	111 (99%)	1 (1%)	75	62
1	B	113/113 (100%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	111/113 (98%)	111 (100%)	0	100	100
1	D	112/113 (99%)	111 (99%)	1 (1%)	75	62
1	E	113/113 (100%)	113 (100%)	0	100	100
1	F	112/113 (99%)	111 (99%)	1 (1%)	75	62
1	G	112/113 (99%)	112 (100%)	0	100	100
1	H	111/113 (98%)	111 (100%)	0	100	100
1	I	111/113 (98%)	111 (100%)	0	100	100
1	J	114/113 (101%)	114 (100%)	0	100	100
1	K	111/113 (98%)	111 (100%)	0	100	100
1	L	112/113 (99%)	112 (100%)	0	100	100
All	All	1344/1356 (99%)	1341 (100%)	3 (0%)	92	86

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

Mol	Chain	Res	Type
1	A	74	VAL
1	D	107	LYS
1	F	54	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	23	GLN
1	A	62	GLN
1	D	14	ASN
1	D	62	GLN
1	E	23	GLN
1	E	104	ASN
1	B	14	ASN
1	B	19	HIS
1	C	14	ASN
1	C	19	HIS
1	C	46	ASN
1	F	62	GLN
1	G	19	HIS
1	H	14	ASN

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Mol	Chain	Res	Type
1	J	14	ASN
1	J	23	GLN
1	K	14	ASN
1	K	19	HIS
1	K	62	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

21 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$
2	A1EL0	H	201	-	46,53,53	1.16	5 (10%)	50,79,79	1.34	6 (12%)
2	A1EL0	C	201	-	46,53,53	1.14	4 (8%)	50,79,79	1.49	9 (18%)
2	A1EL0	D	201	-	46,53,53	1.18	5 (10%)	50,79,79	1.25	4 (8%)
3	GOL	J	202	-	5,5,5	0.32	0	5,5,5	0.29	0
2	A1EL0	E	201	-	46,53,53	1.10	3 (6%)	50,79,79	1.34	6 (12%)
3	GOL	K	202	-	5,5,5	0.25	0	5,5,5	0.37	0
2	A1EL0	J	201	-	46,53,53	1.17	5 (10%)	50,79,79	1.24	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1EL0	F	302	-	46,53,53	1.23	5 (10%)	50,79,79	1.36	5 (10%)
3	GOL	G	202	-	5,5,5	0.33	0	5,5,5	0.57	0
2	A1EL0	B	201	-	46,53,53	1.23	5 (10%)	50,79,79	1.40	9 (18%)
3	GOL	H	202	-	5,5,5	0.28	0	5,5,5	0.66	0
2	A1EL0	L	201	-	46,53,53	1.20	5 (10%)	50,79,79	1.33	6 (12%)
3	GOL	C	202	-	5,5,5	0.38	0	5,5,5	0.43	0
3	GOL	B	202	-	5,5,5	0.38	0	5,5,5	0.42	0
2	A1EL0	I	201	-	46,53,53	1.20	5 (10%)	50,79,79	1.30	7 (14%)
3	GOL	A	202	-	5,5,5	0.32	0	5,5,5	0.19	0
2	A1EL0	K	201	-	46,53,53	1.17	4 (8%)	50,79,79	1.27	7 (14%)
2	A1EL0	A	201	-	46,53,53	1.20	4 (8%)	50,79,79	1.29	5 (10%)
2	A1EL0	G	201	-	46,53,53	1.22	5 (10%)	50,79,79	1.33	8 (16%)
3	GOL	F	301	-	5,5,5	0.25	0	5,5,5	0.49	0
3	GOL	E	202	-	5,5,5	0.28	0	5,5,5	0.34	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	A1EL0	H	201	-	-	0/22/62/62	0/6/6/6
2	A1EL0	C	201	-	-	6/22/62/62	0/6/6/6
2	A1EL0	D	201	-	-	0/22/62/62	0/6/6/6
3	GOL	J	202	-	-	2/4/4/4	-
2	A1EL0	E	201	-	-	1/22/62/62	0/6/6/6
3	GOL	K	202	-	-	0/4/4/4	-
2	A1EL0	J	201	-	-	4/22/62/62	0/6/6/6
2	A1EL0	F	302	-	-	2/22/62/62	0/6/6/6
3	GOL	G	202	-	-	1/4/4/4	-
2	A1EL0	B	201	-	-	0/22/62/62	0/6/6/6
3	GOL	H	202	-	-	0/4/4/4	-
2	A1EL0	L	201	-	-	0/22/62/62	0/6/6/6
3	GOL	C	202	-	-	1/4/4/4	-
3	GOL	B	202	-	-	0/4/4/4	-
2	A1EL0	I	201	-	-	1/22/62/62	0/6/6/6
3	GOL	A	202	-	-	1/4/4/4	-
2	A1EL0	K	201	-	-	1/22/62/62	0/6/6/6
2	A1EL0	A	201	-	-	1/22/62/62	0/6/6/6
2	A1EL0	G	201	-	-	0/22/62/62	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	F	301	-	-	0/4/4/4	-
3	GOL	E	202	-	-	0/4/4/4	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	302	A1EL0	O26-C24	4.17	1.34	1.22
2	B	201	A1EL0	O26-C24	4.15	1.34	1.22
2	G	201	A1EL0	O26-C24	3.90	1.34	1.22
2	J	201	A1EL0	O26-C24	3.87	1.33	1.22
2	H	201	A1EL0	O26-C24	3.86	1.33	1.22
2	I	201	A1EL0	O26-C24	3.86	1.33	1.22
2	A	201	A1EL0	O26-C24	3.82	1.33	1.22
2	L	201	A1EL0	O26-C24	3.79	1.33	1.22
2	K	201	A1EL0	O26-C24	3.71	1.33	1.22
2	C	201	A1EL0	O26-C24	3.62	1.33	1.22
2	E	201	A1EL0	O26-C24	3.61	1.33	1.22
2	D	201	A1EL0	O26-C24	3.58	1.33	1.22
2	I	201	A1EL0	C70-C71	2.73	1.48	1.40
2	G	201	A1EL0	C42-C43	2.63	1.47	1.40
2	L	201	A1EL0	O25-C24	-2.59	1.22	1.30
2	B	201	A1EL0	C70-C71	2.56	1.47	1.40
2	C	201	A1EL0	O25-C24	-2.56	1.22	1.30
2	K	201	A1EL0	C42-C43	2.54	1.47	1.40
2	F	302	A1EL0	O17-C11	2.52	1.44	1.41
2	A	201	A1EL0	C42-C43	2.52	1.47	1.40
2	J	201	A1EL0	C42-C43	2.48	1.47	1.40
2	L	201	A1EL0	C42-C43	2.47	1.47	1.40
2	I	201	A1EL0	C42-C43	2.46	1.47	1.40
2	C	201	A1EL0	C42-C43	2.43	1.47	1.40
2	A	201	A1EL0	O25-C24	-2.43	1.22	1.30
2	K	201	A1EL0	O25-C24	-2.43	1.22	1.30
2	I	201	A1EL0	O25-C24	-2.41	1.22	1.30
2	H	201	A1EL0	C42-C43	2.39	1.47	1.40
2	B	201	A1EL0	C73-N72	2.38	1.35	1.32
2	J	201	A1EL0	O25-C24	-2.38	1.22	1.30
2	D	201	A1EL0	C70-C71	2.37	1.47	1.40
2	C	201	A1EL0	C70-C71	2.35	1.47	1.40
2	D	201	A1EL0	O25-C24	-2.35	1.22	1.30
2	F	302	A1EL0	C42-C43	2.34	1.47	1.40
2	B	201	A1EL0	C42-C43	2.33	1.47	1.40
2	G	201	A1EL0	C70-C71	2.31	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	201	A1EL0	O25-C24	-2.30	1.23	1.30
2	B	201	A1EL0	O25-C24	-2.29	1.23	1.30
2	F	302	A1EL0	O25-C24	-2.29	1.23	1.30
2	K	201	A1EL0	C70-C71	2.29	1.47	1.40
2	D	201	A1EL0	C42-C43	2.26	1.46	1.40
2	J	201	A1EL0	C70-C71	2.25	1.46	1.40
2	F	302	A1EL0	C70-C71	2.25	1.46	1.40
2	H	201	A1EL0	C70-C71	2.24	1.46	1.40
2	D	201	A1EL0	O17-C11	2.24	1.44	1.41
2	L	201	A1EL0	C70-C71	2.23	1.46	1.40
2	A	201	A1EL0	C70-C71	2.22	1.46	1.40
2	H	201	A1EL0	O25-C24	-2.20	1.23	1.30
2	H	201	A1EL0	C73-N72	2.19	1.35	1.32
2	E	201	A1EL0	O25-C24	-2.18	1.23	1.30
2	E	201	A1EL0	C42-C43	2.09	1.46	1.40
2	L	201	A1EL0	C73-N72	2.04	1.35	1.32
2	I	201	A1EL0	C73-N72	2.02	1.35	1.32
2	G	201	A1EL0	O17-C11	2.01	1.43	1.41
2	J	201	A1EL0	C45-N44	2.01	1.35	1.32

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	201	A1EL0	N72-C73-N74	-3.82	122.71	128.68
2	D	201	A1EL0	N72-C73-N74	-3.62	123.02	128.68
2	F	302	A1EL0	N44-C45-N46	-3.61	123.04	128.68
2	E	201	A1EL0	N72-C73-N74	-3.60	123.05	128.68
2	J	201	A1EL0	N44-C45-N46	-3.58	123.08	128.68
2	H	201	A1EL0	N72-C73-N74	-3.53	123.15	128.68
2	C	201	A1EL0	C18-S19-C20	-3.50	91.76	102.27
2	A	201	A1EL0	N72-C73-N74	-3.47	123.26	128.68
2	C	201	A1EL0	O17-C16-C18	3.41	117.61	108.83
2	F	302	A1EL0	N72-C73-N74	-3.38	123.40	128.68
2	H	201	A1EL0	N44-C45-N46	-3.36	123.43	128.68
2	G	201	A1EL0	N72-C73-N74	-3.35	123.44	128.68
2	B	201	A1EL0	N44-C45-N46	-3.33	123.48	128.68
2	B	201	A1EL0	C18-S19-C20	3.28	112.12	102.27
2	J	201	A1EL0	N72-C73-N74	-3.27	123.57	128.68
2	B	201	A1EL0	N72-C73-N74	-3.23	123.62	128.68
2	I	201	A1EL0	N44-C45-N46	-3.22	123.65	128.68
2	C	201	A1EL0	C18-C16-C14	-3.20	107.16	115.02
2	E	201	A1EL0	N44-C45-N46	-3.19	123.69	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	201	A1EL0	N44-C45-N46	-3.09	123.85	128.68
2	D	201	A1EL0	N44-C45-N46	-3.08	123.86	128.68
2	K	201	A1EL0	N72-C73-N74	-3.06	123.90	128.68
2	K	201	A1EL0	N44-C45-N46	-3.01	123.97	128.68
2	A	201	A1EL0	C43-C42-N41	-2.96	106.31	109.40
2	C	201	A1EL0	N44-C45-N46	-2.96	124.06	128.68
2	A	201	A1EL0	N44-C45-N46	-2.95	124.06	128.68
2	I	201	A1EL0	N72-C73-N74	-2.87	124.19	128.68
2	E	201	A1EL0	O25-C24-C22	2.83	123.03	113.38
2	B	201	A1EL0	C12-C14-C16	2.79	108.18	103.22
2	A	201	A1EL0	C18-S19-C20	2.73	110.45	102.27
2	G	201	A1EL0	N44-C45-N46	-2.71	124.45	128.68
2	L	201	A1EL0	N76-C75-N74	2.65	124.07	118.57
2	G	201	A1EL0	C18-S19-C20	2.59	110.04	102.27
2	C	201	A1EL0	N72-C73-N74	-2.56	124.68	128.68
2	L	201	A1EL0	O25-C24-O26	-2.55	118.29	124.09
2	C	201	A1EL0	O25-C24-O26	-2.55	118.31	124.09
2	C	201	A1EL0	C43-C42-N41	-2.54	106.76	109.40
2	K	201	A1EL0	C71-C70-N69	-2.49	106.80	109.40
2	F	302	A1EL0	C18-S19-C20	2.43	109.56	102.27
2	I	201	A1EL0	C43-C42-N41	-2.42	106.88	109.40
2	B	201	A1EL0	N76-C75-N74	2.41	123.57	118.57
2	E	201	A1EL0	O25-C24-O26	-2.40	118.65	124.09
2	D	201	A1EL0	C43-C42-N41	-2.39	106.91	109.40
2	K	201	A1EL0	O25-C24-C22	2.39	121.52	113.38
2	F	302	A1EL0	C45-N46-C47	2.36	122.78	118.75
2	J	201	A1EL0	N76-C75-N74	2.33	123.41	118.57
2	C	201	A1EL0	C45-N46-C47	2.31	122.71	118.75
2	D	201	A1EL0	O25-C24-C22	2.30	121.22	113.38
2	J	201	A1EL0	N48-C47-N46	2.30	123.35	118.57
2	K	201	A1EL0	O25-C24-O26	-2.28	118.91	124.09
2	B	201	A1EL0	C16-C18-S19	-2.28	105.60	113.78
2	G	201	A1EL0	C71-C70-N69	-2.27	107.03	109.40
2	A	201	A1EL0	O25-C24-O26	-2.25	118.97	124.09
2	I	201	A1EL0	C71-C70-N69	-2.24	107.06	109.40
2	I	201	A1EL0	O25-C24-O26	-2.22	119.04	124.09
2	G	201	A1EL0	C43-C42-N41	-2.22	107.09	109.40
2	F	302	A1EL0	N48-C47-N46	2.22	123.17	118.57
2	K	201	A1EL0	C43-C42-N41	-2.21	107.09	109.40
2	J	201	A1EL0	C45-N46-C47	2.20	122.52	118.75
2	H	201	A1EL0	C45-N46-C47	2.19	122.50	118.75
2	K	201	A1EL0	C45-N46-C47	2.19	122.50	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	201	A1EL0	C21-C20-S19	-2.18	108.42	113.31
2	B	201	A1EL0	C43-C42-N41	-2.15	107.16	109.40
2	C	201	A1EL0	O25-C24-C22	2.14	120.67	113.38
2	J	201	A1EL0	C73-N74-C75	2.10	122.35	118.75
2	H	201	A1EL0	C18-S19-C20	2.09	108.55	102.27
2	H	201	A1EL0	O25-C24-C22	2.09	120.51	113.38
2	G	201	A1EL0	N48-C47-N46	2.09	122.92	118.57
2	H	201	A1EL0	N76-C75-N74	2.09	122.91	118.57
2	B	201	A1EL0	N48-C47-N46	2.09	122.90	118.57
2	G	201	A1EL0	O25-C24-C22	2.08	120.46	113.38
2	J	201	A1EL0	O25-C24-C22	2.06	120.41	113.38
2	I	201	A1EL0	C73-N74-C75	2.05	122.27	118.75
2	L	201	A1EL0	C73-N74-C75	2.04	122.24	118.75
2	B	201	A1EL0	O25-C24-O26	-2.03	119.47	124.09
2	E	201	A1EL0	C45-N46-C47	2.02	122.21	118.75
2	E	201	A1EL0	C73-N74-C75	2.01	122.20	118.75
2	G	201	A1EL0	C73-N74-C75	2.01	122.19	118.75
2	L	201	A1EL0	C43-C42-N41	-2.01	107.31	109.40

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201	A1EL0	C20-C21-C22-C24
2	C	201	A1EL0	O17-C16-C18-S19
2	J	201	A1EL0	C31-O30-P27-O29
3	C	202	GOL	O1-C1-C2-C3
3	G	202	GOL	O1-C1-C2-C3
3	J	202	GOL	O1-C1-C2-C3
2	F	302	A1EL0	O30-C31-C32-C33
2	C	201	A1EL0	C20-C21-C22-N23
2	C	201	A1EL0	C21-C22-C24-O25
2	I	201	A1EL0	C31-O30-P27-O28
2	J	201	A1EL0	C31-O30-P27-O28
2	J	201	A1EL0	C21-C20-S19-C18
2	C	201	A1EL0	C21-C22-C24-O26
2	F	302	A1EL0	O30-C31-C32-O38
2	J	201	A1EL0	C31-O30-P27-O15
3	A	202	GOL	O1-C1-C2-O2
2	E	201	A1EL0	N23-C22-C24-O26
3	J	202	GOL	O1-C1-C2-O2
2	A	201	A1EL0	C31-O30-P27-O28

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Mol	Chain	Res	Type	Atoms
2	C	201	A1EL0	C31-O30-P27-O28
2	K	201	A1EL0	C31-O30-P27-O28

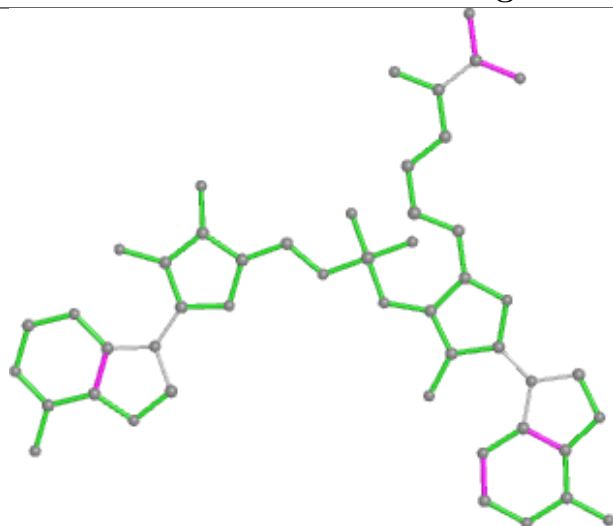
There are no ring outliers.

5 monomers are involved in 7 short contacts:

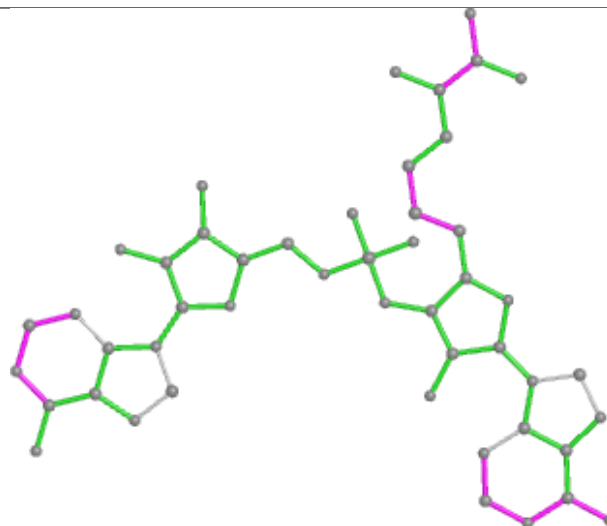
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	201	A1EL0	1	0
2	C	201	A1EL0	2	0
2	D	201	A1EL0	2	0
2	J	201	A1EL0	1	0
2	F	302	A1EL0	1	0

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

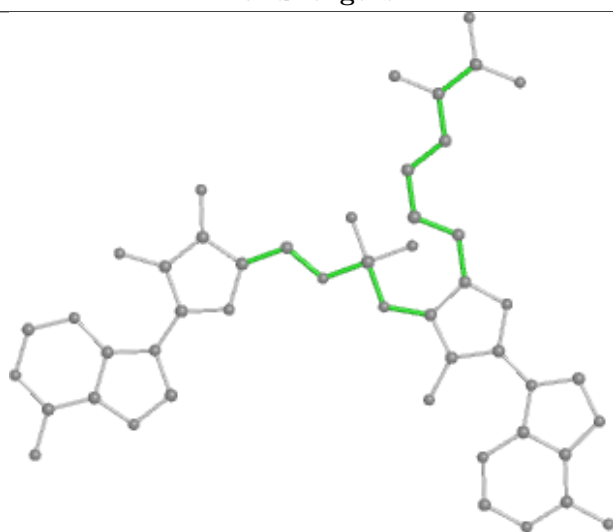
Ligand A1EL0 H 201



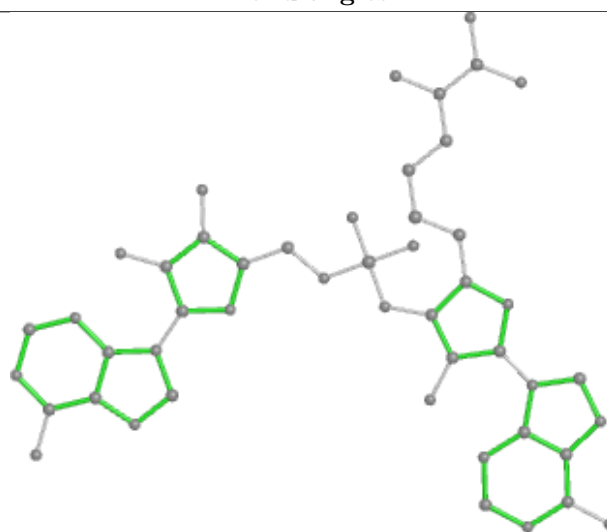
Bond lengths



Bond angles

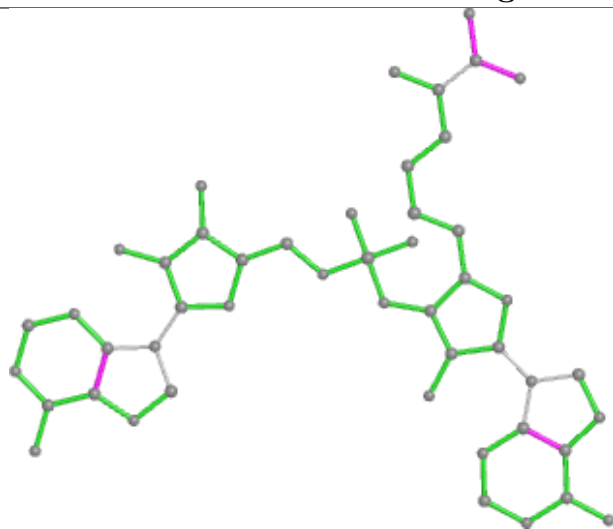


Torsions

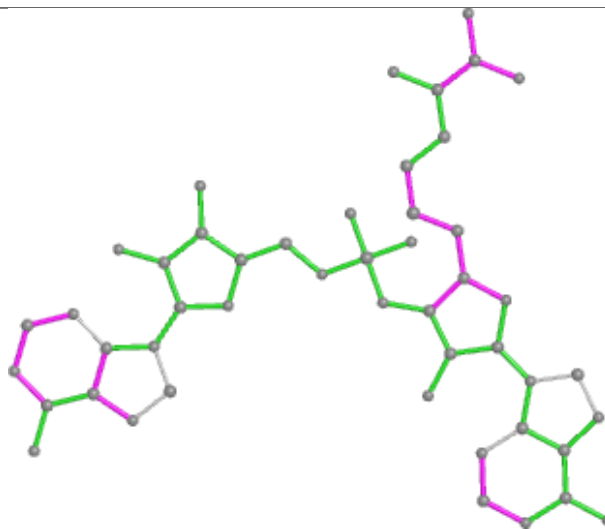


Rings

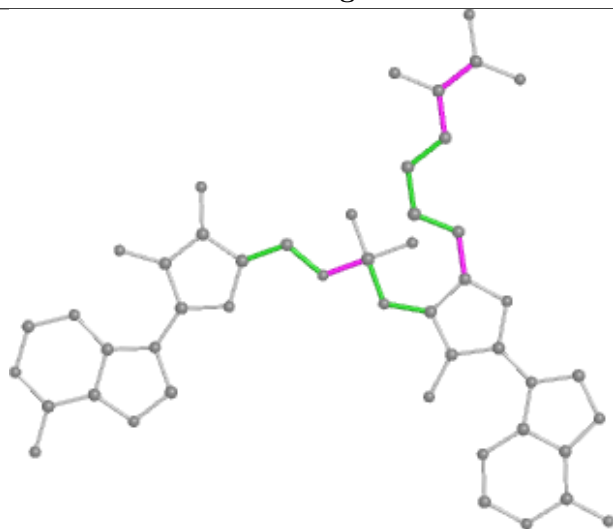
Ligand A1EL0 C 201



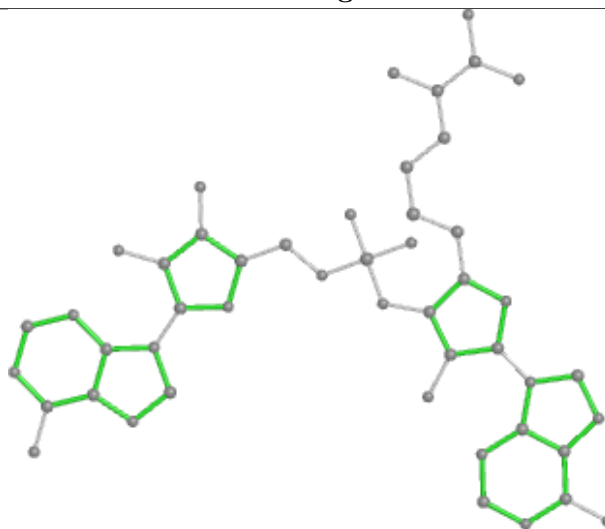
Bond lengths



Bond angles

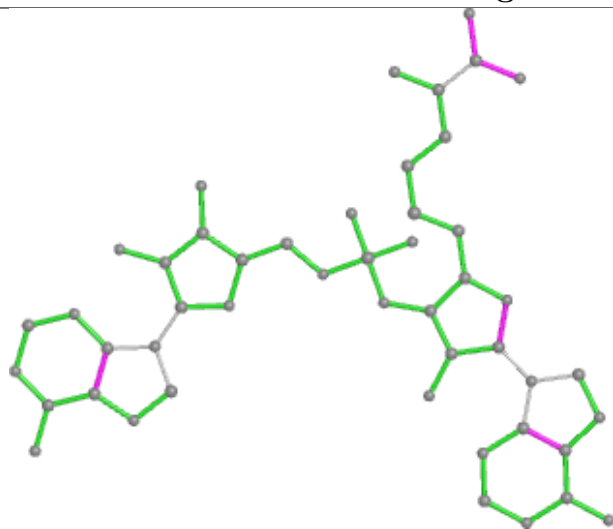


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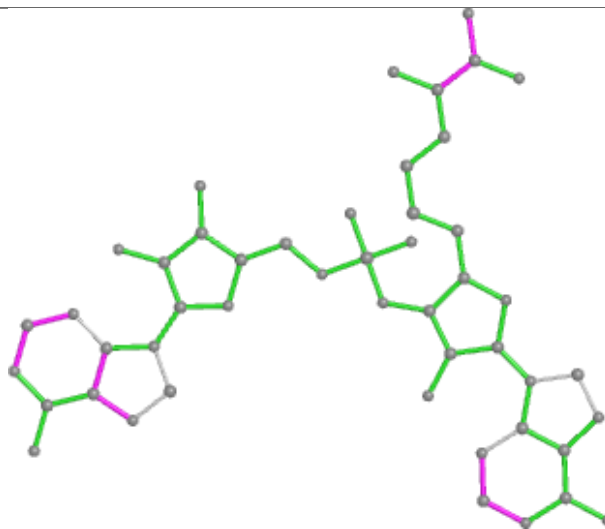


Rings

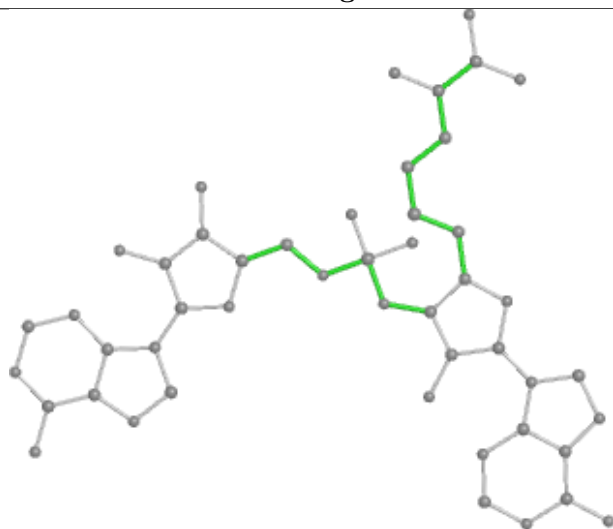
Ligand A1EL0 D 201



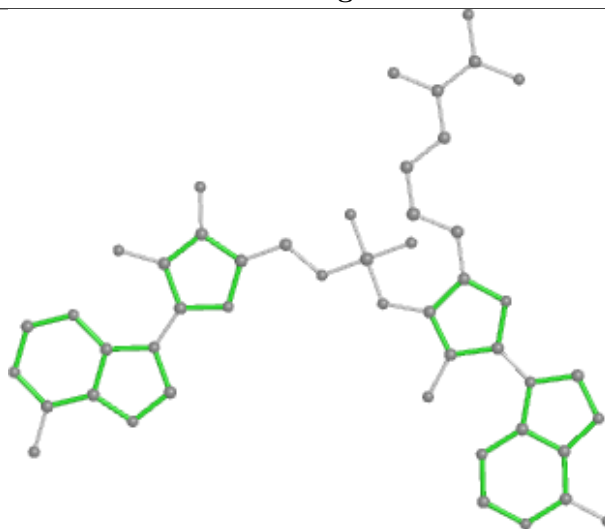
Bond lengths



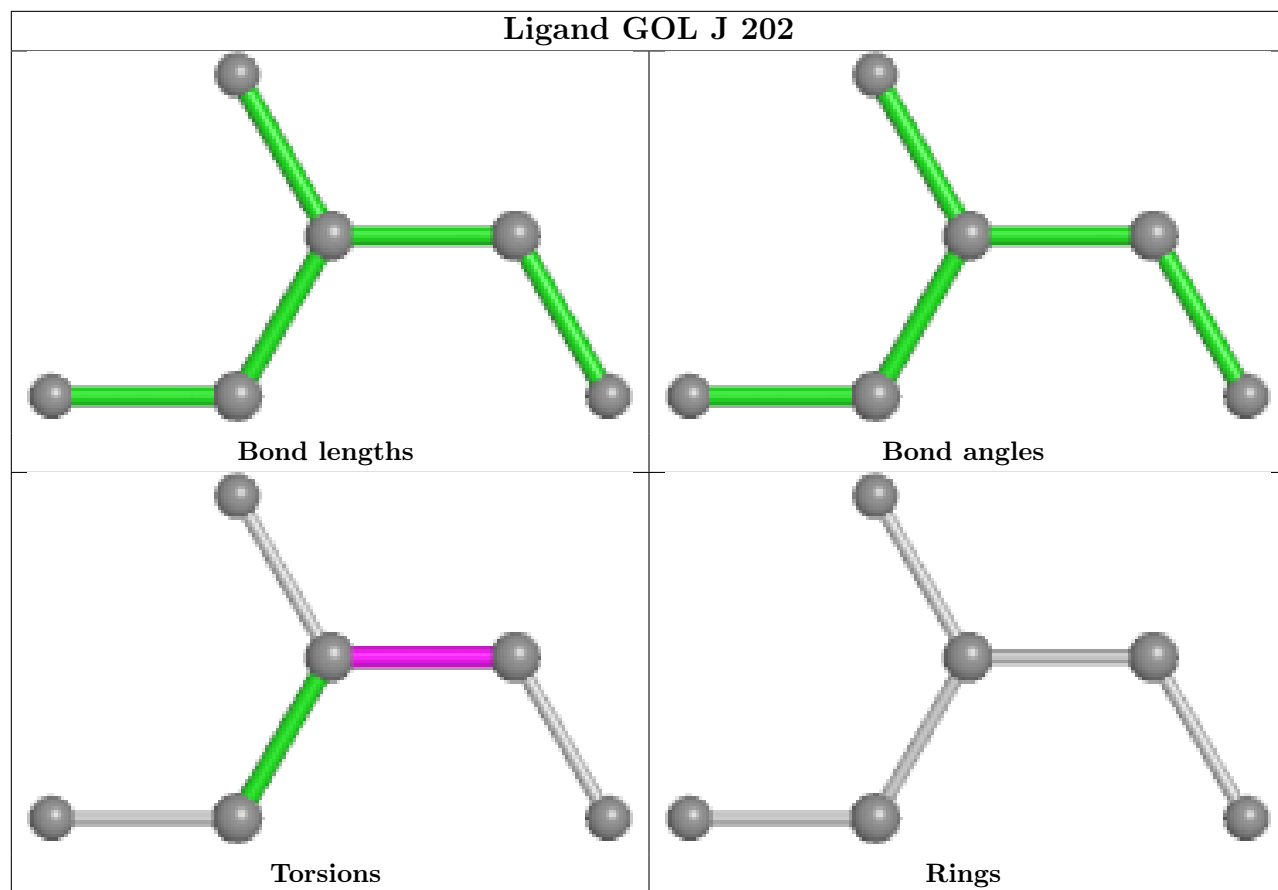
Bond angles



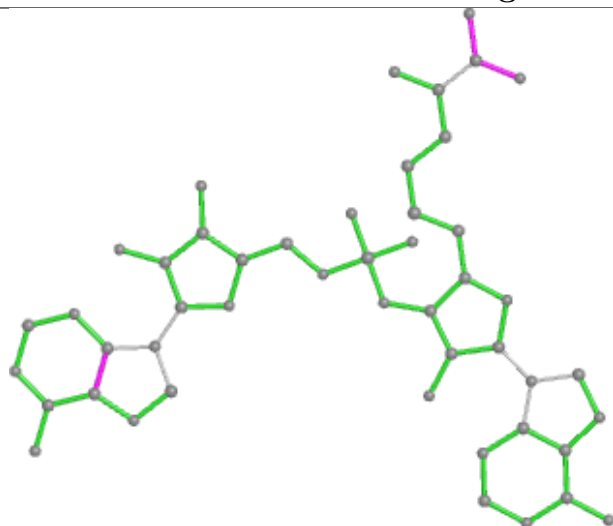
Torsions



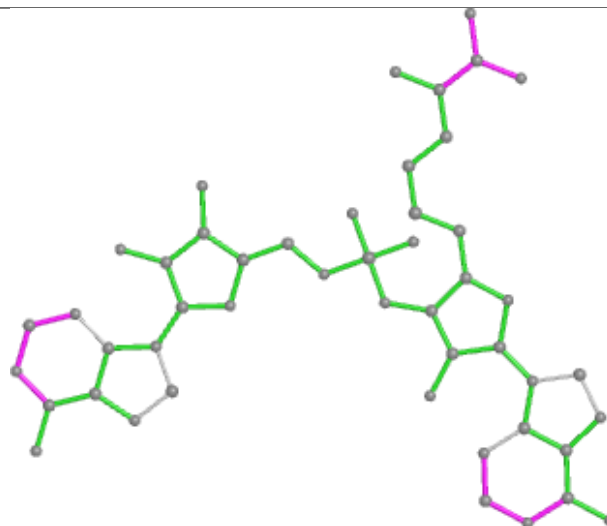
Rings



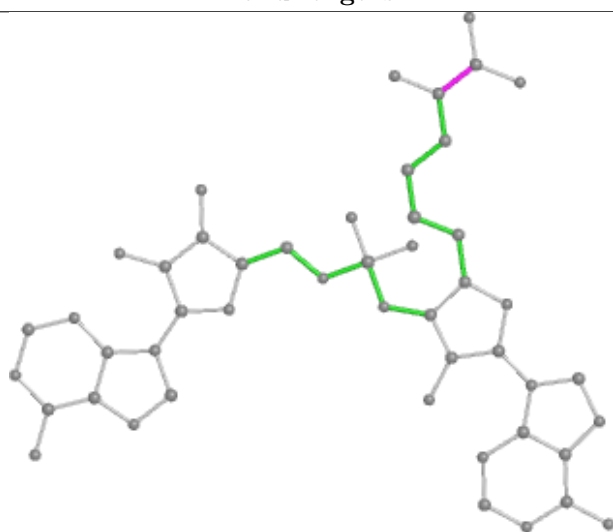
Ligand A1EL0 E 201



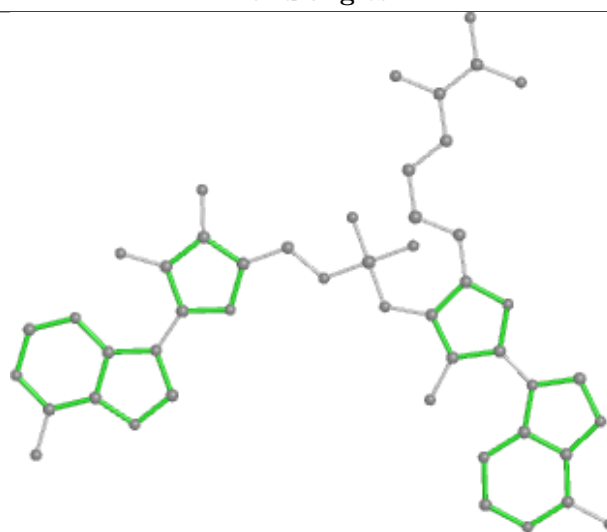
Bond lengths



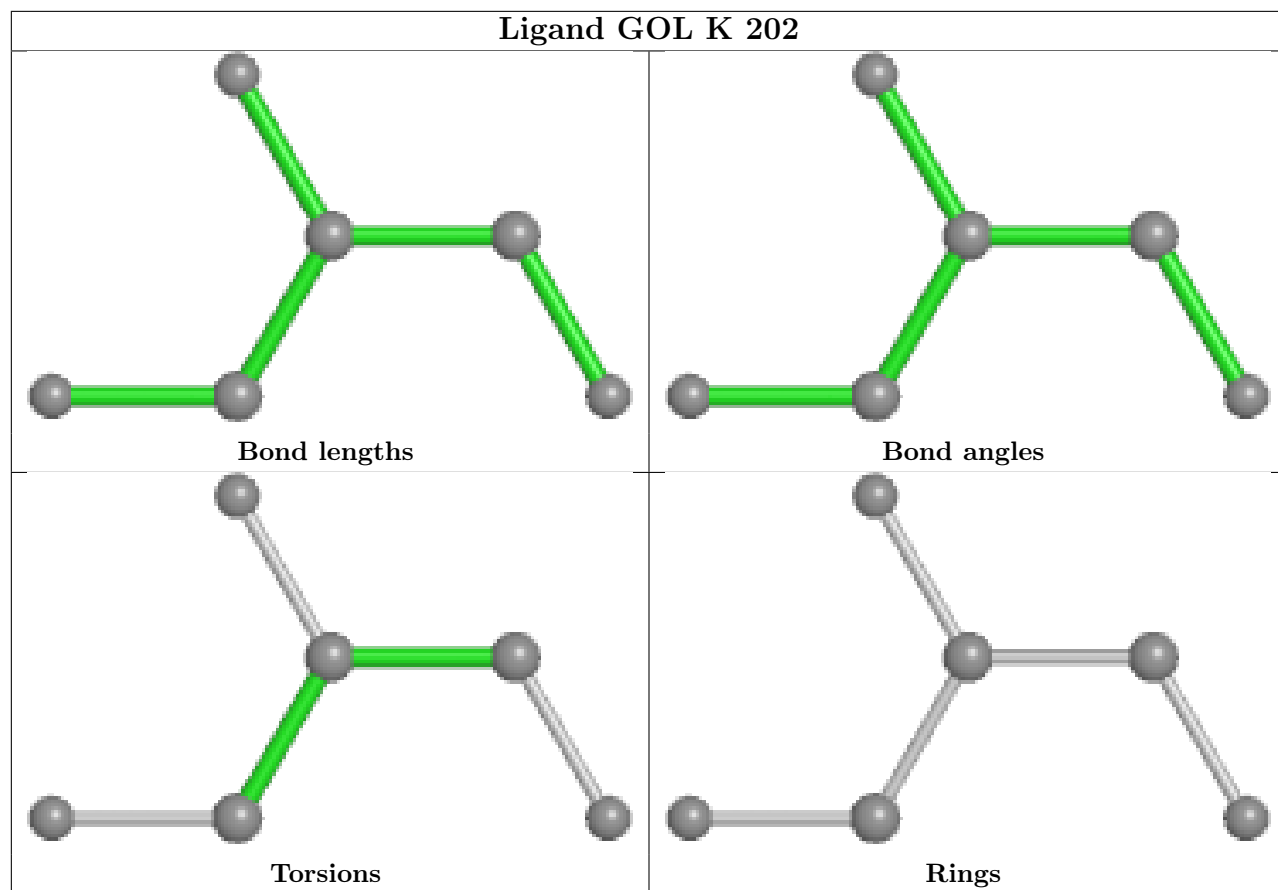
Bond angles



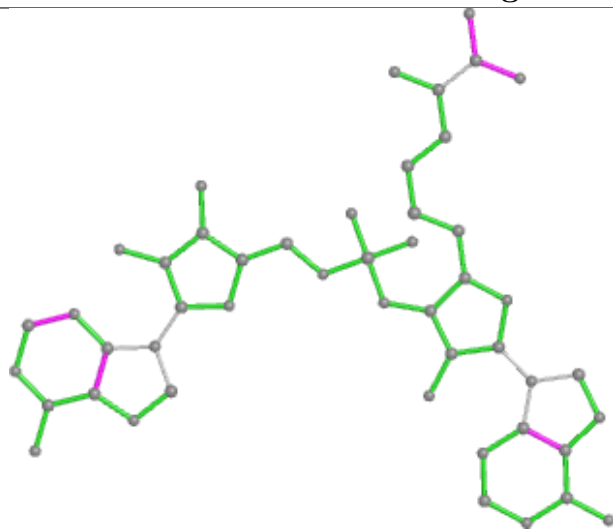
Torsions



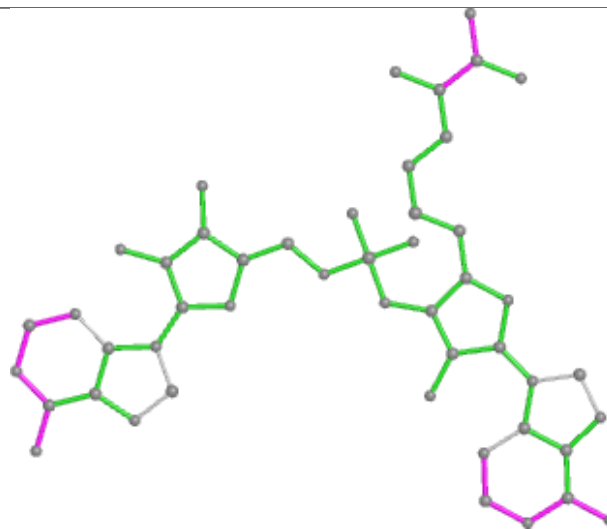
Rings



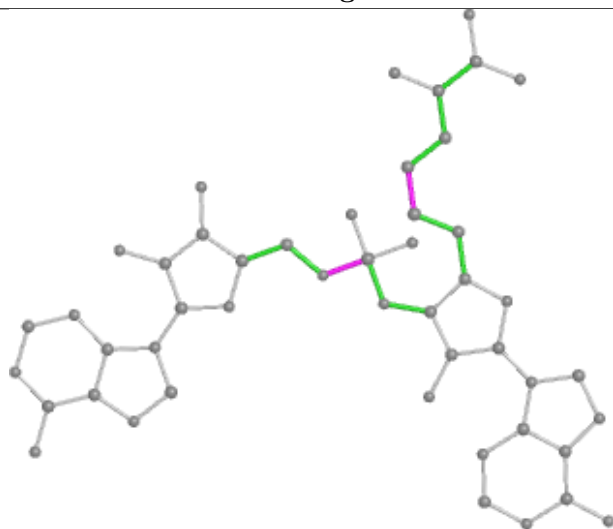
Ligand A1EL0 J 201



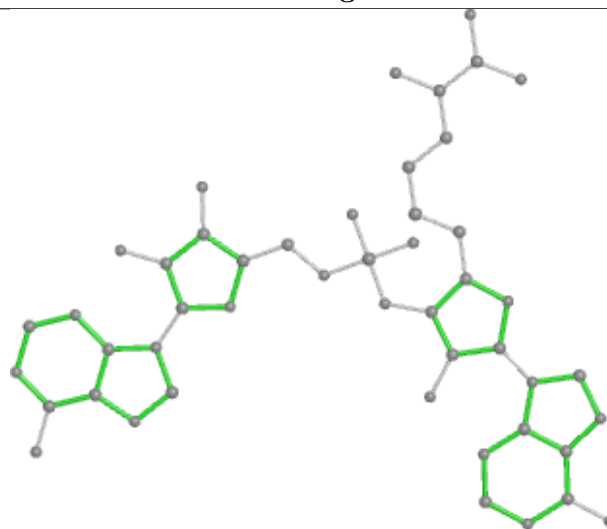
Bond lengths



Bond angles

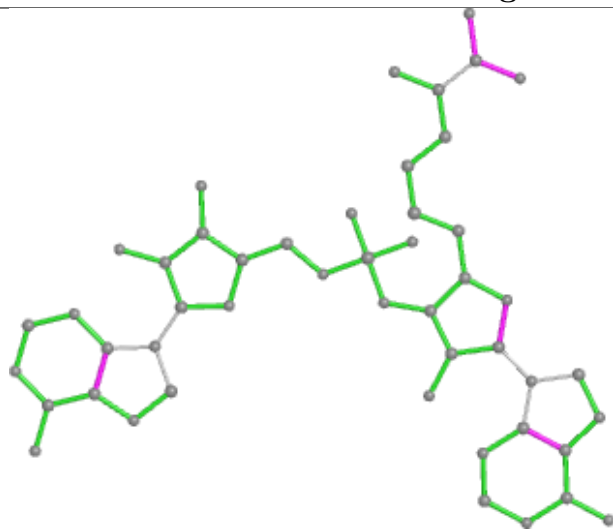


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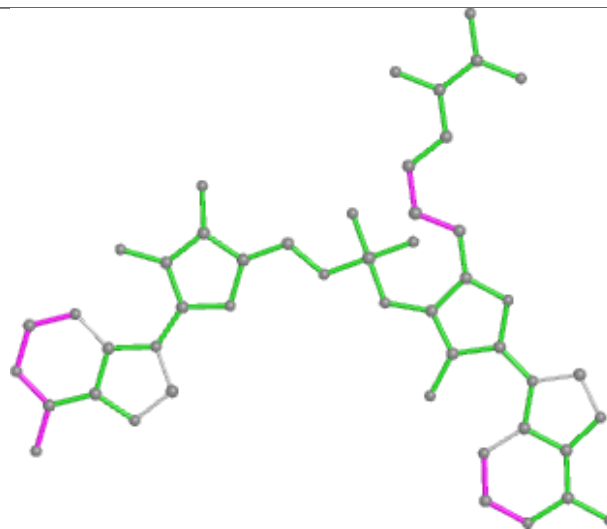


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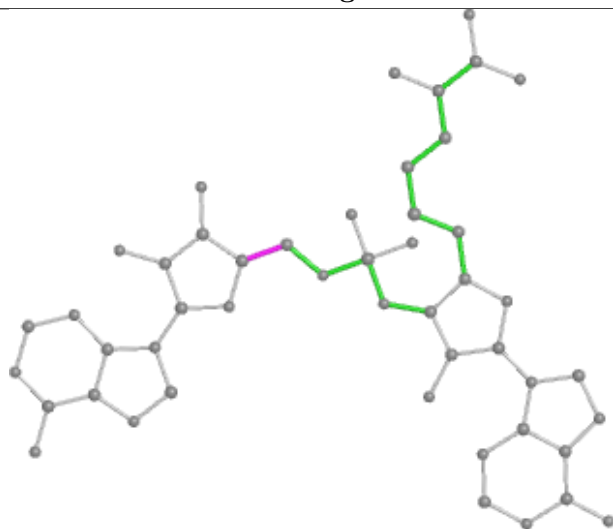
Ligand A1EL0 F 302



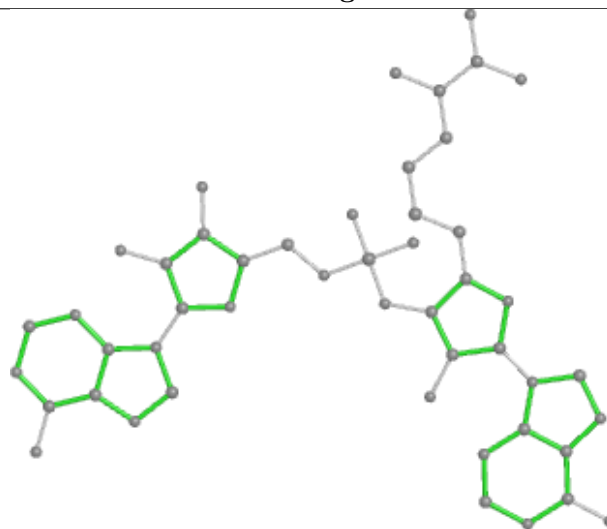
Bond lengths



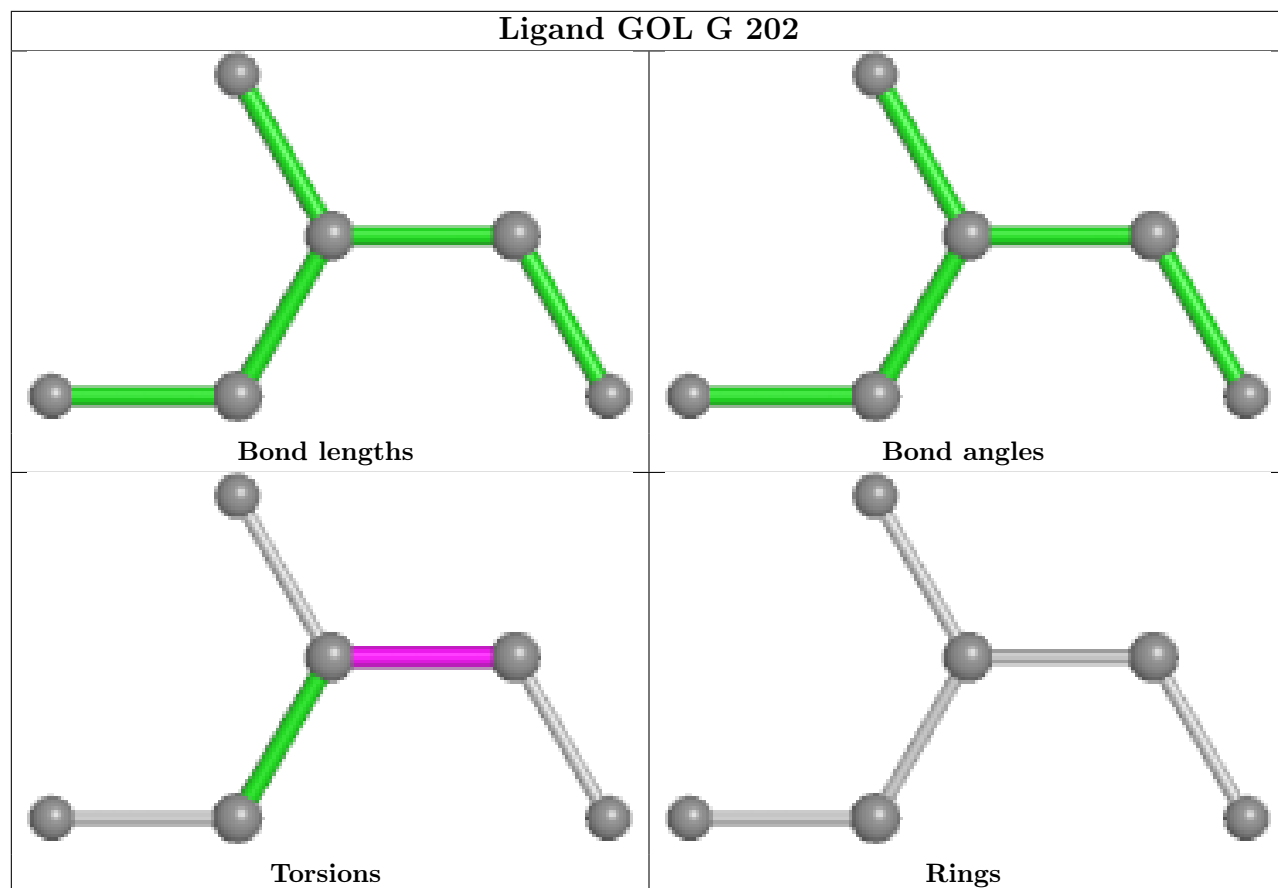
Bond angles



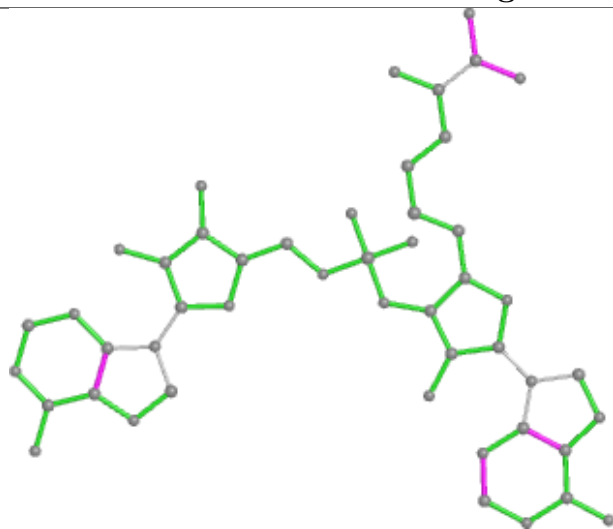
Torsions



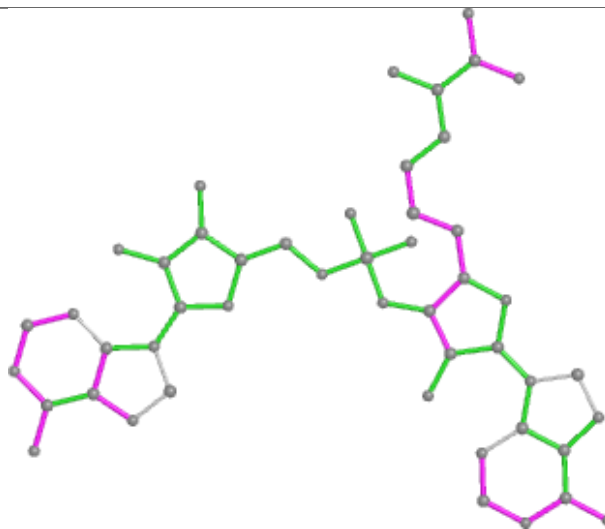
Rings



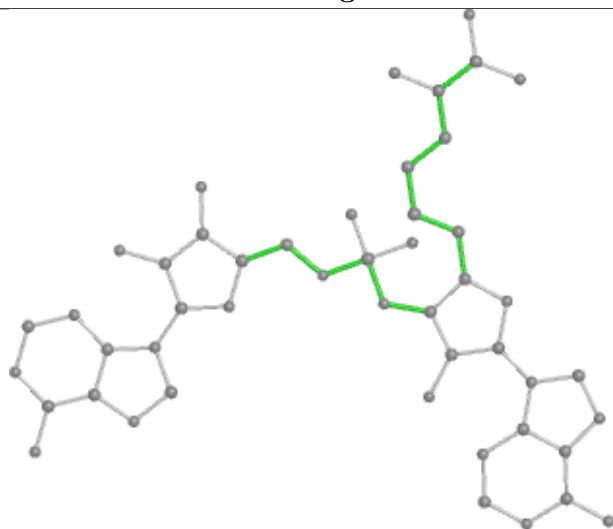
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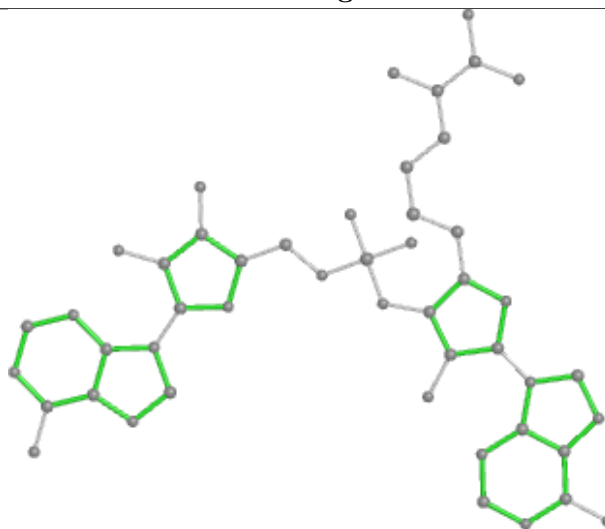
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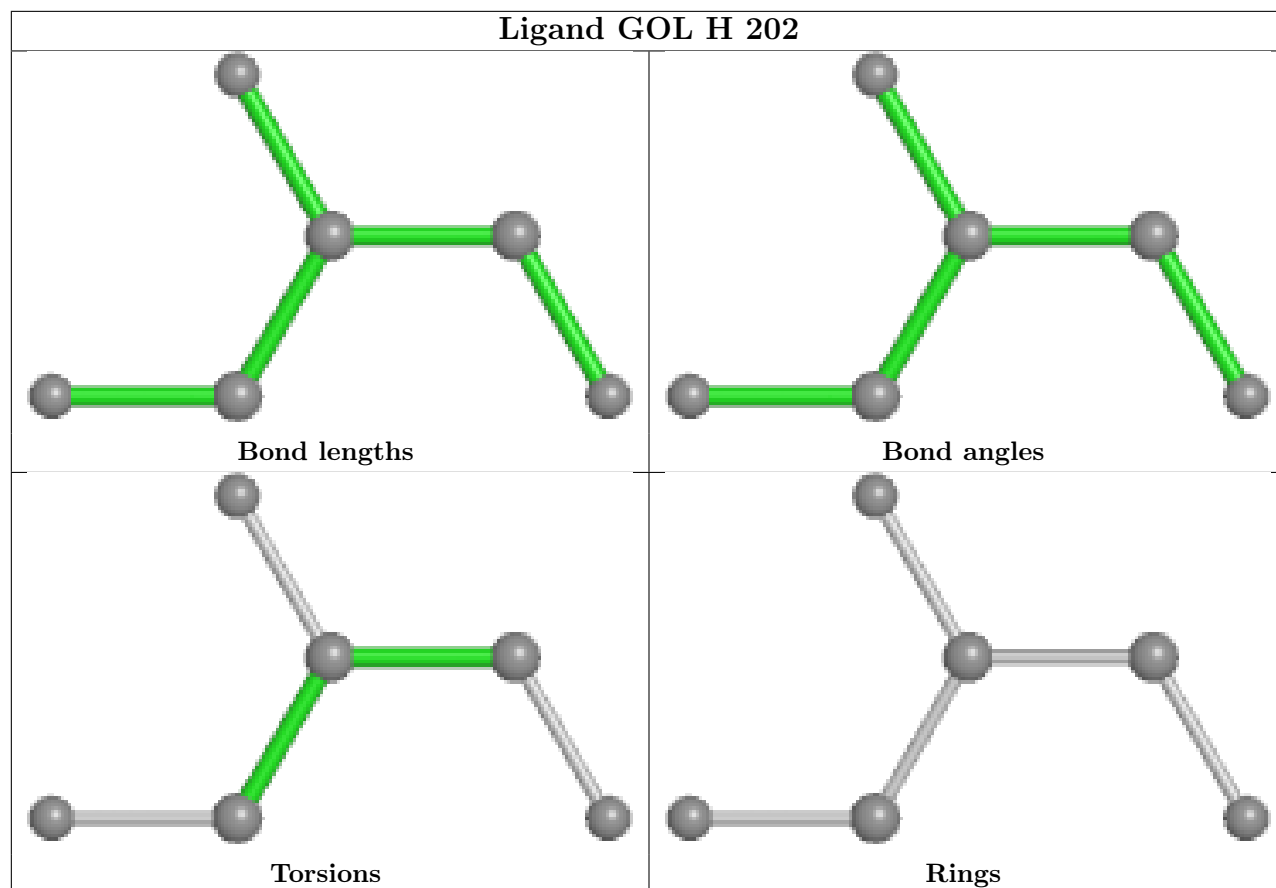
Bond angles



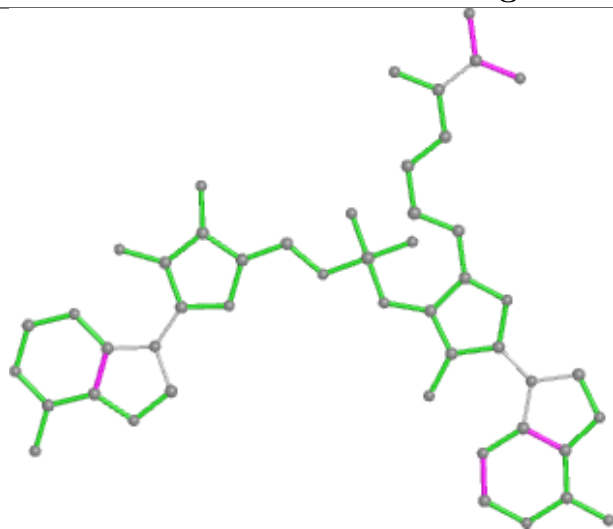
Torsions



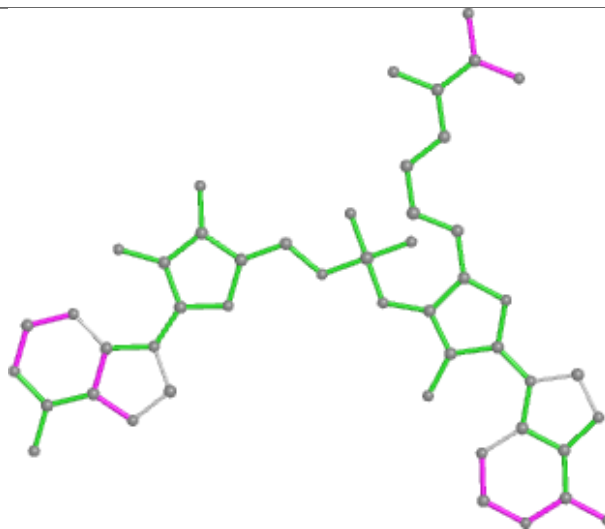
Rings



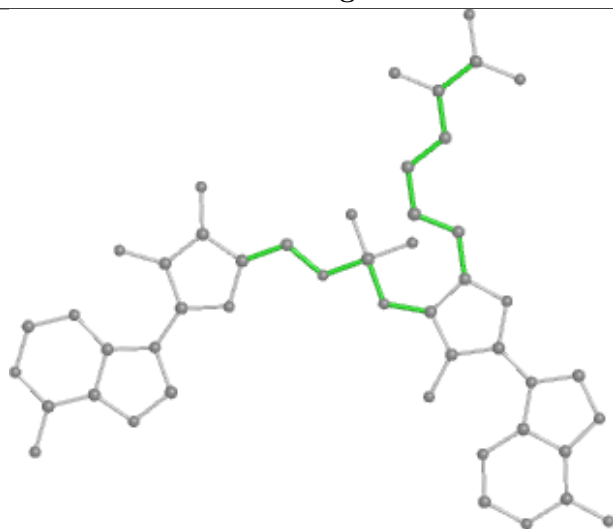
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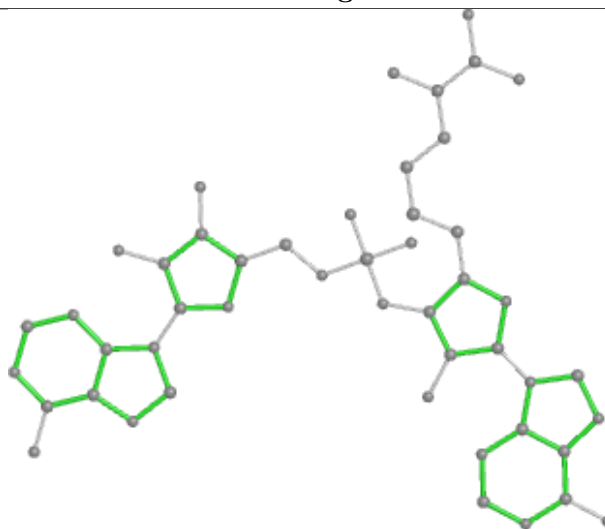
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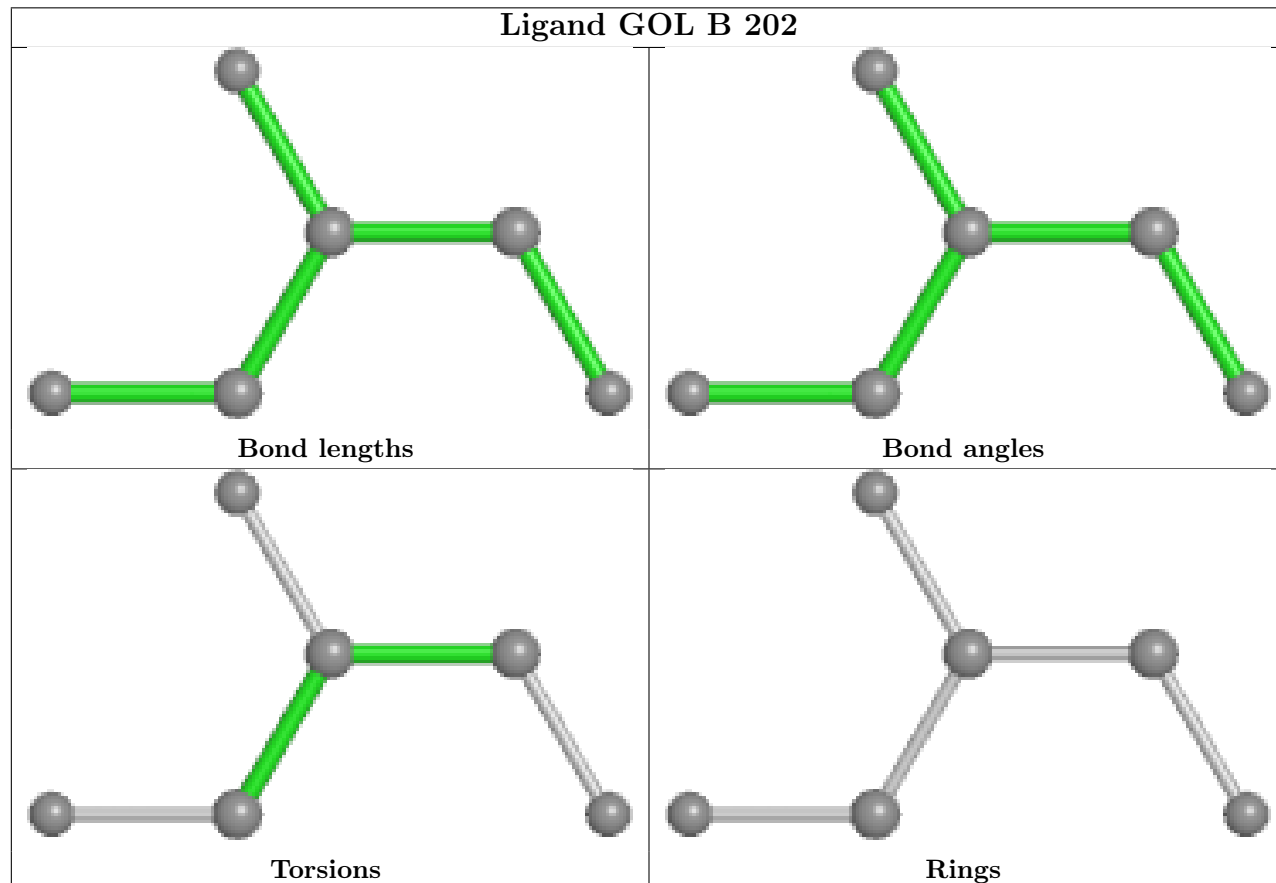
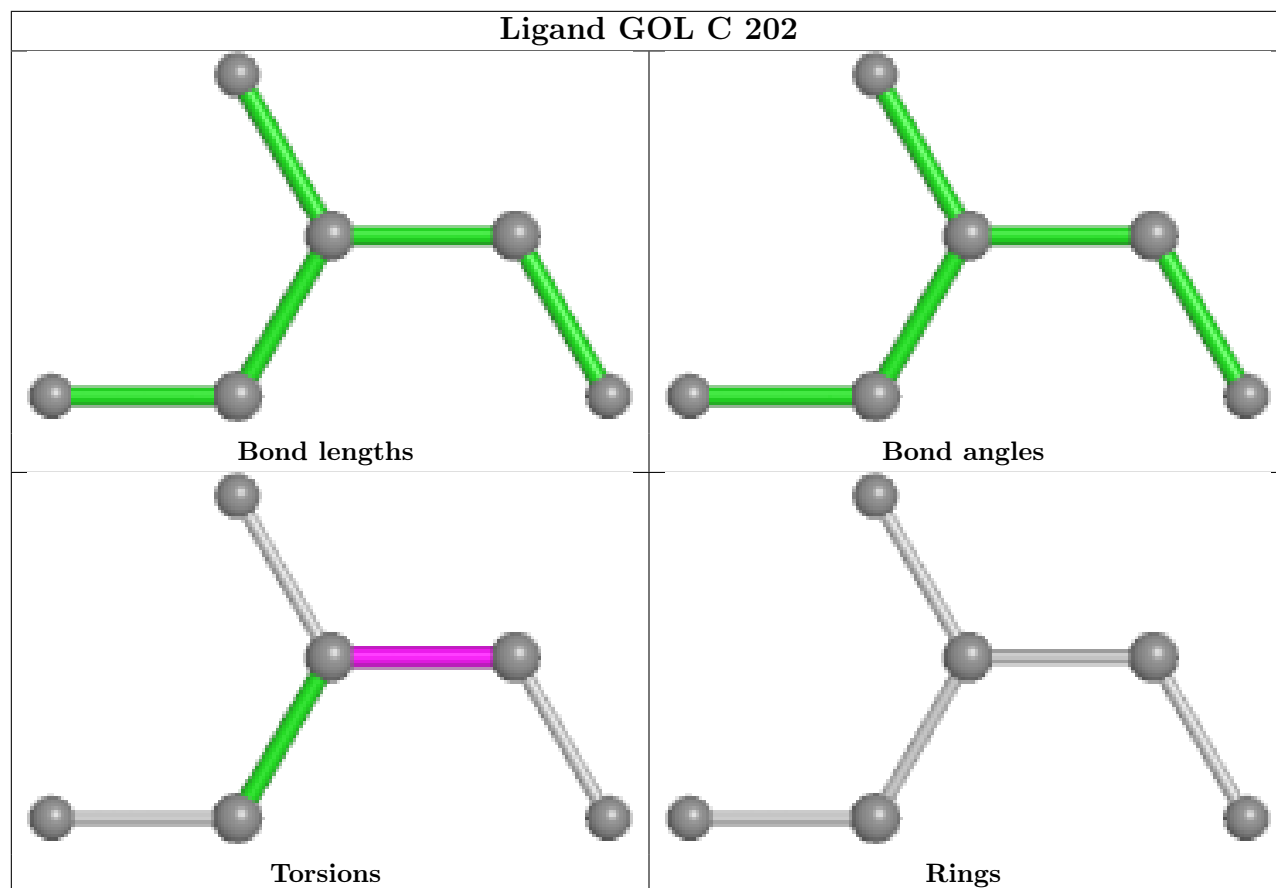
Bond angles



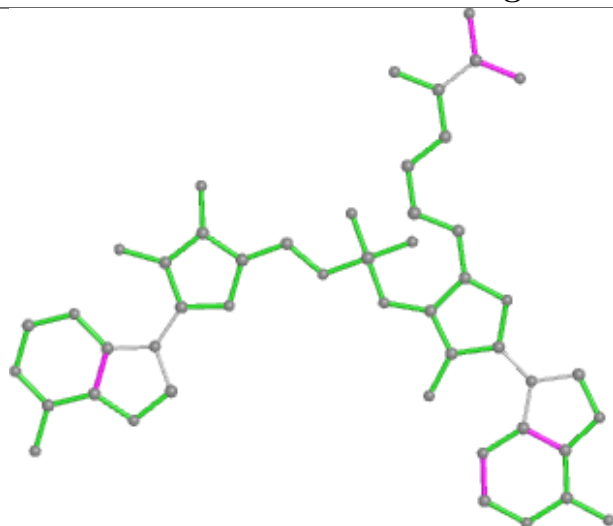
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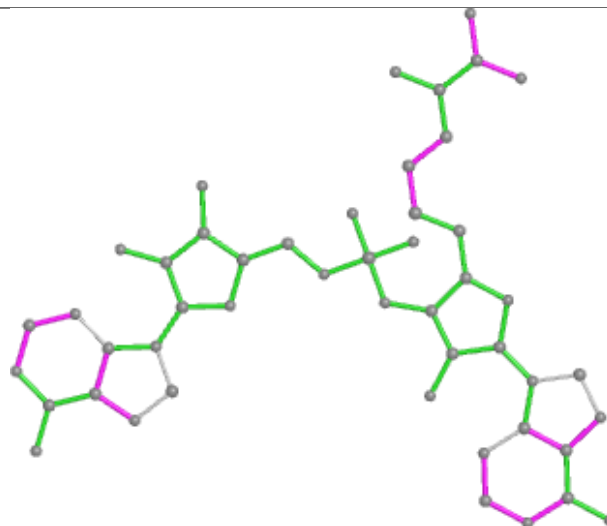
Rings



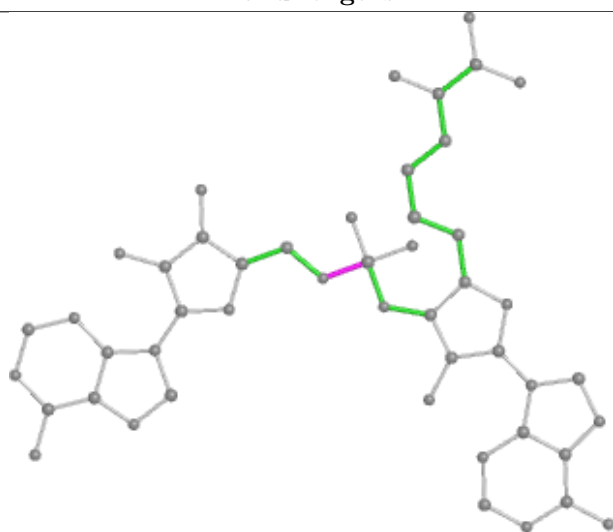
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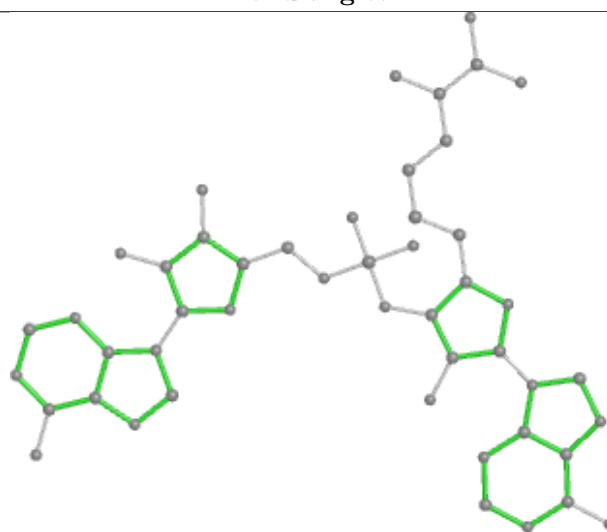
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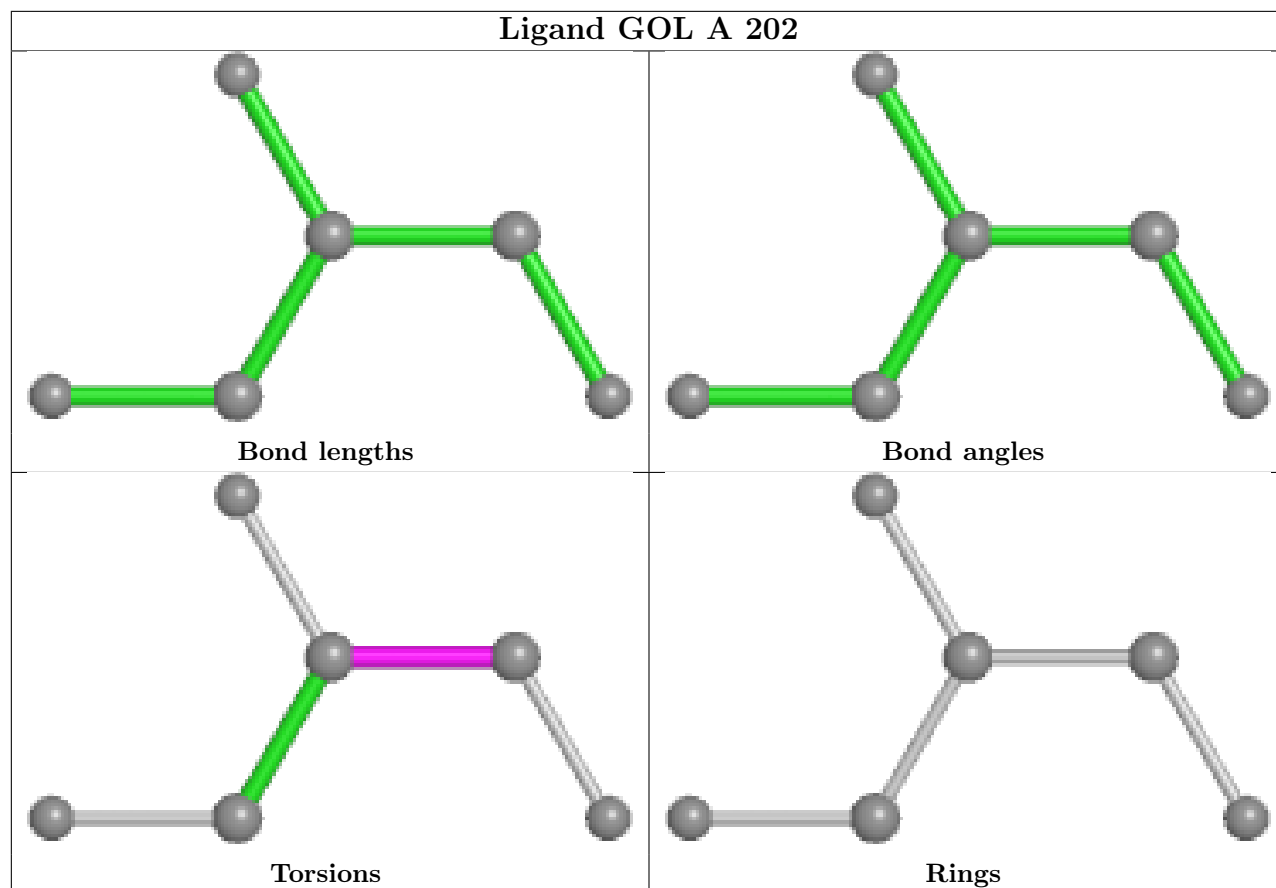
Bond angles



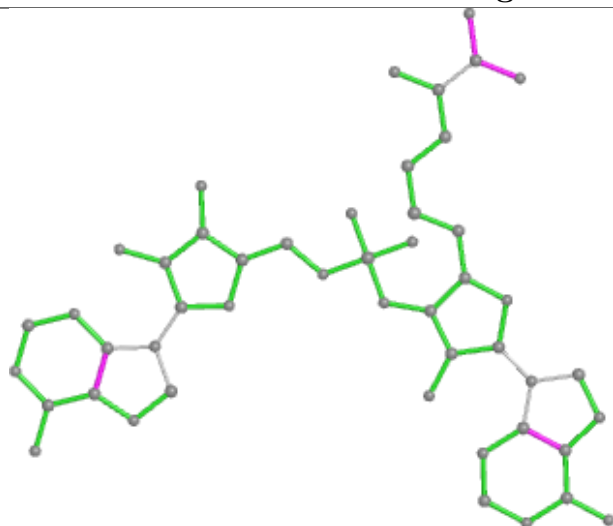
Torsions



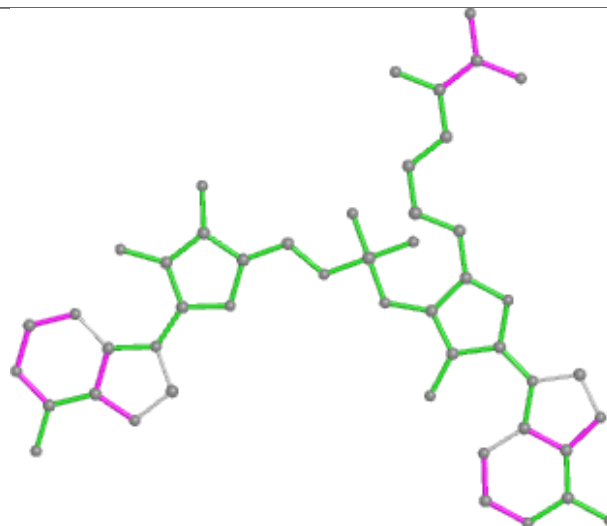
Rings



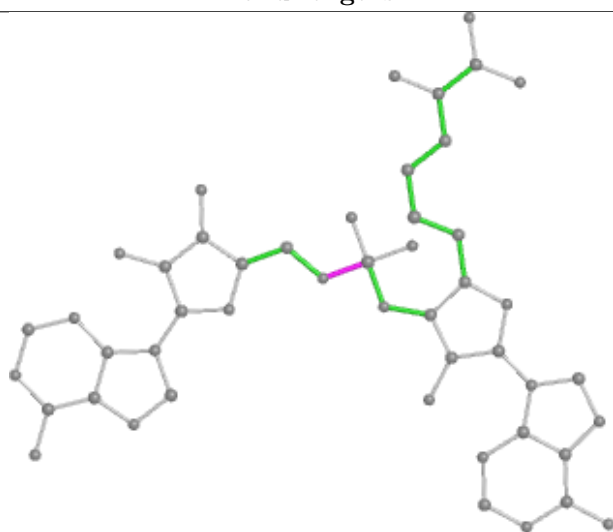
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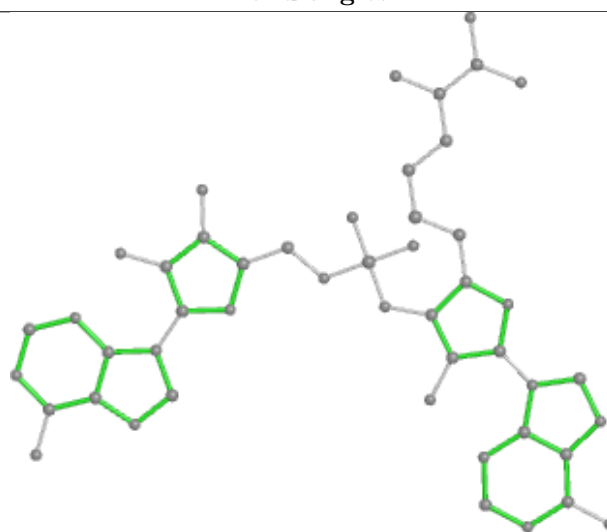
Bond lengths



Bond angles

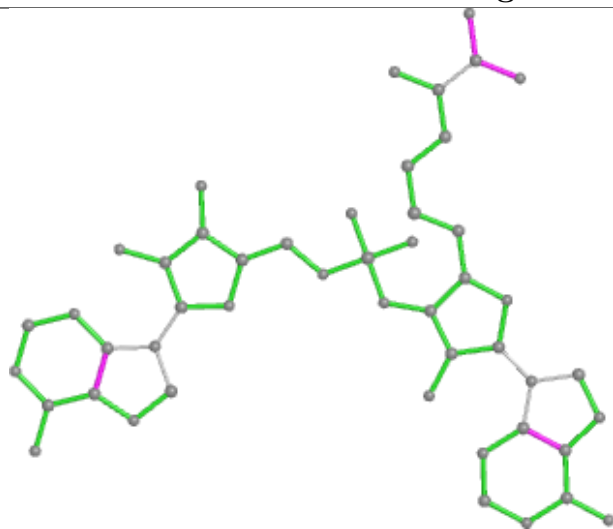


Torsions

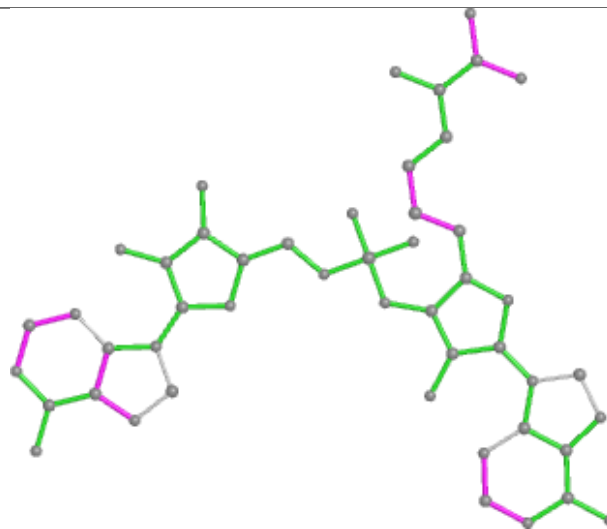


Rings

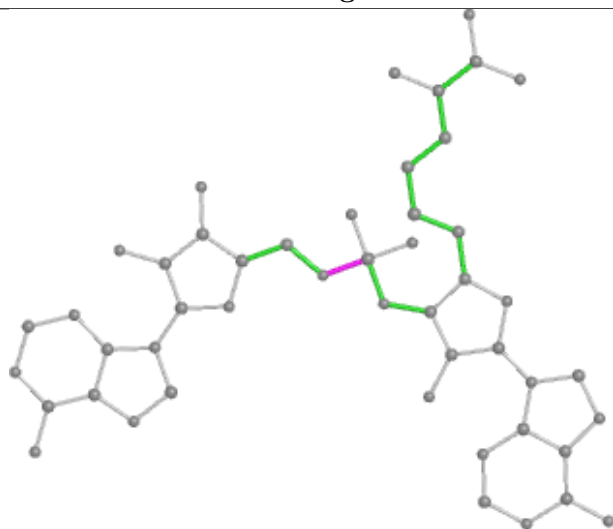
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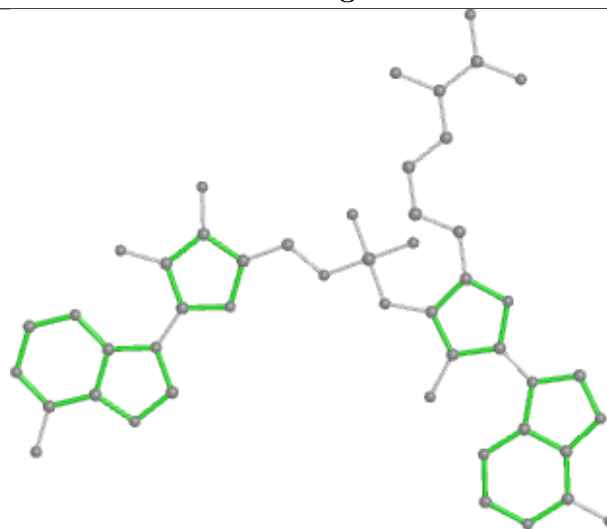
Bond lengths



Bond angles

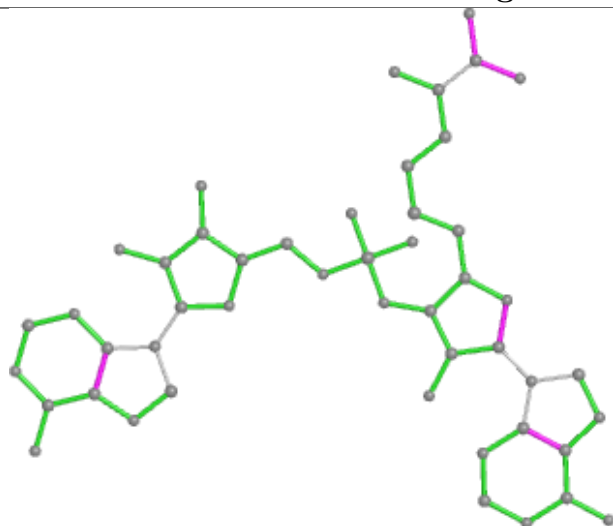


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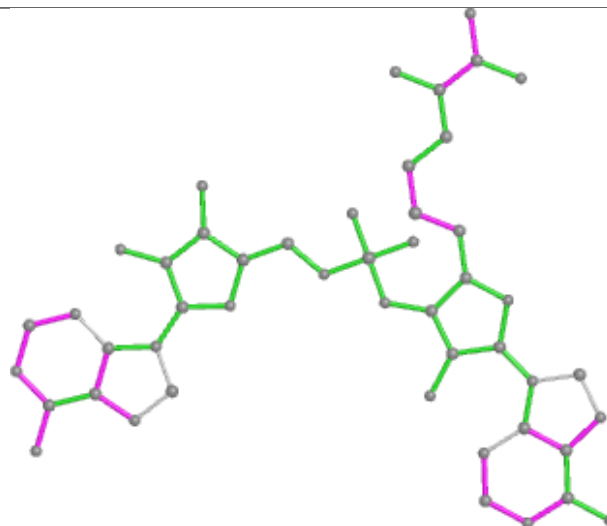


Rings

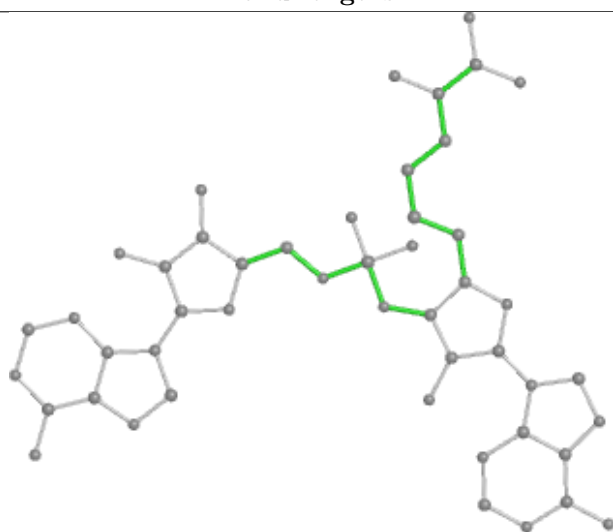
Ligand A1EL0 G 201



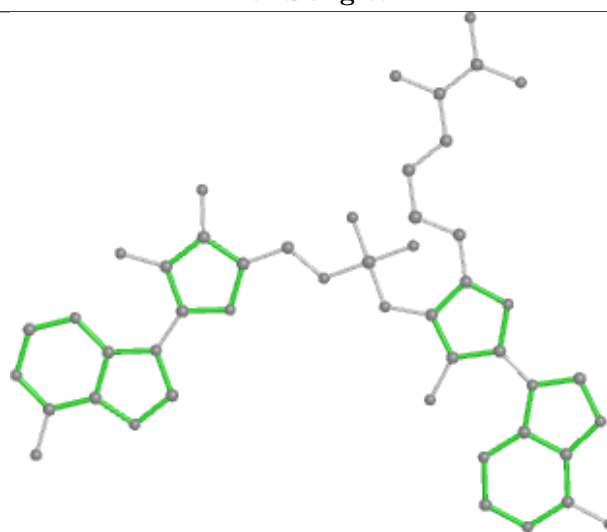
Bond lengths



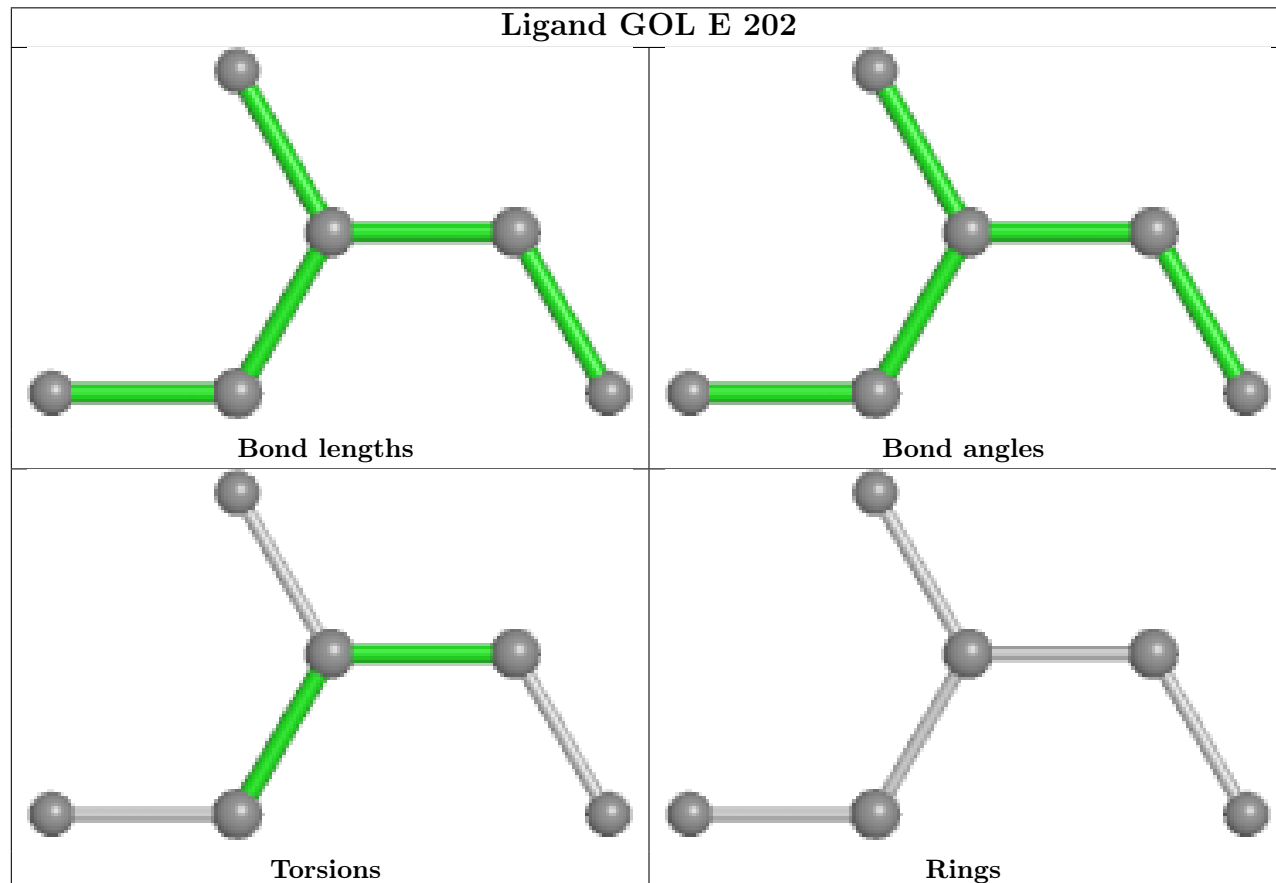
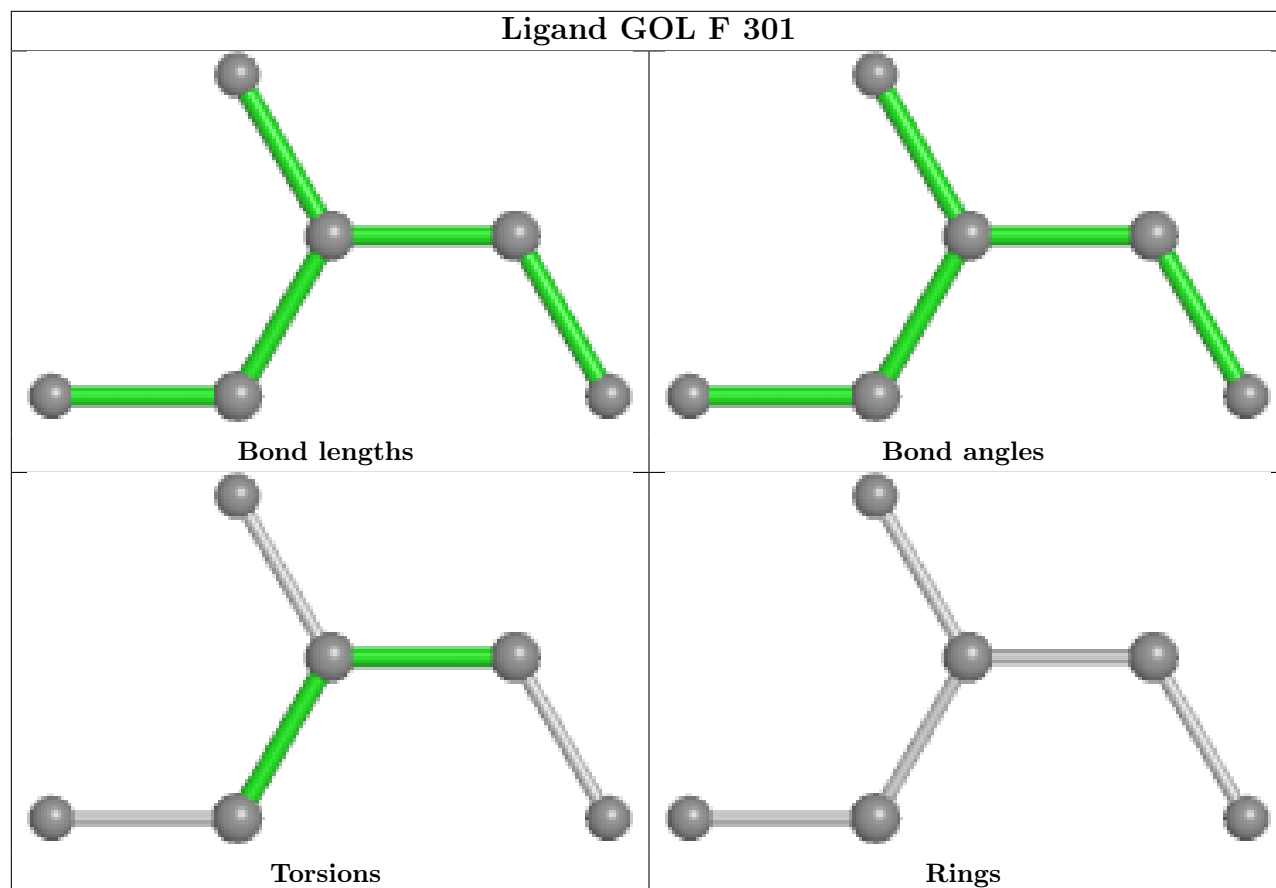
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	123/125 (98%)	0.45	12 (9%) 14 13	11, 21, 47, 55	1 (0%)
1	B	125/125 (100%)	-0.13	2 (1%) 70 73	9, 17, 32, 49	0
1	C	123/125 (98%)	-0.05	6 (4%) 36 35	10, 16, 33, 51	0
1	D	122/125 (97%)	0.17	5 (4%) 42 42	10, 20, 37, 44	1 (0%)
1	E	124/125 (99%)	-0.07	2 (1%) 70 73	8, 18, 32, 42	1 (0%)
1	F	123/125 (98%)	-0.09	2 (1%) 70 73	8, 18, 31, 45	1 (0%)
1	G	123/125 (98%)	0.26	9 (7%) 22 22	10, 20, 43, 56	1 (0%)
1	H	122/125 (97%)	0.20	4 (3%) 49 50	12, 19, 38, 48	0
1	I	123/125 (98%)	0.12	1 (0%) 82 85	13, 20, 32, 39	0
1	J	125/125 (100%)	-0.06	5 (4%) 43 43	10, 17, 37, 46	1 (0%)
1	K	123/125 (98%)	0.10	2 (1%) 70 73	11, 19, 36, 48	0
1	L	122/125 (97%)	0.09	7 (5%) 30 30	8, 18, 40, 52	1 (0%)
All	All	1478/1500 (98%)	0.08	57 (3%) 44 44	8, 19, 38, 56	7 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	0	SER	5.1
1	C	21	ASN	3.6
1	L	3[A]	LYS	3.6
1	A	2	GLY	3.6
1	G	20	THR	3.4
1	G	22	SER	3.4
1	C	85	VAL	3.3
1	A	24	SER	3.3
1	G	85	VAL	3.2
1	I	85	VAL	3.2
1	L	21	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	17	TYR	2.9
1	D	68	GLU	2.9
1	B	21	ASN	2.9
1	A	85	VAL	2.9
1	L	20	THR	2.8
1	A	15	LYS	2.7
1	A	18	PHE	2.7
1	G	18	PHE	2.7
1	J	1	MET	2.7
1	G	19	HIS	2.6
1	K	21	ASN	2.6
1	H	85	VAL	2.6
1	D	19	HIS	2.5
1	H	16	GLY	2.5
1	L	19	HIS	2.5
1	J	86	ASP	2.5
1	L	18	PHE	2.5
1	A	3	LYS	2.5
1	H	17	TYR	2.5
1	G	21	ASN	2.5
1	A	19	HIS	2.4
1	H	19	HIS	2.4
1	G	24	SER	2.4
1	C	68	GLU	2.4
1	L	16	GLY	2.4
1	E	1	MET	2.3
1	D	21	ASN	2.3
1	C	82	GLU	2.3
1	A	28	ASP	2.3
1	C	20	THR	2.3
1	G	64	TRP	2.3
1	E	21	ASN	2.3
1	A	29	LEU	2.3
1	D	16	GLY	2.2
1	K	2	GLY	2.2
1	F	21	ASN	2.2
1	A	25	GLU	2.2
1	G	63	GLU	2.2
1	B	23	GLN	2.2
1	L	17	TYR	2.1
1	J	21	ASN	2.1
1	C	2	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	3	LYS	2.0
1	J	85	VAL	2.0
1	A	16	GLY	2.0
1	F	86	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

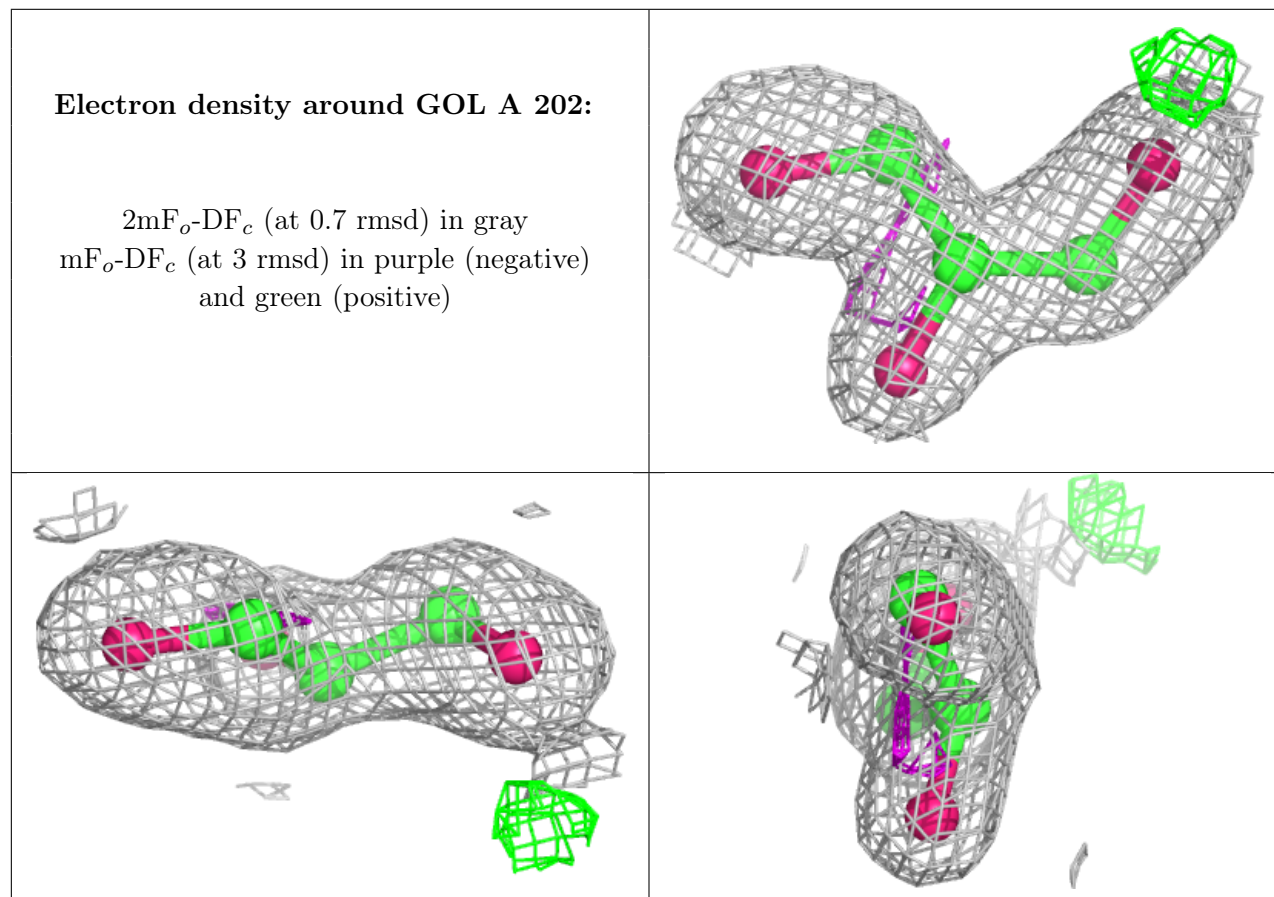
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	202	6/6	0.92	0.11	18,22,24,26	0
3	GOL	H	202	6/6	0.93	0.08	20,24,29,29	0
3	GOL	K	202	6/6	0.93	0.09	18,21,23,24	0
2	A1EL0	A	201	48/48	0.94	0.09	15,24,35,39	0
3	GOL	C	202	6/6	0.95	0.10	16,18,22,23	0
2	A1EL0	G	201	48/48	0.95	0.08	14,21,32,43	0
2	A1EL0	F	302	48/48	0.95	0.08	11,16,28,31	0
2	A1EL0	E	201	48/48	0.96	0.06	9,16,22,32	0
3	GOL	E	202	6/6	0.96	0.11	18,21,23,23	0
3	GOL	B	202	6/6	0.96	0.06	18,20,21,23	0
2	A1EL0	B	201	48/48	0.96	0.07	9,14,26,32	0
3	GOL	F	301	6/6	0.96	0.07	16,18,20,23	0
2	A1EL0	I	201	48/48	0.96	0.07	13,20,26,32	0
2	A1EL0	L	201	48/48	0.96	0.07	12,18,28,31	0
2	A1EL0	J	201	48/48	0.97	0.06	12,15,22,27	0
2	A1EL0	K	201	48/48	0.97	0.06	12,16,28,35	0
2	A1EL0	C	201	48/48	0.97	0.06	9,13,31,34	0
3	GOL	G	202	6/6	0.97	0.06	14,18,20,20	0
2	A1EL0	H	201	48/48	0.97	0.06	10,14,28,32	0

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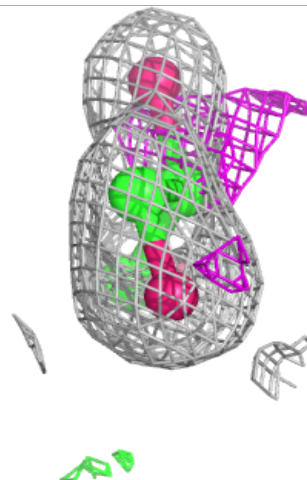
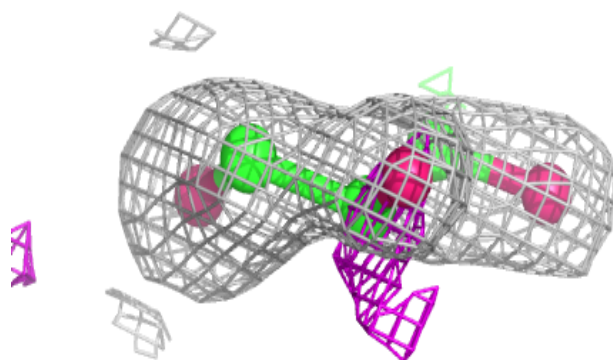
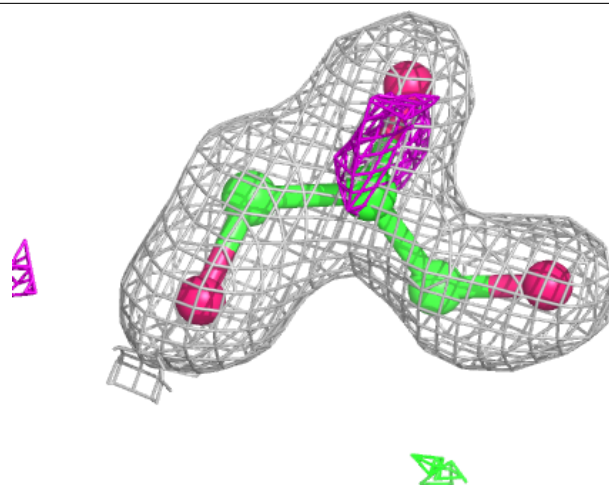
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	J	202	6/6	0.97	0.07	16,18,18,20	0
2	A1EL0	D	201	48/48	0.97	0.06	12,17,28,29	0

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.



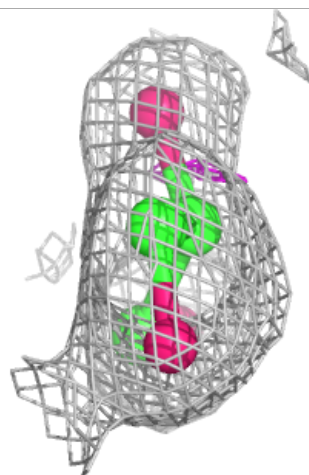
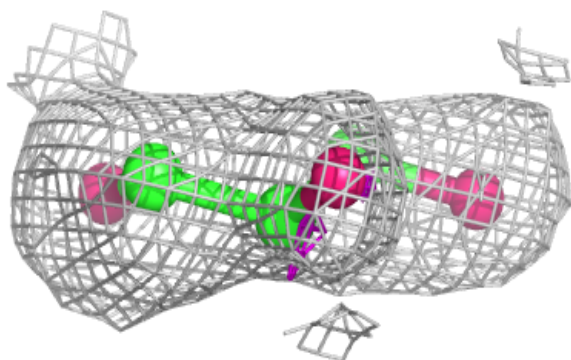
Electron density around GOL H 202:

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



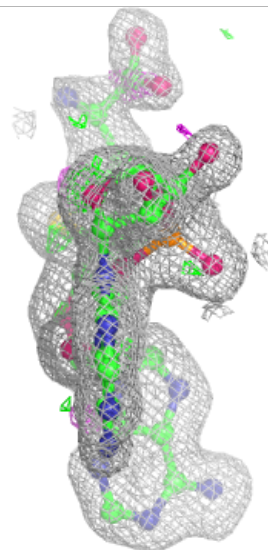
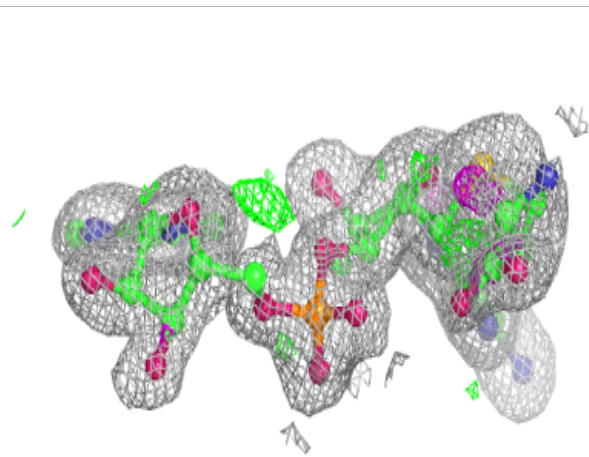
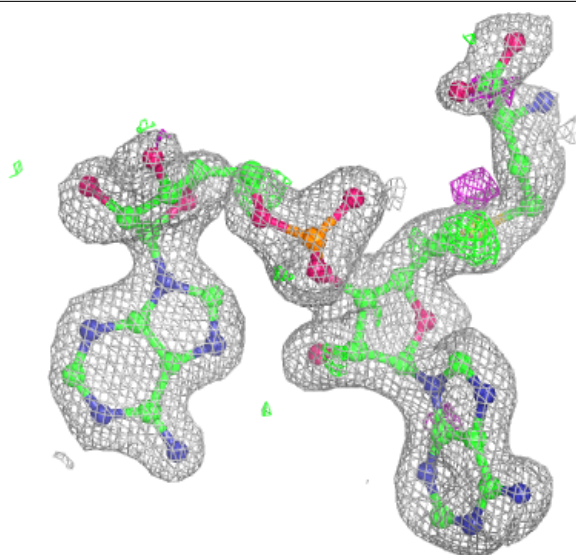
Electron density around GOL K 202:

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



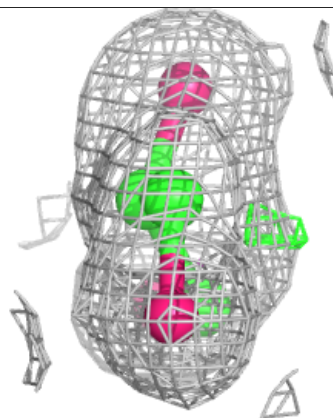
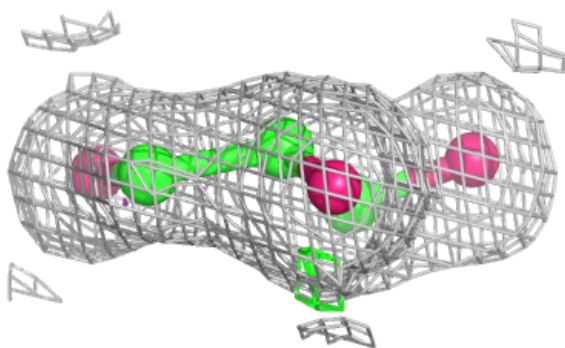
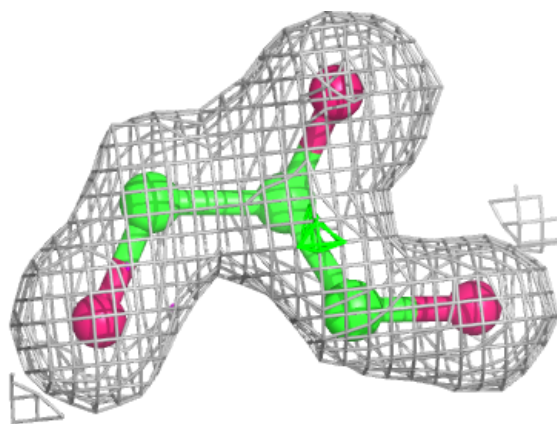
Electron density around A1EL0 A 201:

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



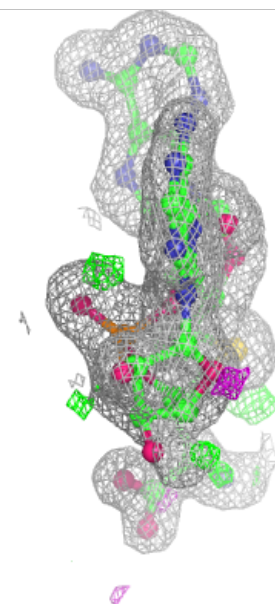
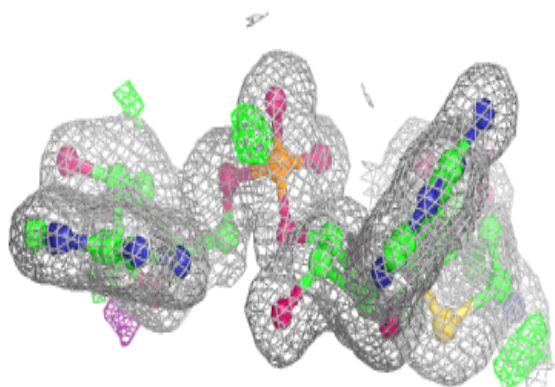
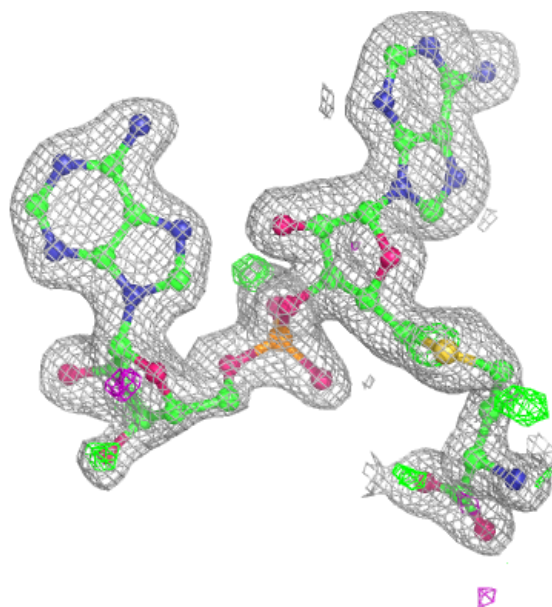
Electron density around GOL C 202:

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



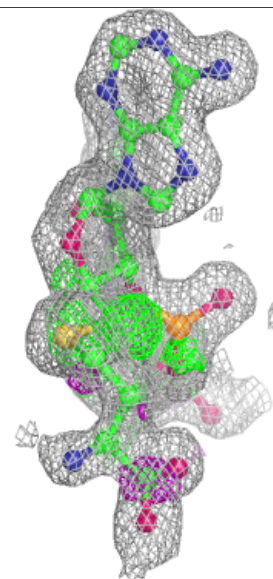
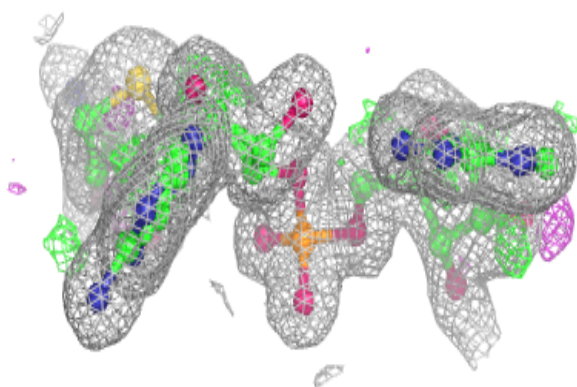
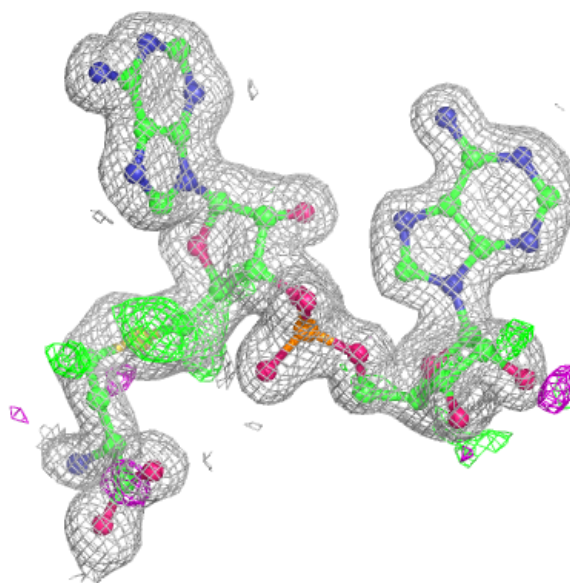
Electron density around A1EL0 G 201:

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



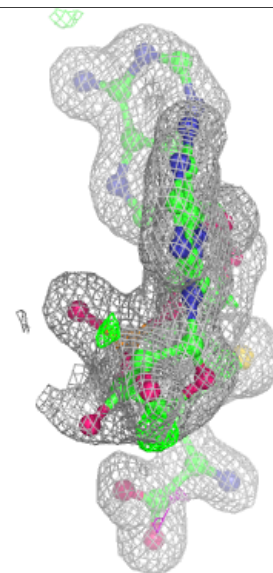
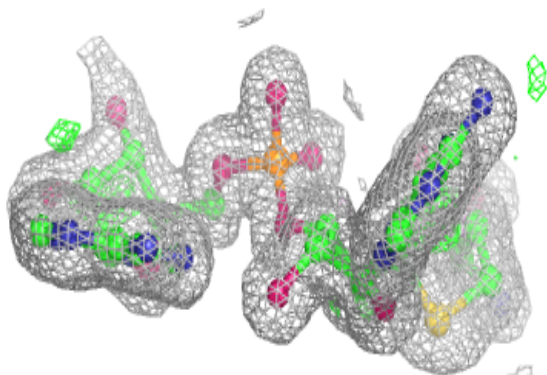
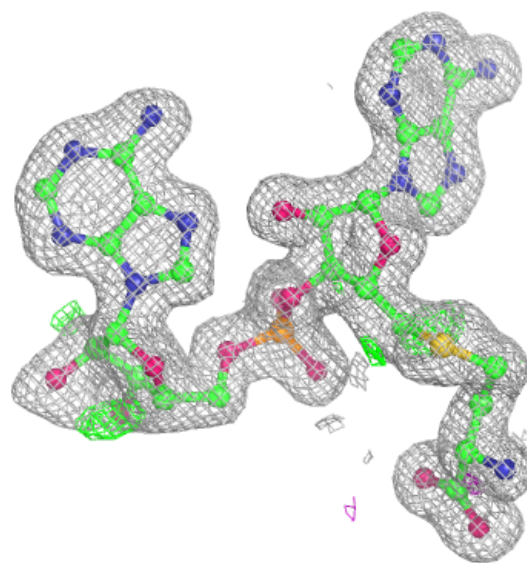
Electron density around A1EL0 F 302:

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



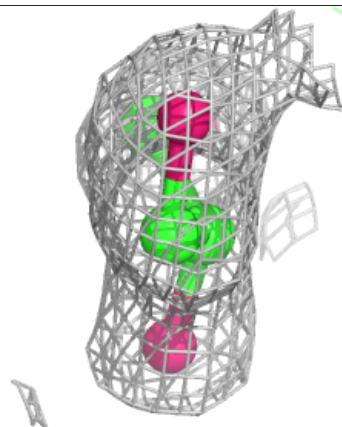
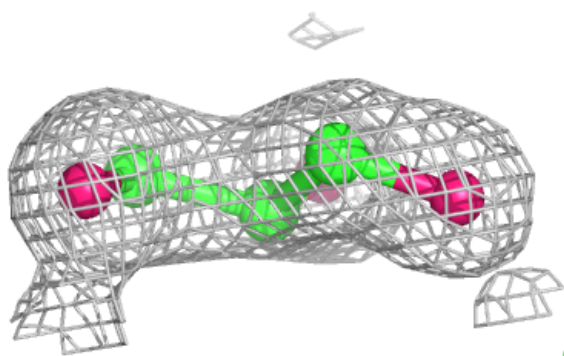
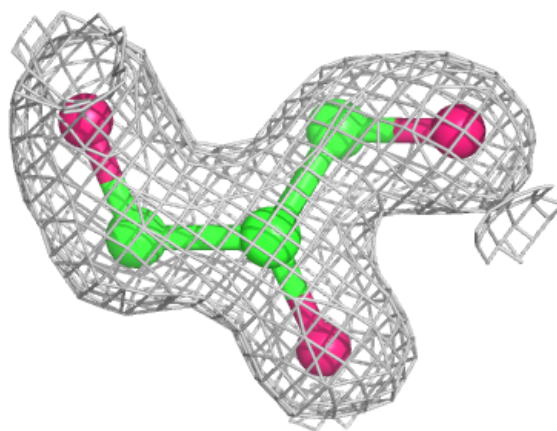
Electron density around A1EL0 E 201:

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and green (positive)



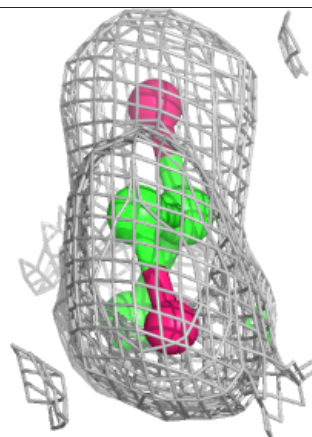
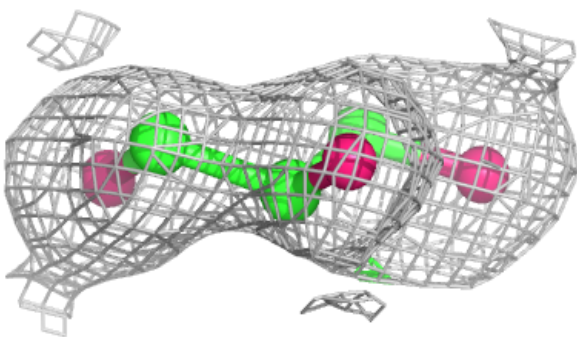
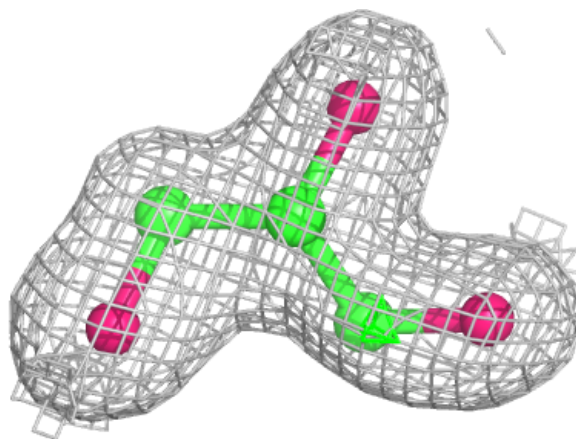
Electron density around GOL E 202:

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and green (positive)



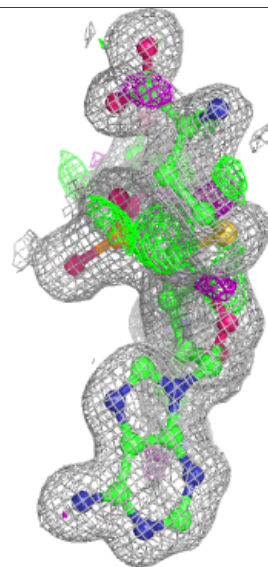
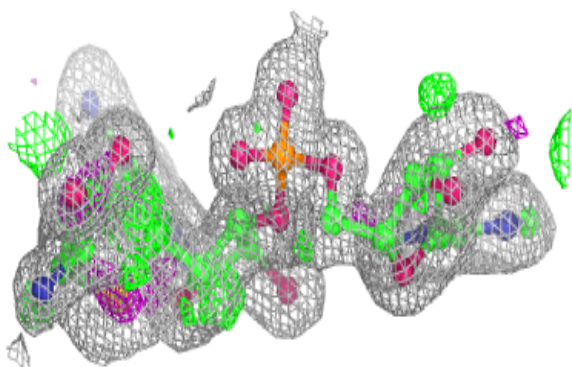
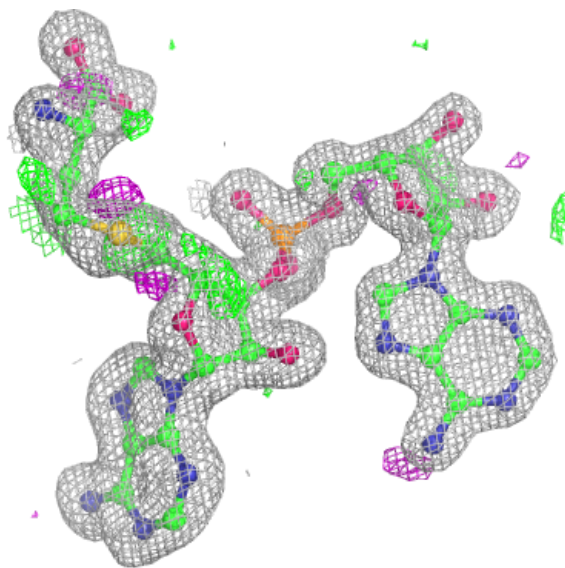
Electron density around GOL B 202:

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and green (positive)



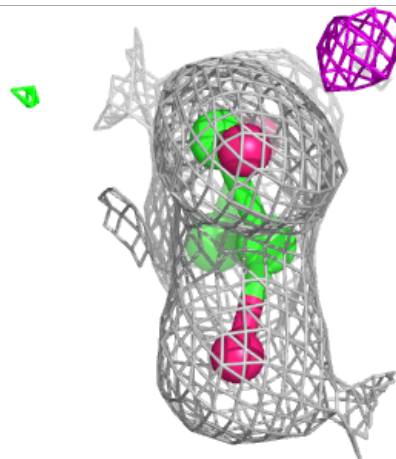
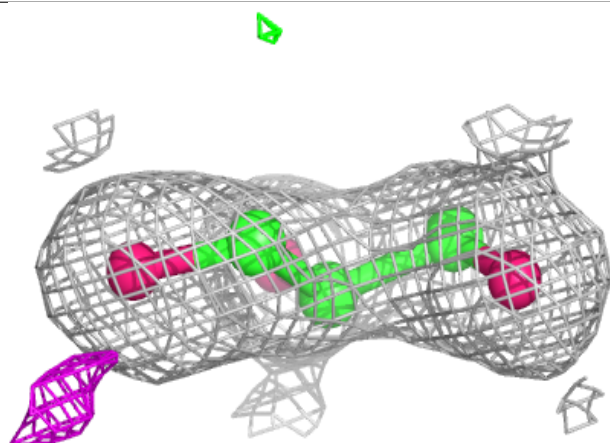
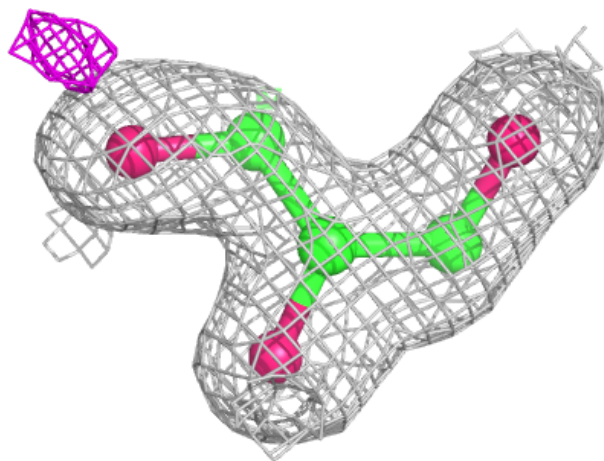
Electron density around A1EL0 B 201:

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and green (positive)



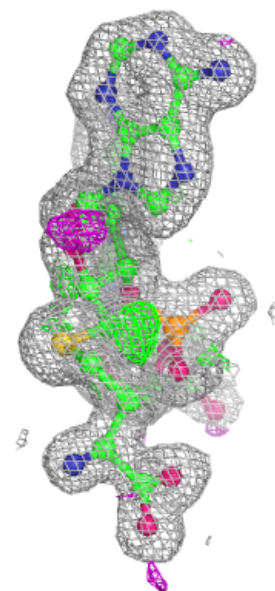
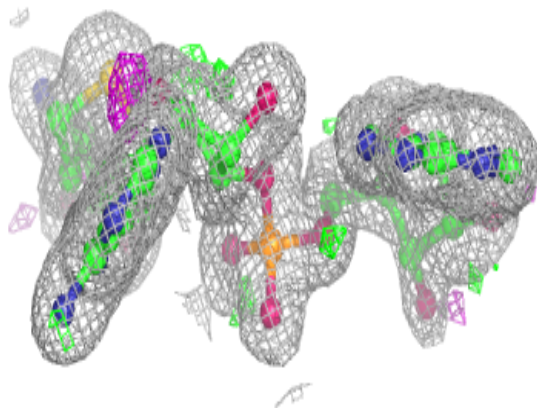
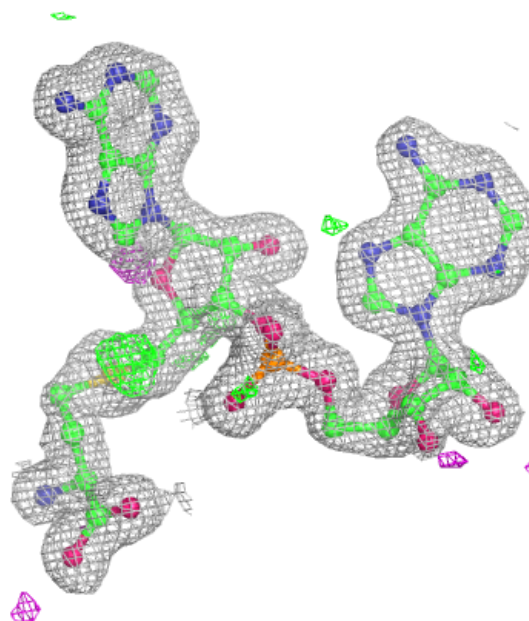
Electron density around GOL F 301:

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



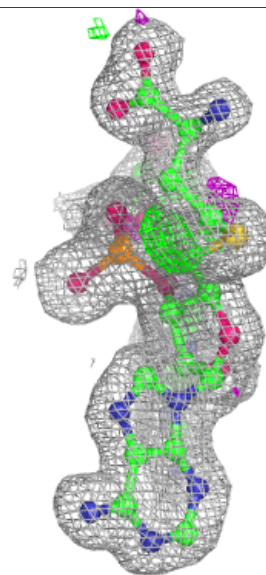
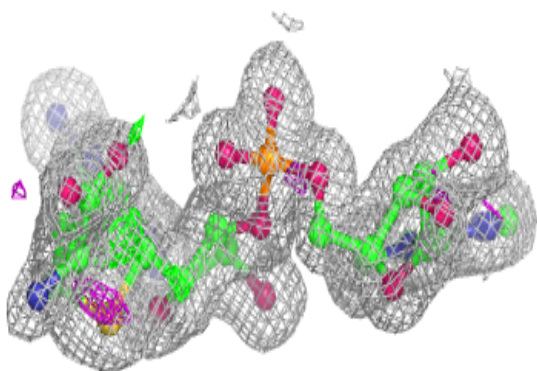
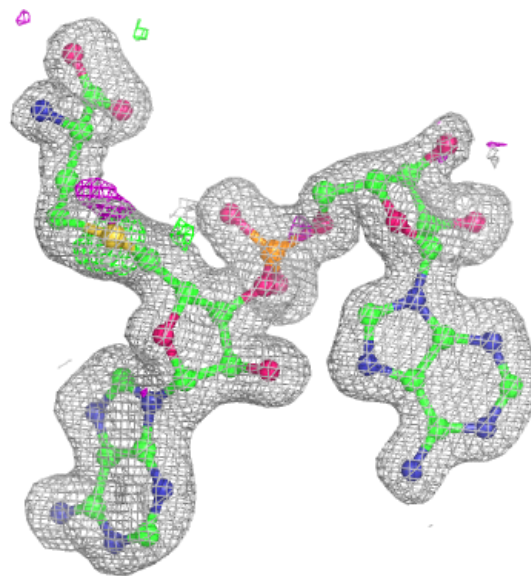
Electron density around A1EL0 I 201:

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



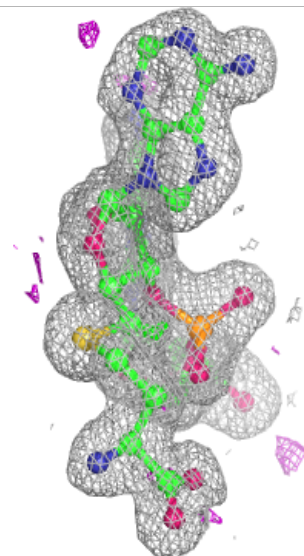
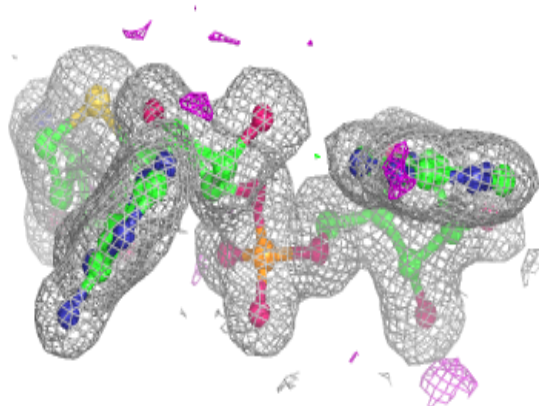
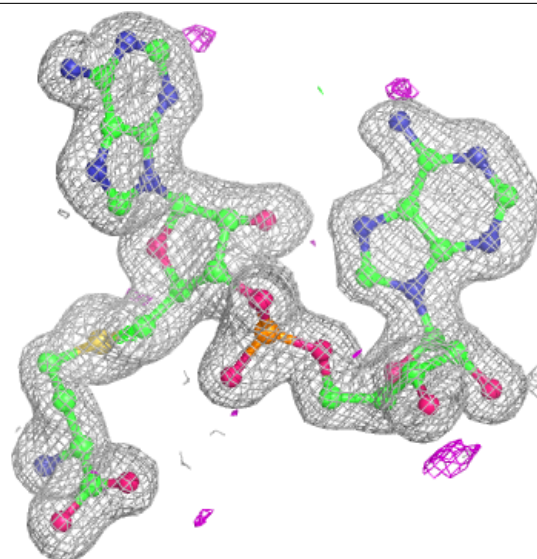
Electron density around A1EL0 L 201:

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and green (positive)



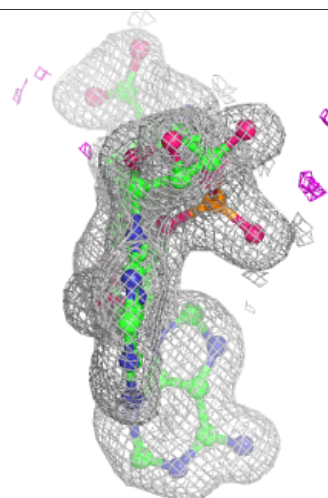
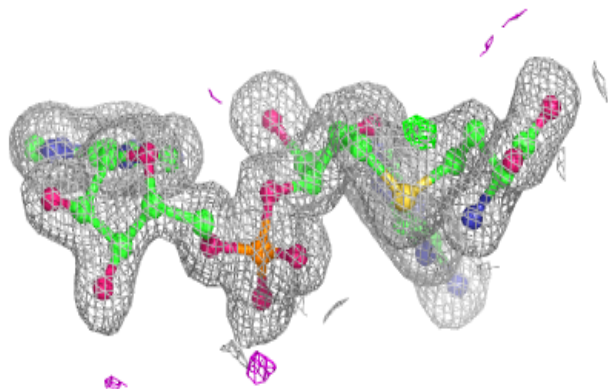
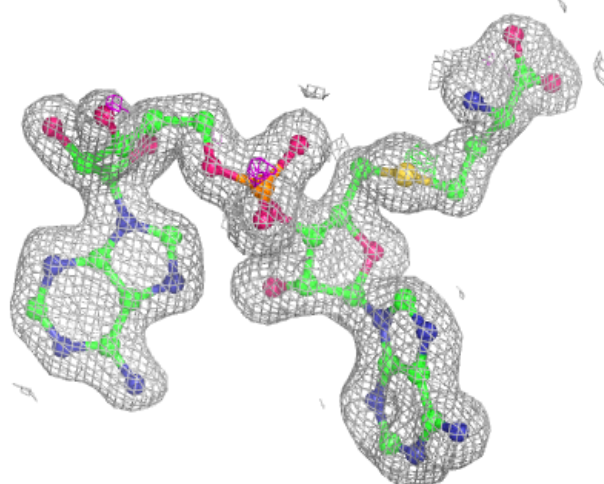
Electron density around A1EL0 J 201:

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and green (positive)



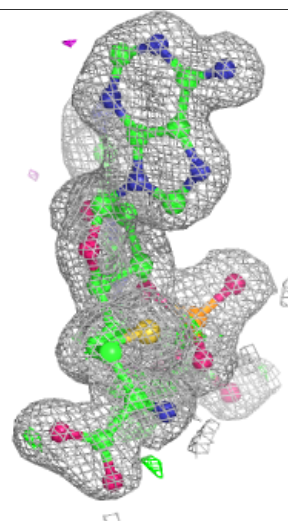
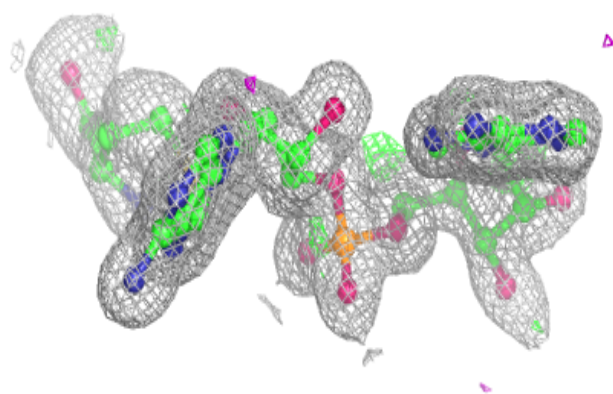
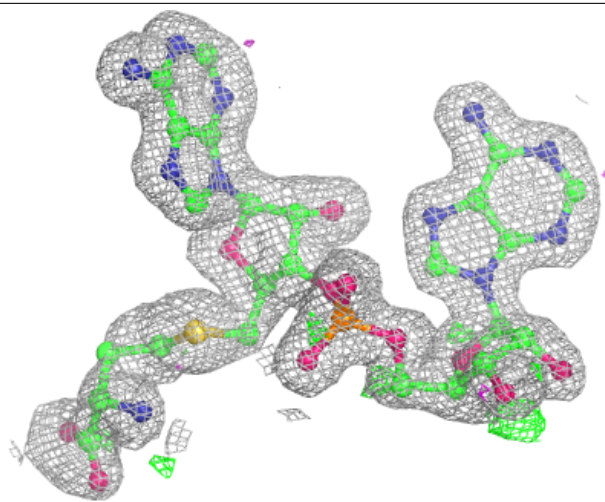
Electron density around A1EL0 K 201:

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and green (positive)



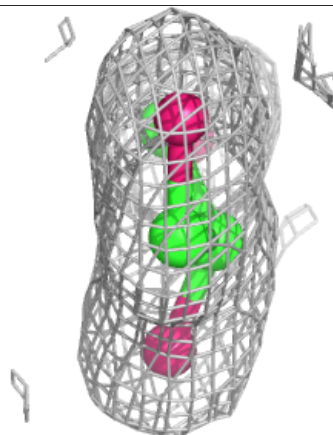
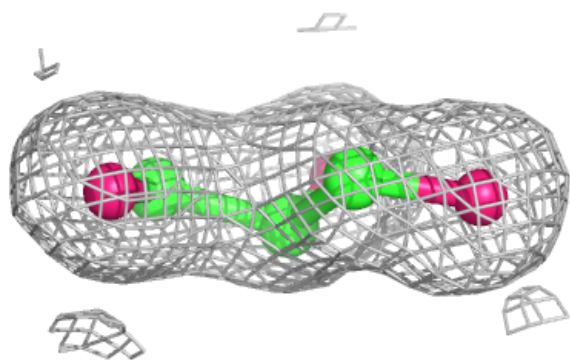
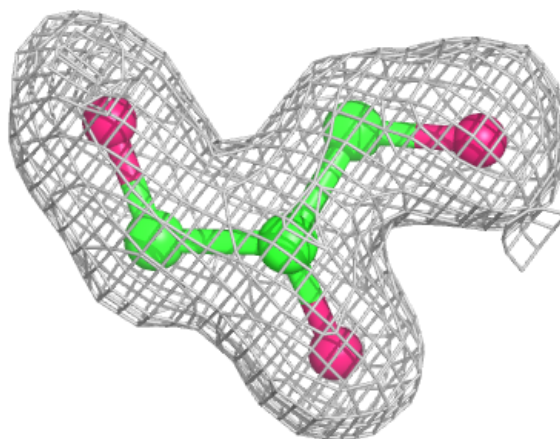
Electron density around A1EL0 C 201:

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and green (positive)



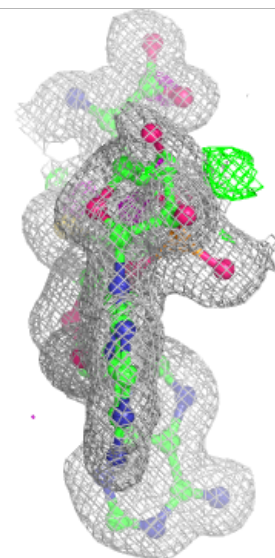
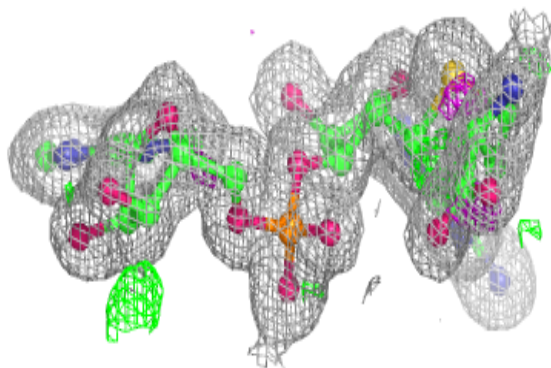
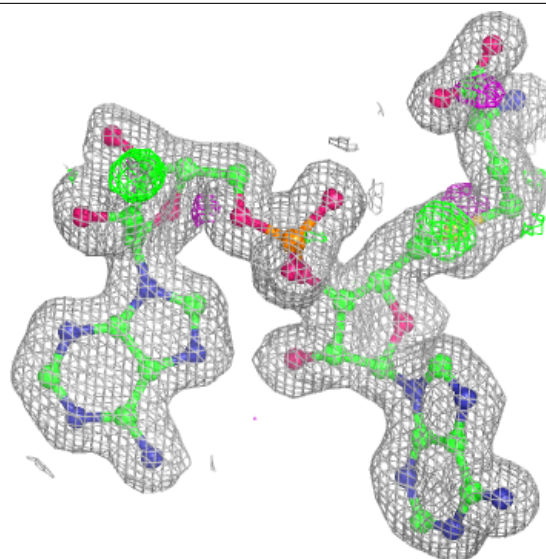
Electron density around GOL G 202:

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



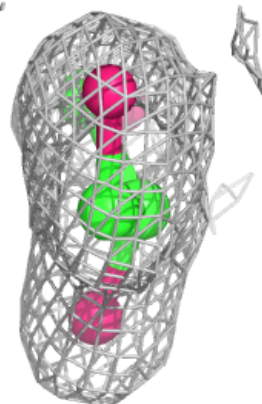
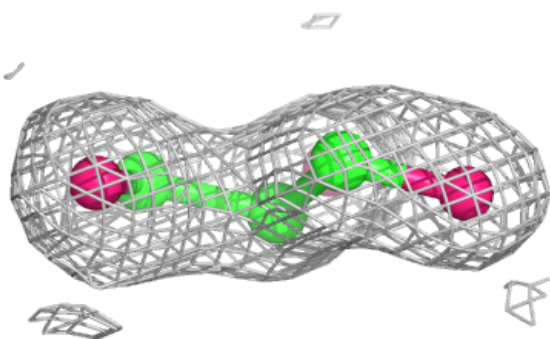
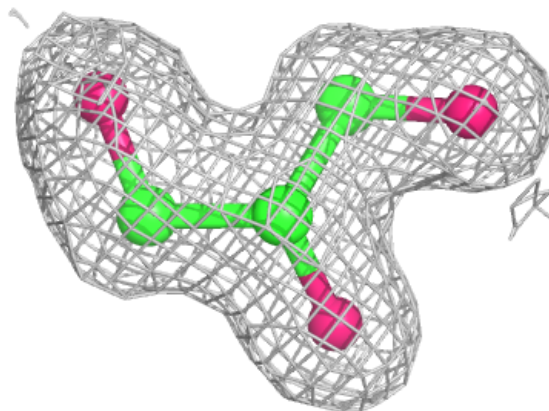
Electron density around A1EL0 H 201:

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



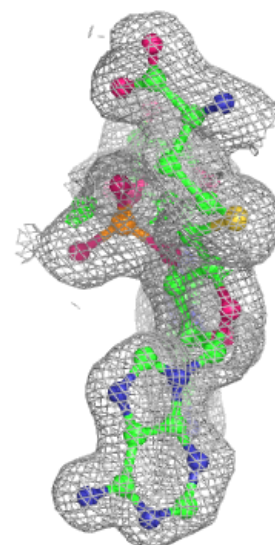
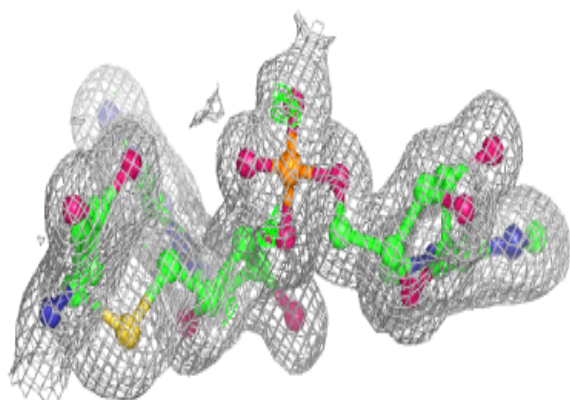
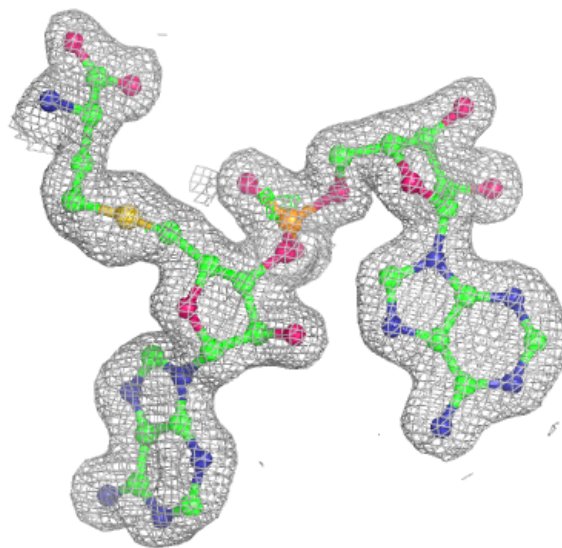
Electron density around GOL J 202:

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



Electron density around A1EL0 D 201:

$2mF_o-DF_c$ (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.