



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2022 – 04:42 PM EST

PDB ID : 7SZF  
Title : Structure of the Rieske Non-heme Iron Oxygenase GxtA with beta-Saxitoxinol Bound  
Authors : Bridwell-Rabb, J.; Liu, J.  
Deposited on : 2021-11-27  
Resolution : 1.79 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.25  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.25

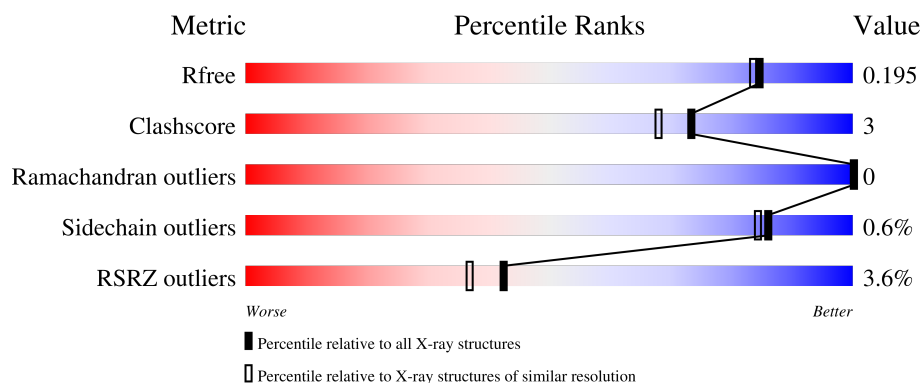
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	334	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>6% • 5%</div> </div> </div>
1	B	334	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>7% 5%</div> </div> </div>
1	C	334	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>7% •</div> </div> </div>

## 2 Entry composition [i](#)

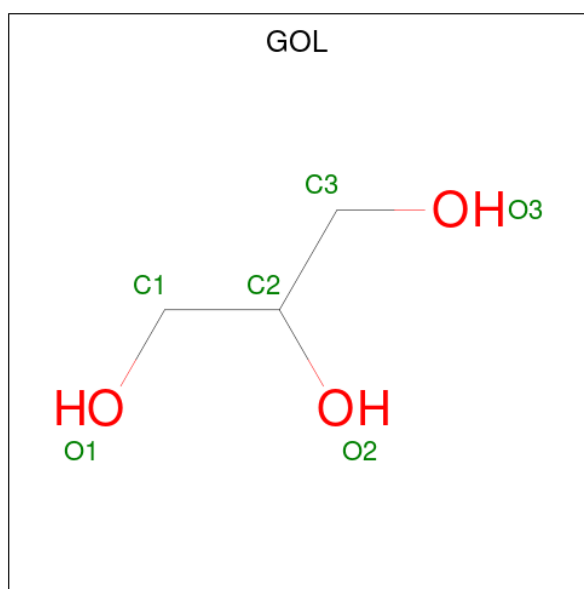
There are 7 unique types of molecules in this entry. The entry contains 8988 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SxtDIOX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	7	0
			2592	1644	448	481	19			
1	B	318	Total	C	N	O	S	0	12	0
			2633	1671	455	486	21			
1	C	326	Total	C	N	O	S	0	8	0
			2672	1689	464	498	21			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ) (labeled as "Ligand of Interest" by depositor).



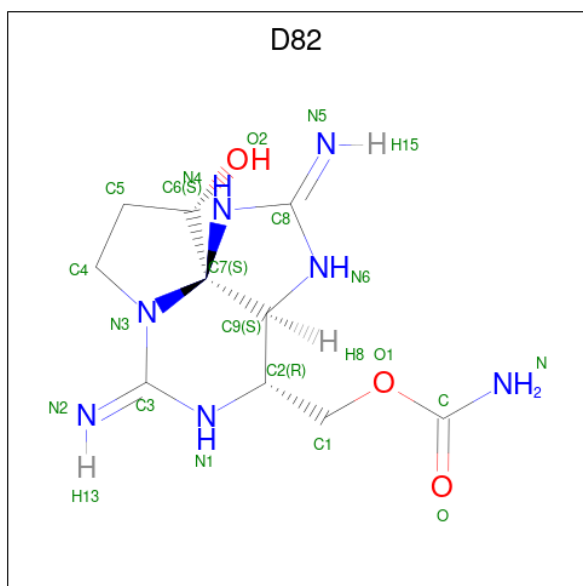
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 3 is beta-Saxitoxinol (three-letter code: D82) (formula:  $C_{10}H_{17}N_7O_3$ ) (labeled as "Ligand of Interest" by depositor).

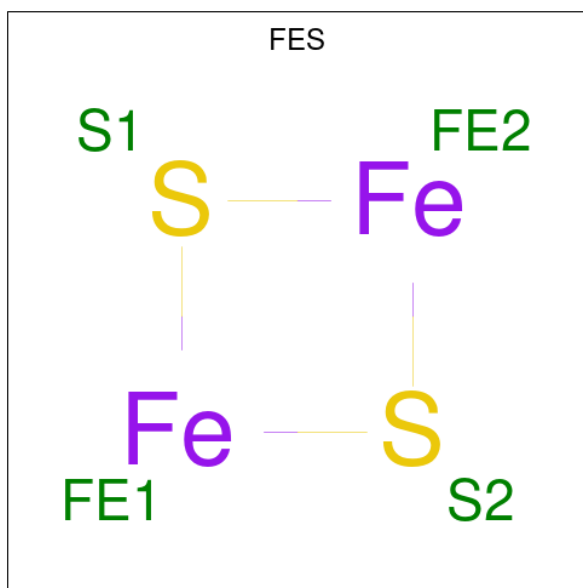


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	10	7	3		
3	B	1	Total	C	N	O	0	0
			20	10	7	3		
3	C	1	Total	C	N	O	0	0
			20	10	7	3		

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Fe	0	0
			1	1		
4	B	1	Total	Fe	0	0
			1	1		
4	C	1	Total	Fe	0	0
			1	1		

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			4	2	2		
5	B	1	Total	Fe	S	0	0
			4	2	2		
5	C	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total 4	Cl 4	0	0
6	B	1	Total 1	Cl 1	0	0
6	C	2	Total 2	Cl 2	0	0

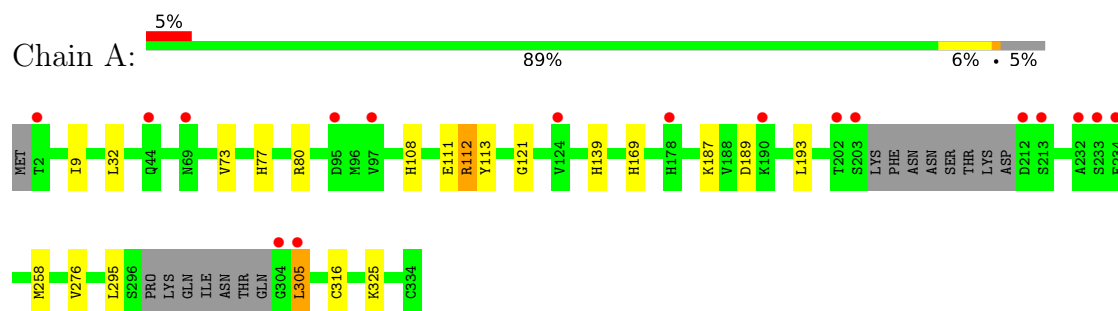
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	323	Total 323	O 323	0	2
7	B	270	Total 270	O 270	0	1
7	C	332	Total 332	O 332	0	1

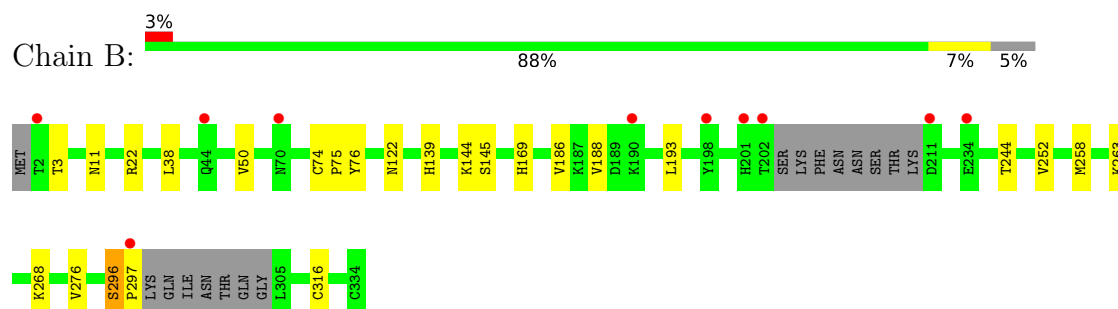
### 3 Residue-property plots [i](#)

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.

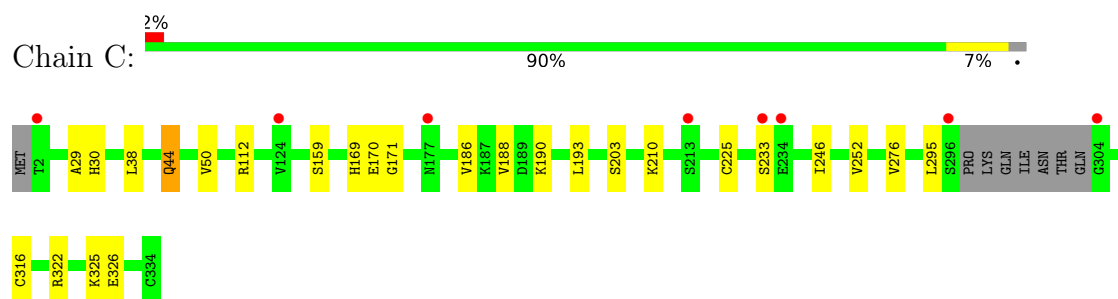
#### • Molecule 1: SxtDIOX



#### • Molecule 1: SxtDIOX



#### • Molecule 1: SxtDIOX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.73Å 96.93Å 80.81Å 90.00° 106.97° 90.00°	Depositor
Resolution (Å)	46.19 – 1.79 46.19 – 1.78	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.19-1.79) 97.5 (46.19-1.78)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.158 , 0.196 0.157 , 0.195	Depositor DCC
$R_{free}$ test set	5146 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8988	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D82, FE, GOL, FES, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.38	0/2678	0.57	0/3653
1	B	0.36	0/2721	0.56	0/3710
1	C	0.39	0/2751	0.59	1/3753 (0.0%)
All	All	0.38	0/8150	0.57	1/11116 (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	C	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	GLN	CB-CA-C	5.14	120.68	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	159[B]	SER	Mainchain
1	C	159[C]	SER	Mainchain

## 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	2592	0	2518	14	0
1	B	2633	0	2568	21	0
1	C	2672	0	2582	19	0
2	A	30	0	40	1	0
2	B	24	0	32	2	0
2	C	30	0	40	3	0
3	A	20	0	0	0	0
3	B	20	0	0	0	0
3	C	20	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	4	0	0	1	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
6	A	4	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	1	0
7	A	323	0	0	0	0
7	B	270	0	0	7	0
7	C	332	0	0	6	0
All	All	8988	0	7780	53	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (53) 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)
6:C:509:CL:CL	7:C:891:HOH:O	2.27	0.89
1:A:305:LEU:O	1:A:305:LEU:HD12	1.85	0.77
1:C:30:HIS:HD1	2:C:505:GOL:H12	1.49	0.75
1:B:22:ARG:HH21	1:C:44:GLN:HG2	1.50	0.74
1:B:11[B]:ASN:ND2	7:B:603:HOH:O	2.25	0.68
1:B:22:ARG:NH2	1:C:44:GLN:HG2	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225[B]:CYS:SG	7:C:733:HOH:O	2.43	0.61
1:A:112[B]:ARG:NH1	1:A:113:TYR:OH	2.35	0.60
1:B:193[A]:LEU:HD21	1:B:316[A]:CYS:SG	2.43	0.59
1:B:122:ASN:ND2	7:B:605:HOH:O	2.26	0.58
1:C:322[A]:ARG:NH1	7:C:606:HOH:O	2.36	0.58
1:A:111:GLU:O	1:A:112[A]:ARG:NH1	2.37	0.57
1:B:263[A]:LYS:NZ	7:B:608:HOH:O	2.37	0.57
1:C:169:HIS:CE1	1:C:276:VAL:HG13	2.40	0.56
1:C:186:VAL:HG22	1:C:316[B]:CYS:SG	2.45	0.55
1:A:295:LEU:O	1:A:325:LYS:NZ	2.35	0.55
1:C:295:LEU:O	1:C:325:LYS:NZ	2.39	0.55
1:B:38:LEU:HG	1:B:50:VAL:HG22	1.91	0.53
1:A:73:VAL:HG22	1:A:80:ARG:HG2	1.90	0.53
1:C:246:ILE:HD11	1:C:252:VAL:HG23	1.91	0.52
1:C:38:LEU:HG	1:C:50:VAL:HG22	1.91	0.51
1:C:171:GLY:HA2	1:C:203:SER:HB2	1.92	0.50
1:B:268:LYS:NZ	7:B:612:HOH:O	2.45	0.49
1:C:188:VAL:HG22	1:C:193:LEU:HD13	1.95	0.48
1:C:112:ARG:HD2	7:C:816:HOH:O	2.14	0.47
1:A:193:LEU:HD21	1:A:316[A]:CYS:SG	2.54	0.47
1:B:169:HIS:CE1	1:B:276[A]:VAL:HG13	2.50	0.47
1:B:169:HIS:CE1	1:B:276[B]:VAL:HG13	2.50	0.47
1:A:9:ILE:HG22	1:A:121:GLY:HA3	1.96	0.47
1:B:139:HIS:HB3	2:B:502:GOL:H12	1.98	0.46
1:A:108:HIS:HA	2:A:804:GOL:H2	1.97	0.46
1:C:210:LYS:HE3	1:C:233:SER:HB3	1.96	0.46
1:B:144:LYS:HB2	7:B:809:HOH:O	2.15	0.46
1:B:145[B]:SER:OG	7:B:601:HOH:O	2.20	0.46
1:A:169:HIS:CE1	1:A:276:VAL:HG13	2.52	0.44
1:B:139:HIS:ND1	2:B:502:GOL:O3	2.40	0.44
1:B:74:CYS:SG	1:B:75:PRO:HD2	2.57	0.44
1:A:187:LYS:HE2	1:A:189:ASP:HB3	1.98	0.44
1:C:190:LYS:NZ	7:C:617:HOH:O	2.51	0.44
1:A:139:HIS:O	1:A:258:MET:HA	2.18	0.43
1:B:186:VAL:HG22	1:B:316[B]:CYS:SG	2.58	0.43
1:C:188:VAL:HG21	7:C:606:HOH:O	2.18	0.43
1:B:296:SER:HA	1:B:297:PRO:HD3	1.88	0.43
1:A:77:HIS:HB2	5:A:808:FES:S1	2.59	0.42
1:C:29:ALA:HA	2:C:505:GOL:H31	2.01	0.42
1:A:9:ILE:HD13	1:A:32:LEU:HD13	2.02	0.42
1:B:3:THR:HG22	7:B:611:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:HIS:ND1	2:C:505:GOL:H12	2.26	0.41
1:B:139:HIS:O	1:B:258:MET:HA	2.20	0.41
1:C:322[B]:ARG:O	1:C:326:GLU:HG3	2.21	0.41
1:A:193:LEU:C	1:A:193:LEU:HD23	2.41	0.41
1:B:188:VAL:HG22	1:B:193[B]:LEU:HD13	2.03	0.41
1:B:244:THR:HB	1:B:252:VAL:HB	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/334 (96%)	309 (97%)	10 (3%)	0	100	100
1	B	323/334 (97%)	315 (98%)	8 (2%)	0	100	100
1	C	330/334 (99%)	321 (97%)	9 (3%)	0	100	100
All	All	972/1002 (97%)	945 (97%)	27 (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	295/304 (97%)	292 (99%)	3 (1%)	76	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	301/304 (99%)	299 (99%)	2 (1%)	84	81
1	C	304/304 (100%)	303 (100%)	1 (0%)	92	91
All	All	900/912 (99%)	894 (99%)	6 (1%)	86	81

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112[A]	ARG
1	A	112[B]	ARG
1	A	305	LEU
1	B	76	TYR
1	B	296	SER
1	C	170	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 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	GOL	C	506	-	5,5,5	0.92	0	5,5,5	1.14	1 (20%)
3	D82	C	504	-	17,22,22	0.55	0	14,34,34	0.93	1 (7%)
2	GOL	C	507	-	5,5,5	0.73	0	5,5,5	1.11	0
5	FES	C	501	1	0,4,4	-	-	-	-	-
2	GOL	A	805	-	5,5,5	0.92	0	5,5,5	0.98	0
5	FES	A	808	1	0,4,4	-	-	-	-	-
2	GOL	C	502	-	5,5,5	0.89	0	5,5,5	1.17	1 (20%)
2	GOL	A	801	-	5,5,5	0.96	0	5,5,5	0.89	0
2	GOL	B	506	-	5,5,5	0.83	0	5,5,5	1.04	0
2	GOL	B	502	-	5,5,5	1.01	0	5,5,5	1.00	0
2	GOL	B	504	-	5,5,5	0.84	0	5,5,5	1.06	0
2	GOL	C	505	-	5,5,5	1.06	0	5,5,5	1.00	0
2	GOL	C	503	-	5,5,5	1.02	0	5,5,5	0.86	0
2	GOL	A	806	-	5,5,5	0.79	0	5,5,5	1.08	1 (20%)
3	D82	B	505	-	17,22,22	0.60	1 (5%)	14,34,34	0.94	0
2	GOL	A	804	-	5,5,5	0.96	0	5,5,5	0.91	0
3	D82	A	803	-	17,22,22	0.57	0	14,34,34	0.87	1 (7%)
5	FES	B	501	1	0,4,4	-	-	-	-	-
2	GOL	A	802	-	5,5,5	1.14	1 (20%)	5,5,5	0.95	0
2	GOL	B	503	-	5,5,5	0.85	0	5,5,5	0.92	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	GOL	C	506	-	-	2/4/4/4	-
3	D82	C	504	-	-	0/5/49/49	0/3/3/3
2	GOL	C	507	-	-	0/4/4/4	-
5	FES	C	501	1	-	-	0/1/1/1
2	GOL	A	805	-	-	4/4/4/4	-
5	FES	A	808	1	-	-	0/1/1/1
2	GOL	C	502	-	-	2/4/4/4	-
2	GOL	A	801	-	-	2/4/4/4	-
2	GOL	B	506	-	-	2/4/4/4	-
2	GOL	B	502	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	504	-	-	2/4/4/4	-
2	GOL	C	505	-	-	0/4/4/4	-
2	GOL	C	503	-	-	4/4/4/4	-
2	GOL	A	806	-	-	1/4/4/4	-
3	D82	B	505	-	-	0/5/49/49	0/3/3/3
2	GOL	A	804	-	-	2/4/4/4	-
3	D82	A	803	-	-	0/5/49/49	0/3/3/3
5	FES	B	501	1	-	-	0/1/1/1
2	GOL	A	802	-	-	3/4/4/4	-
2	GOL	B	503	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	GOL	C3-C2	2.04	1.60	1.51
3	B	505	D82	O2-C6	-2.03	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	504	D82	O2-C6-C7	-2.39	104.21	110.50
2	C	506	GOL	C3-C2-C1	-2.23	103.05	111.70
3	A	803	D82	O2-C6-C7	-2.07	105.06	110.50
2	C	502	GOL	C3-C2-C1	-2.01	103.90	111.70
2	A	806	GOL	C3-C2-C1	-2.01	103.90	111.70

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	802	GOL	O1-C1-C2-C3
2	A	804	GOL	C1-C2-C3-O3
2	C	503	GOL	C1-C2-C3-O3
2	C	506	GOL	O1-C1-C2-C3
2	A	801	GOL	O2-C2-C3-O3
2	C	503	GOL	O2-C2-C3-O3
2	A	801	GOL	C1-C2-C3-O3
2	A	805	GOL	O1-C1-C2-C3
2	B	502	GOL	O1-C1-C2-C3
2	B	502	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	506	GOL	O1-C1-C2-C3
2	C	502	GOL	C1-C2-C3-O3
2	C	503	GOL	O1-C1-C2-C3
2	A	802	GOL	O1-C1-C2-O2
2	B	506	GOL	O1-C1-C2-O2
2	C	506	GOL	O1-C1-C2-O2
2	A	804	GOL	O2-C2-C3-O3
2	C	502	GOL	O2-C2-C3-O3
2	B	502	GOL	O1-C1-C2-O2
2	B	502	GOL	O2-C2-C3-O3
2	A	805	GOL	O1-C1-C2-O2
2	A	805	GOL	O2-C2-C3-O3
2	A	806	GOL	O1-C1-C2-C3
2	B	504	GOL	O1-C1-C2-C3
2	A	802	GOL	O2-C2-C3-O3
2	A	805	GOL	C1-C2-C3-O3
2	B	504	GOL	O2-C2-C3-O3
2	C	503	GOL	O1-C1-C2-O2

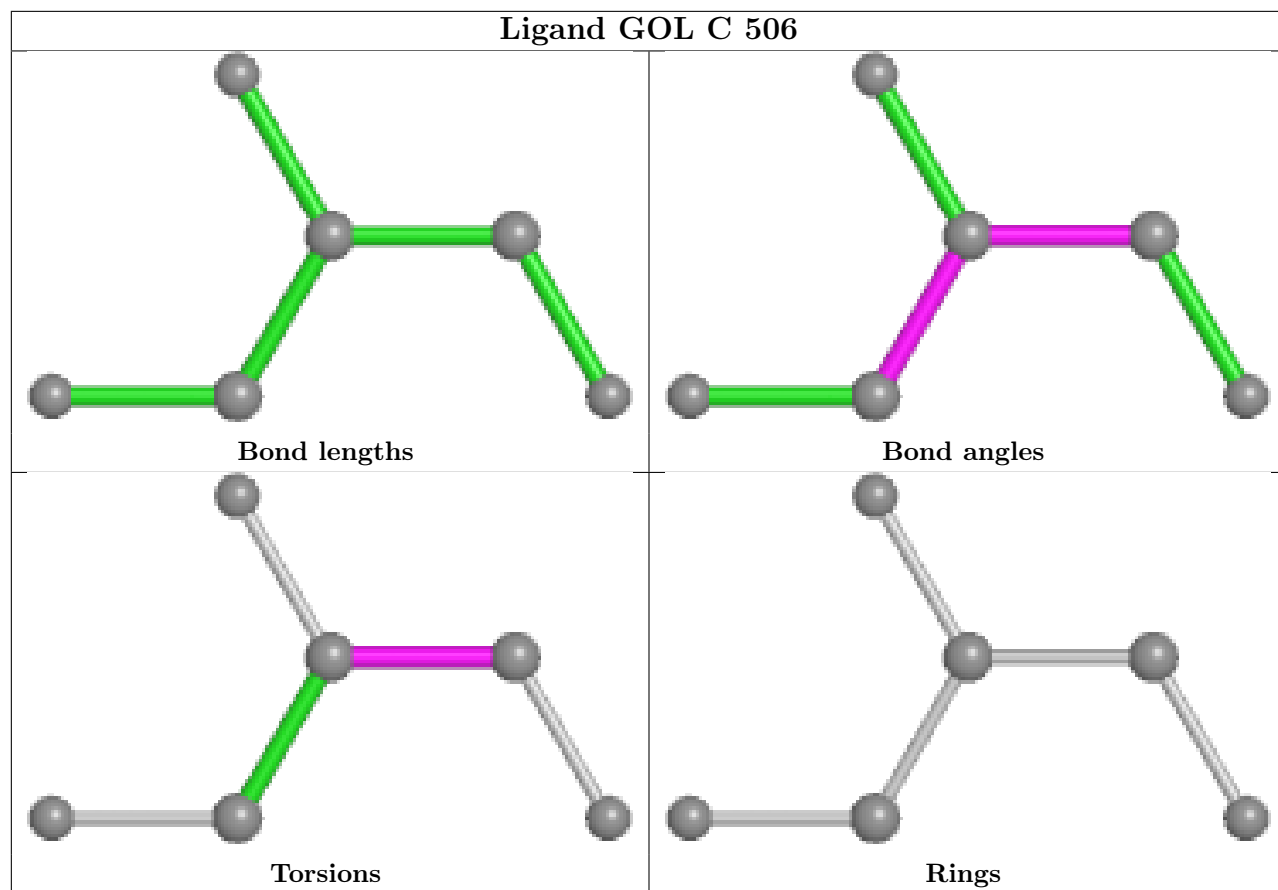
There are no ring outliers.

4 monomers are involved in 7 short contacts:

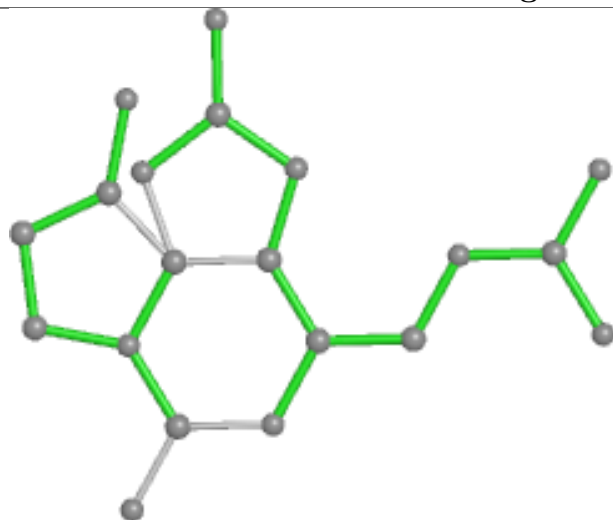
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	808	FES	1	0
2	B	502	GOL	2	0
2	C	505	GOL	3	0
2	A	804	GOL	1	0

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

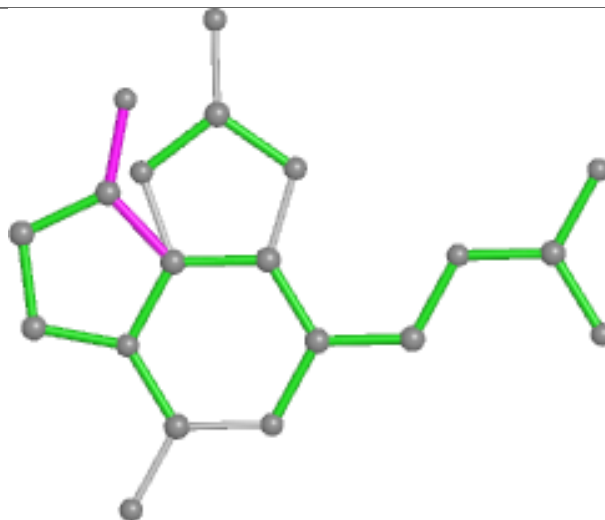




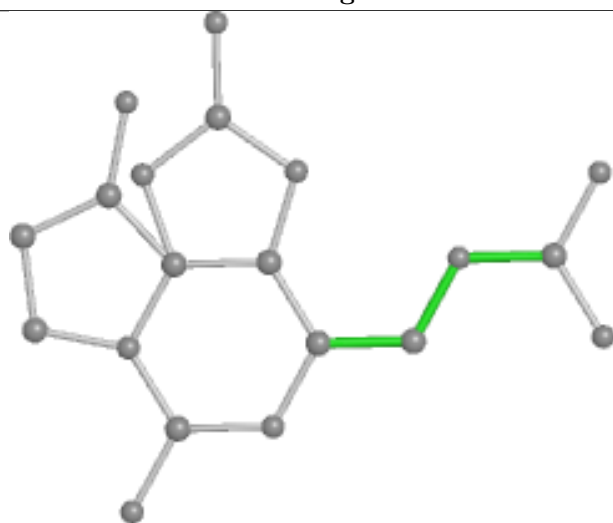
## Ligand D82 C 504



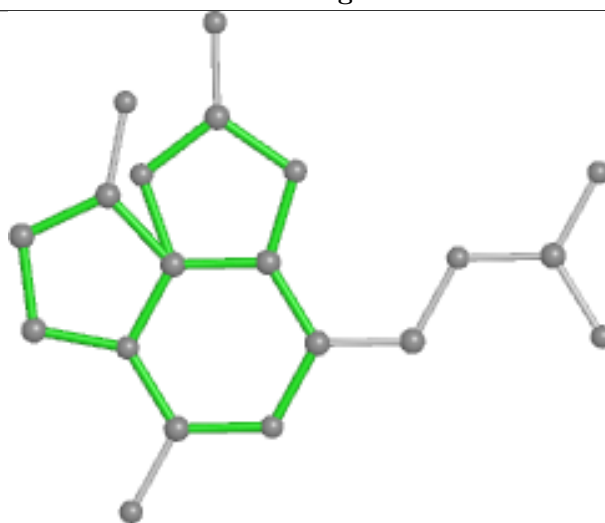
Bond lengths



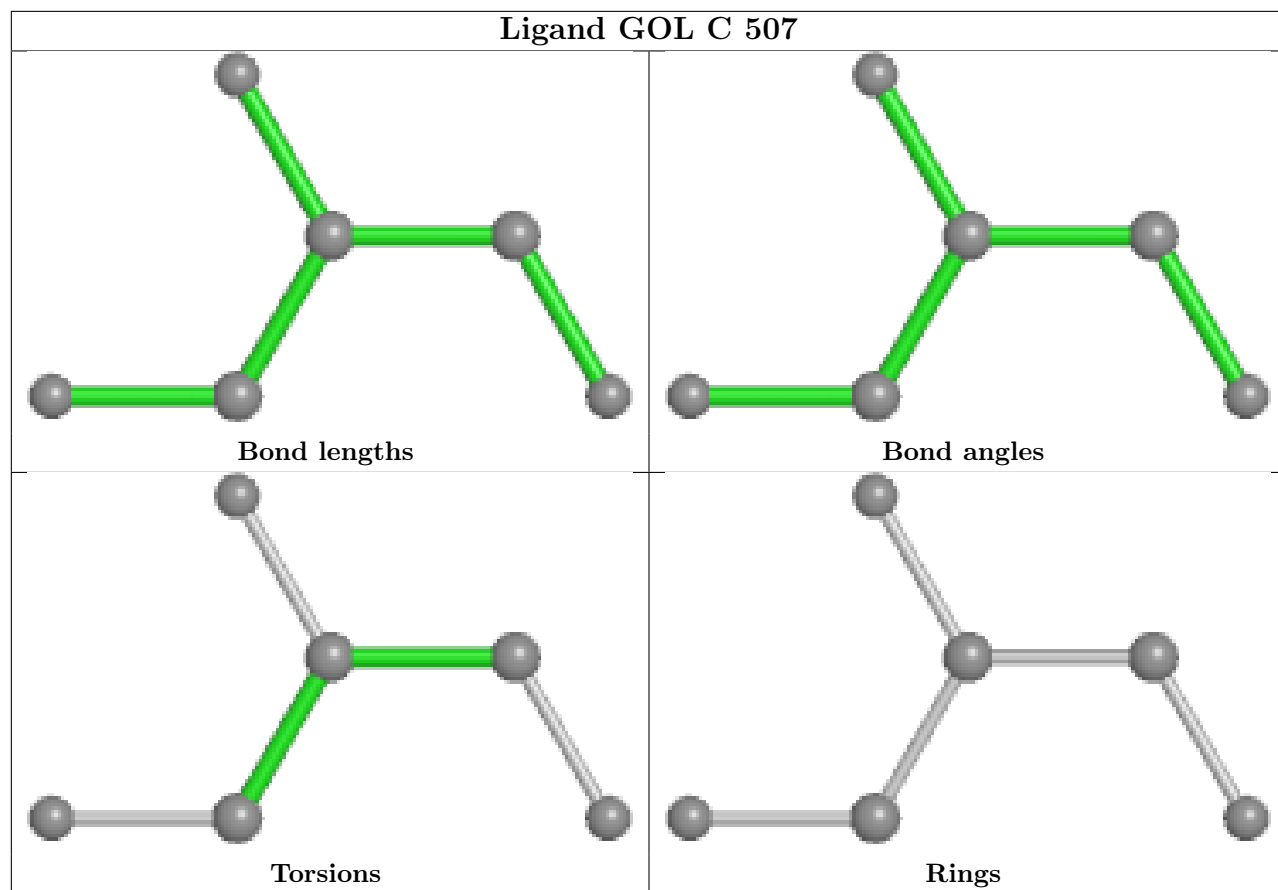
Bond angles

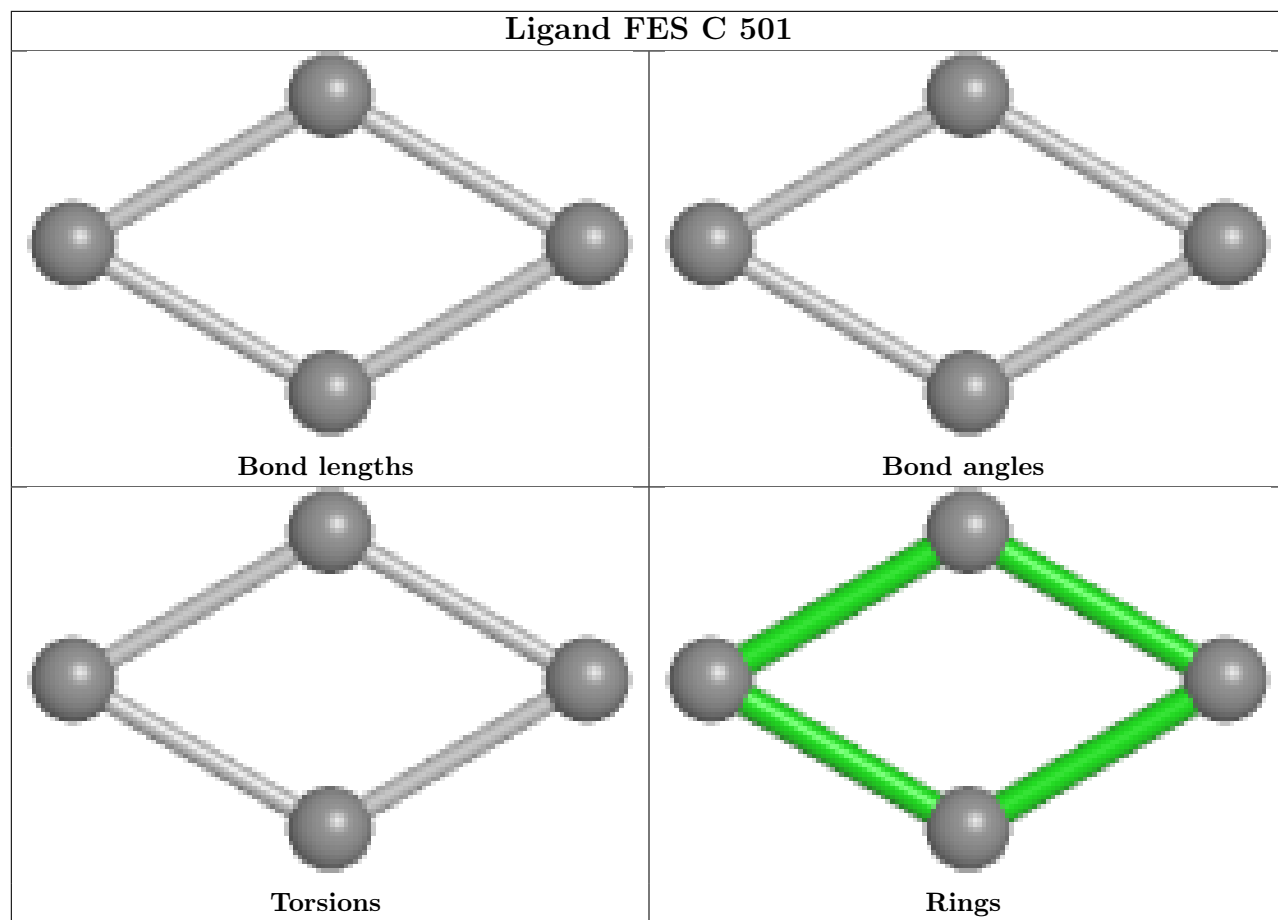


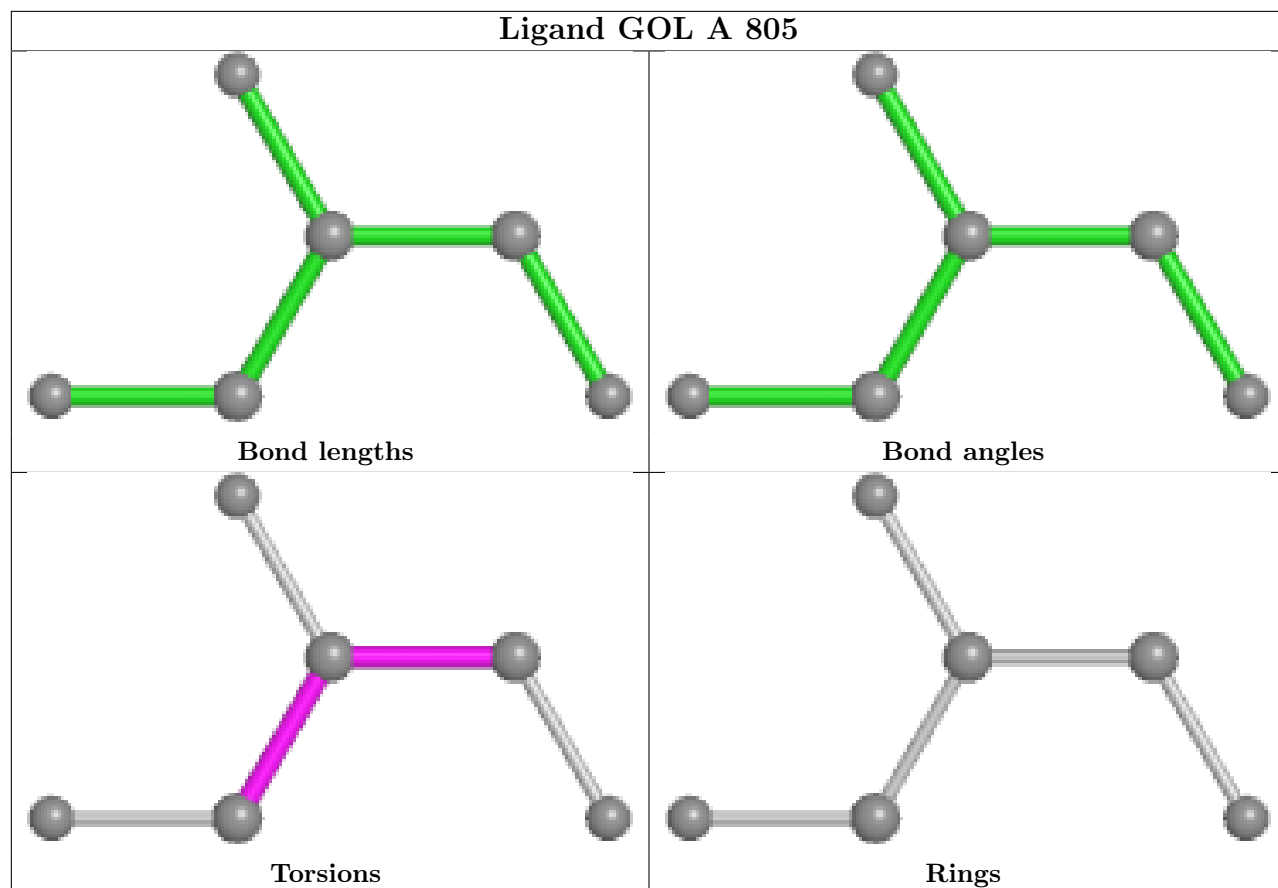
Torsions

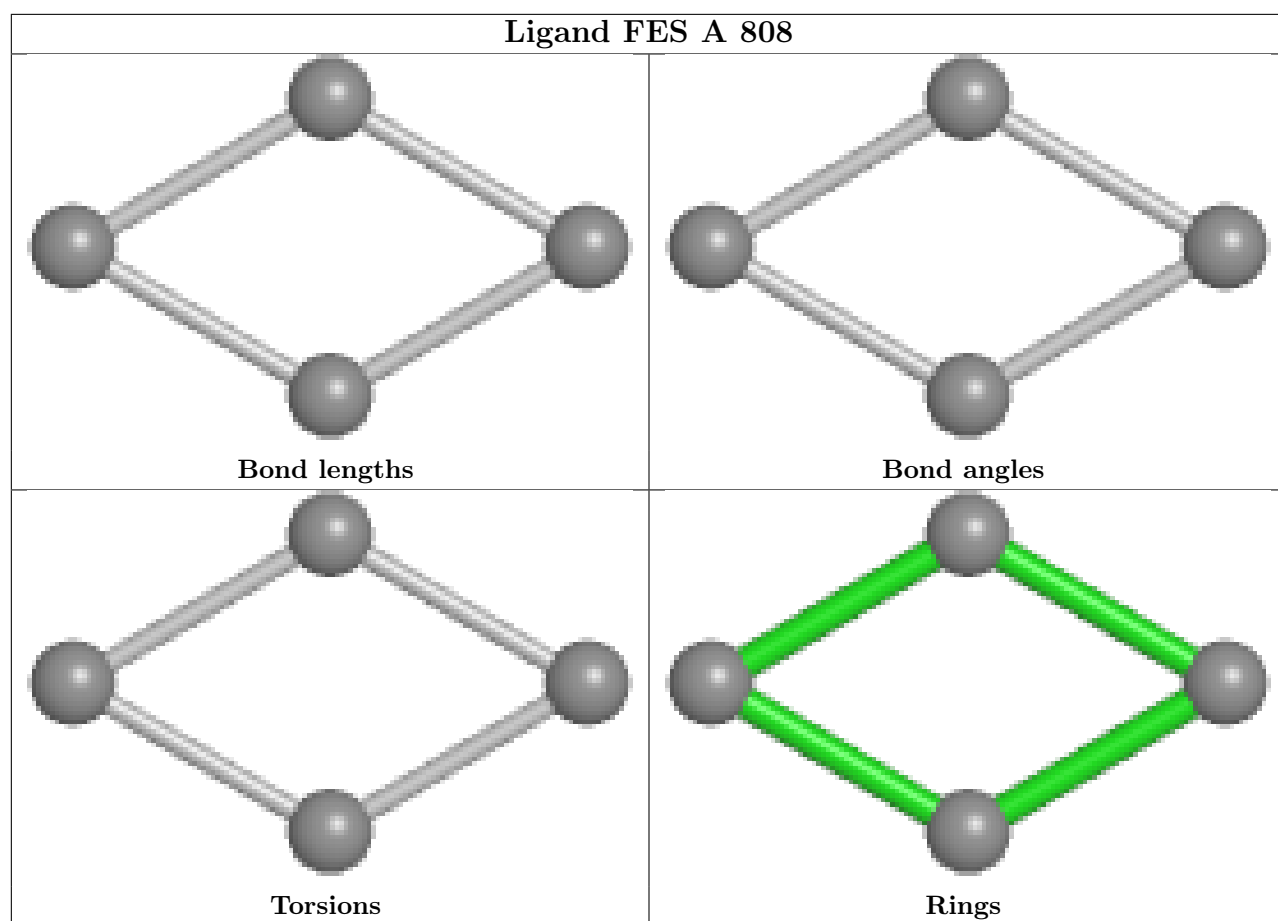


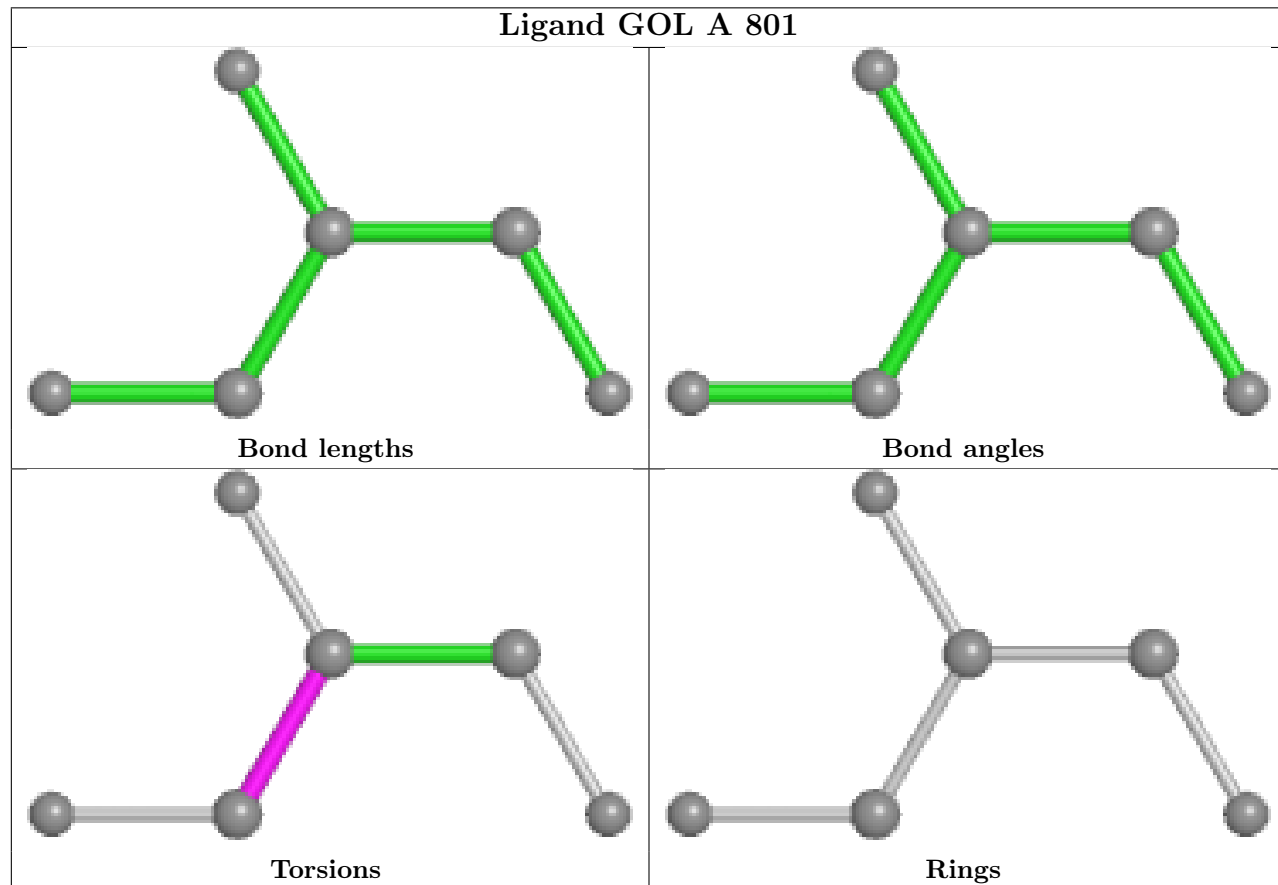
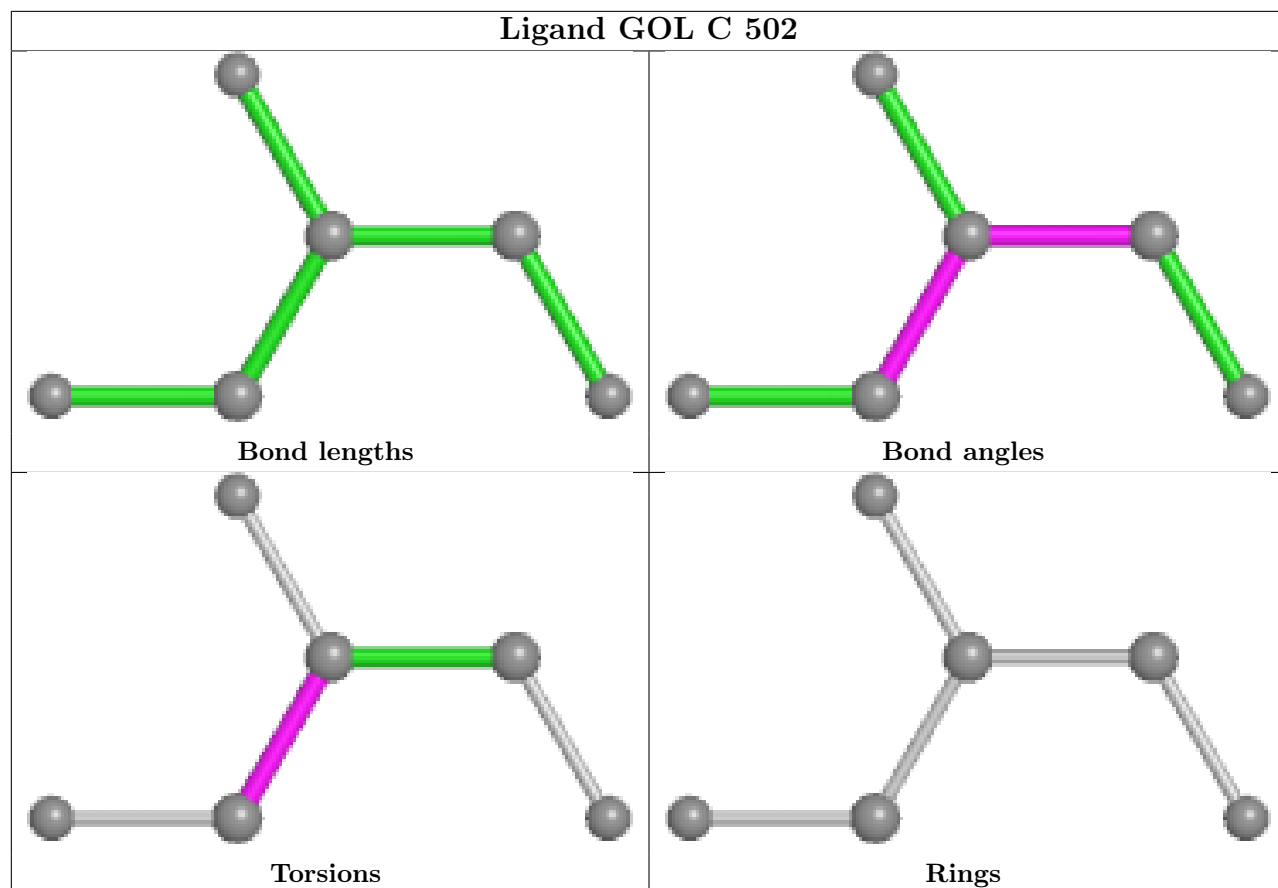
Rings

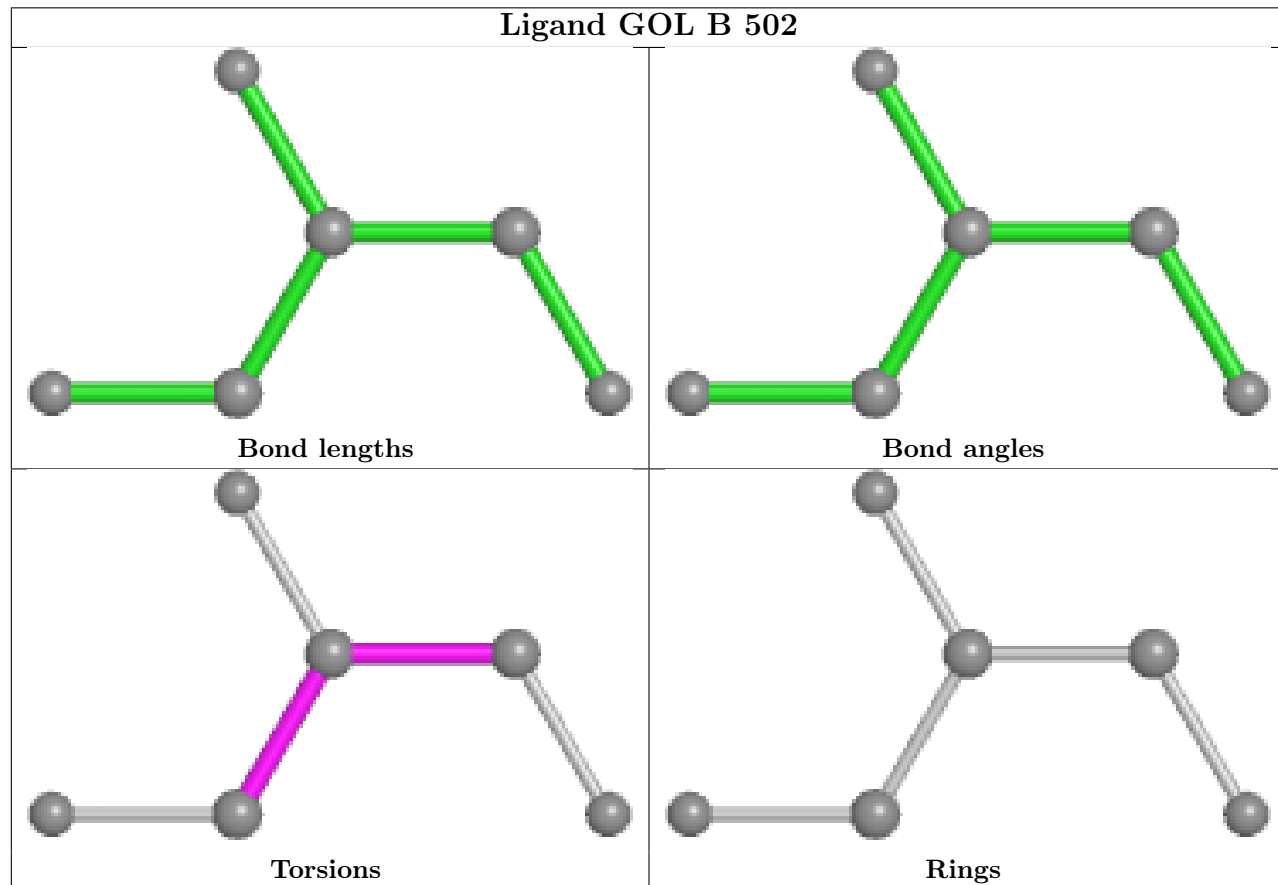
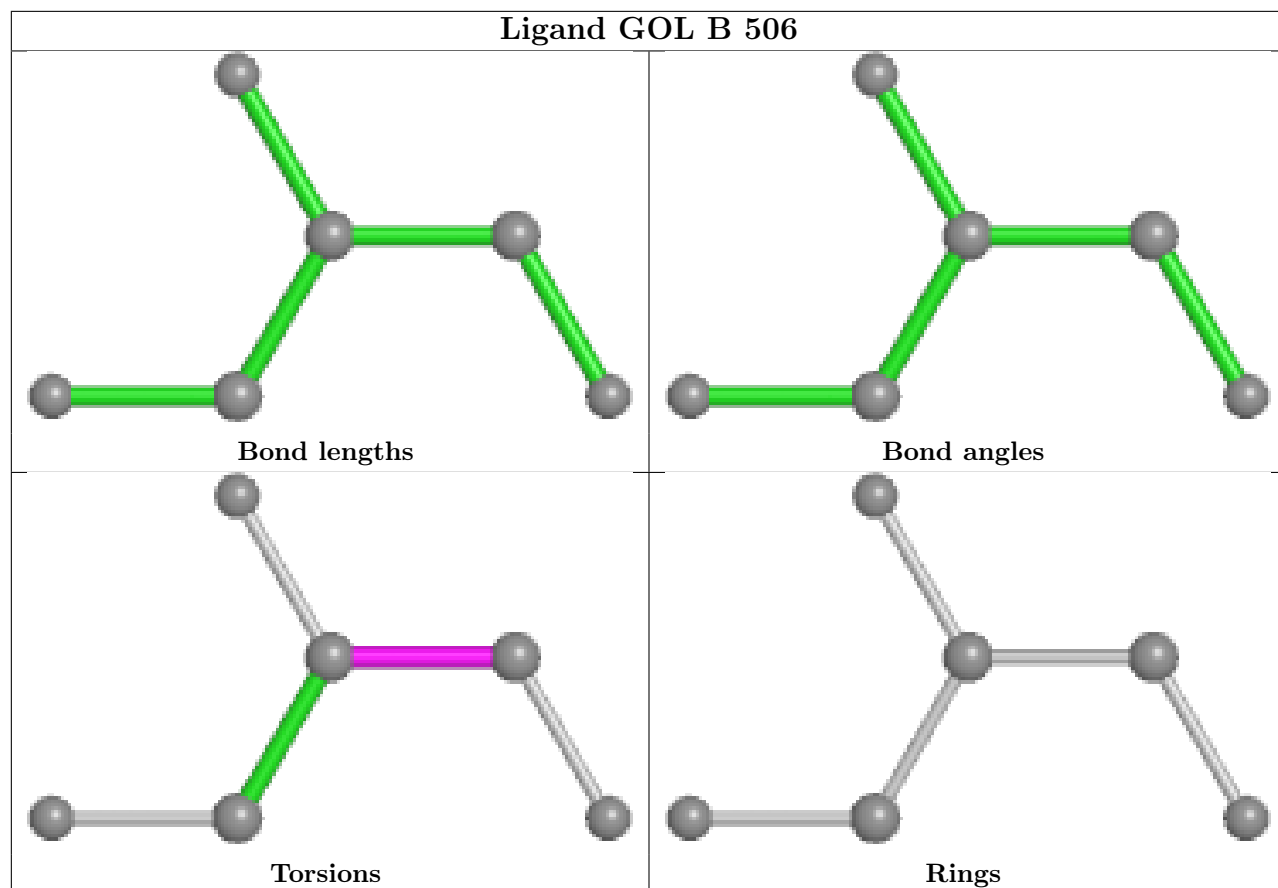




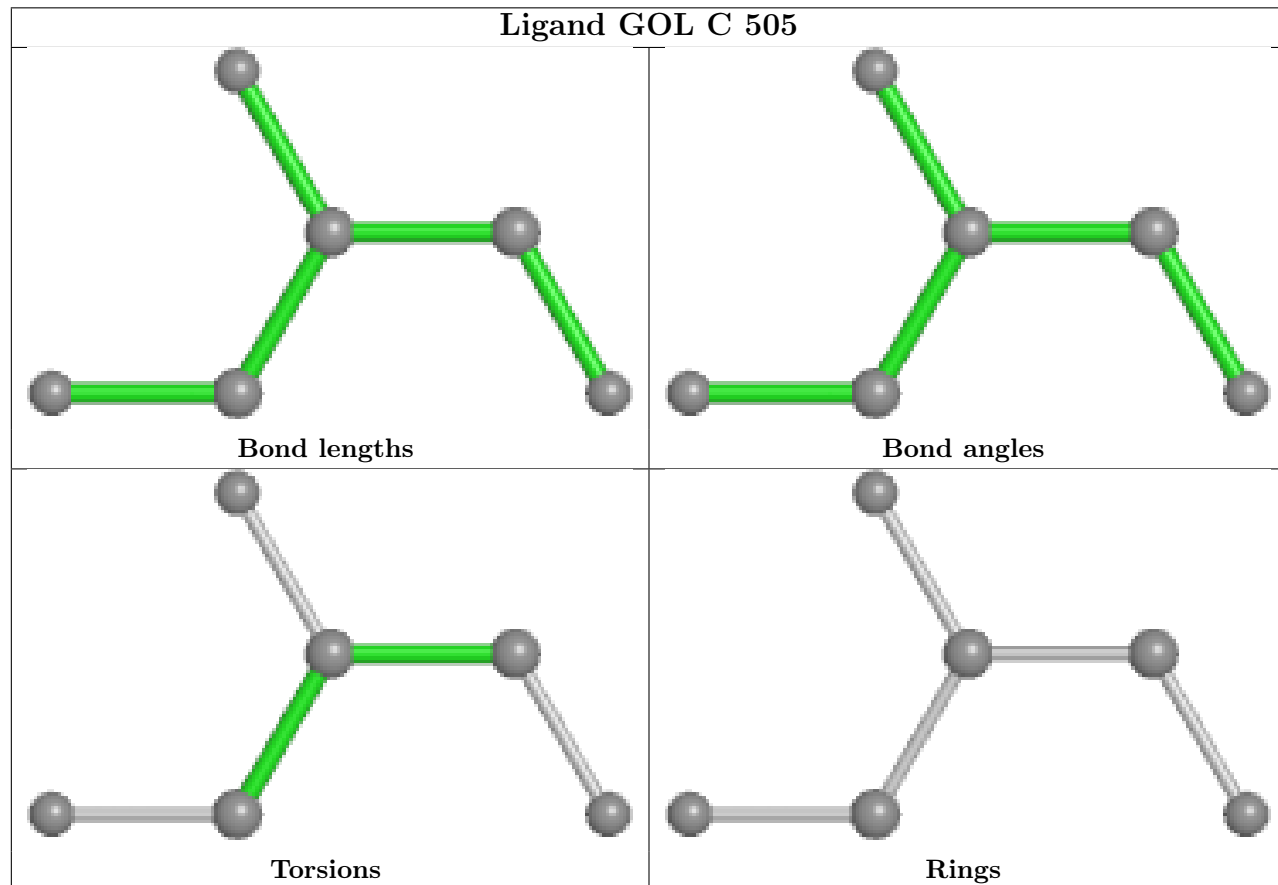
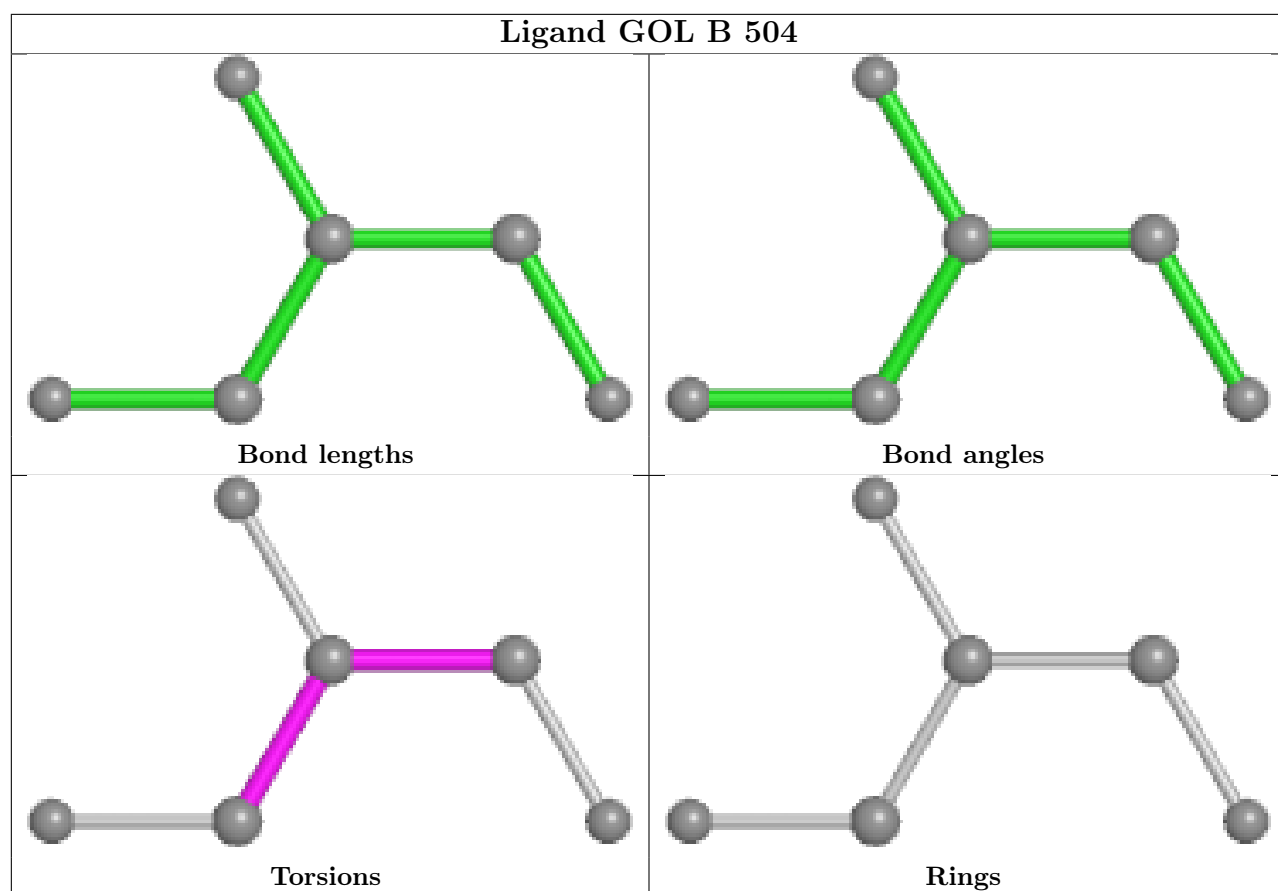


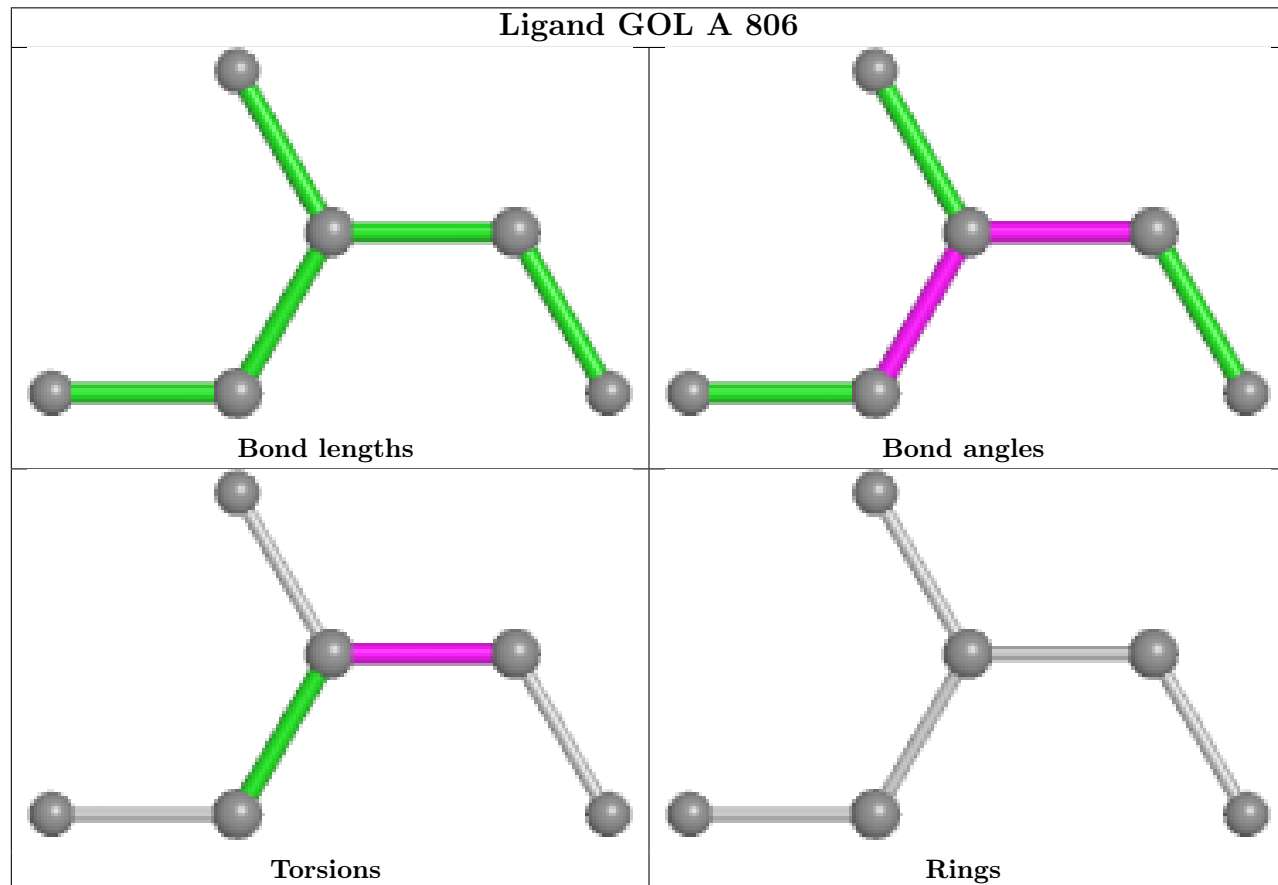
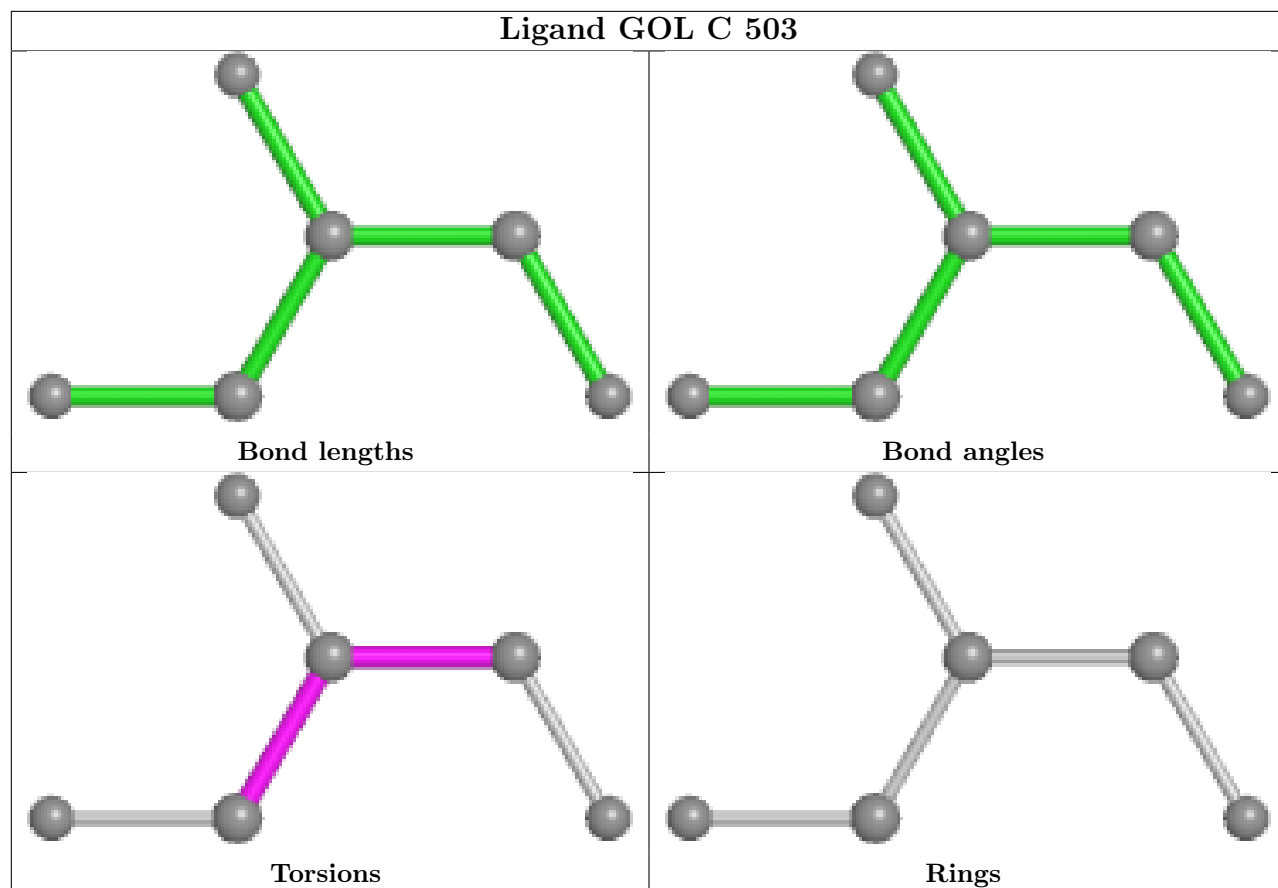




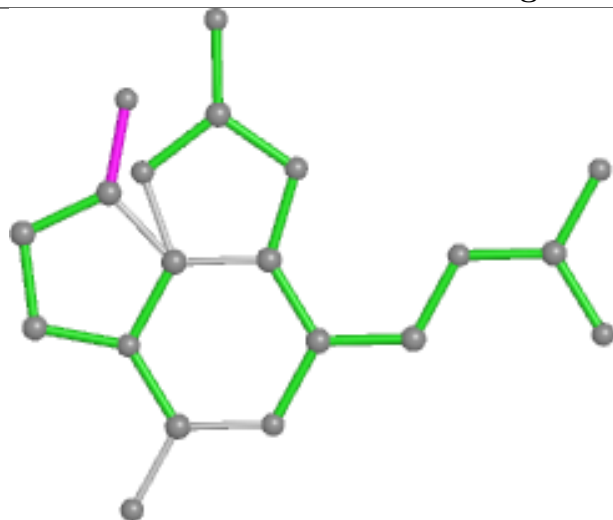




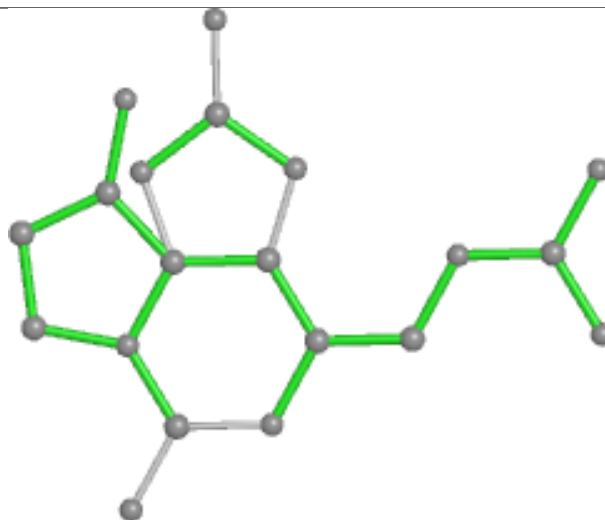




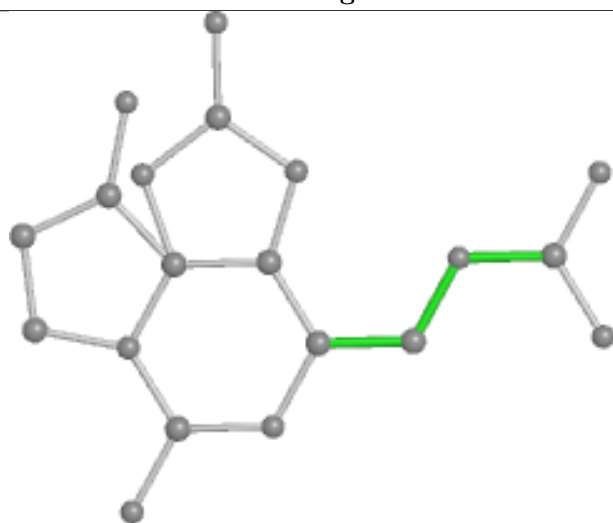
## Ligand D82 B 505



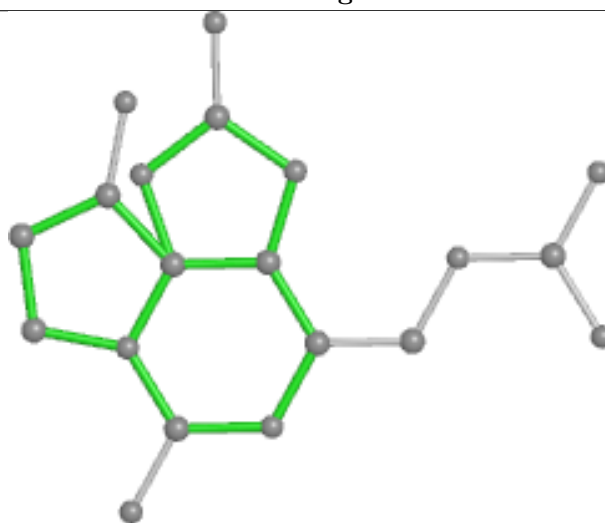
Bond lengths



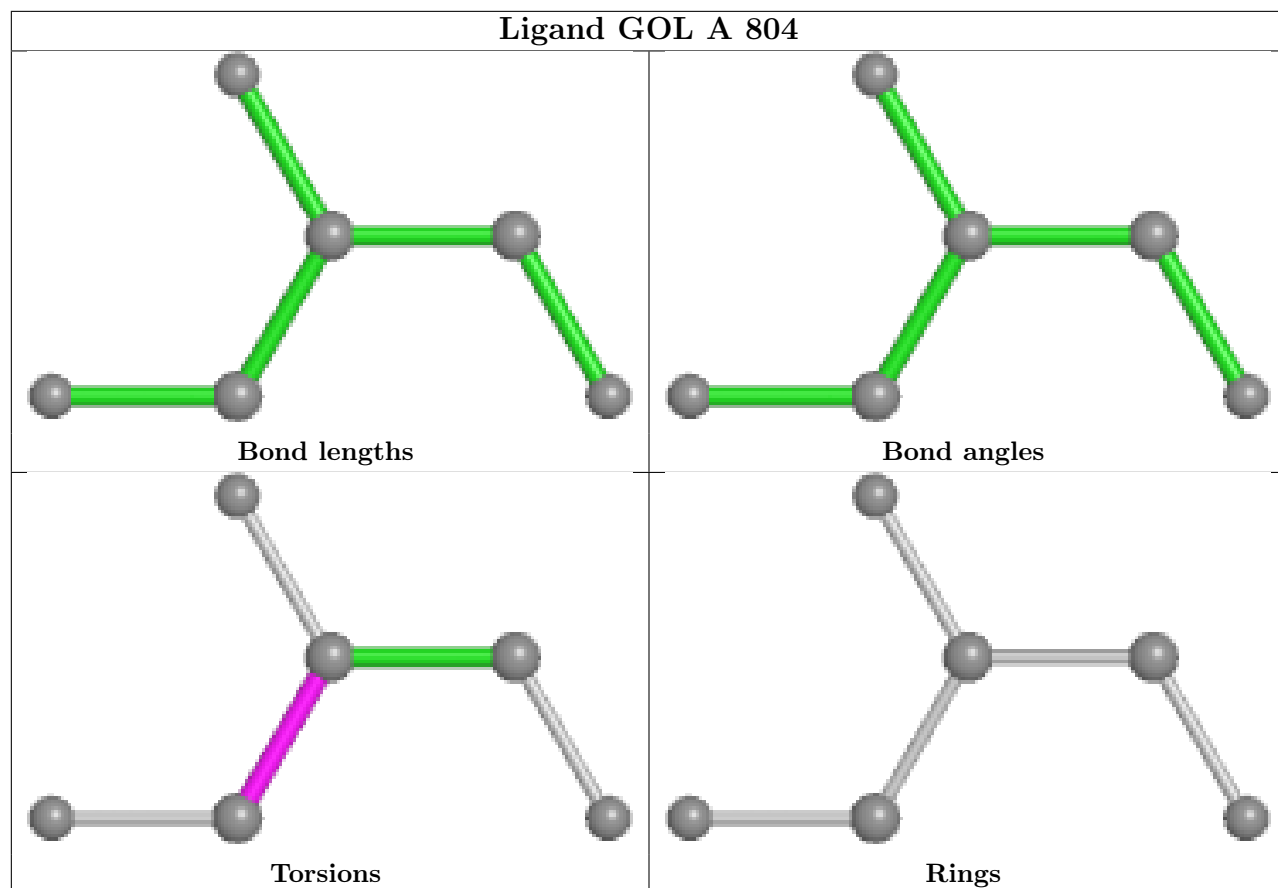
Bond angles



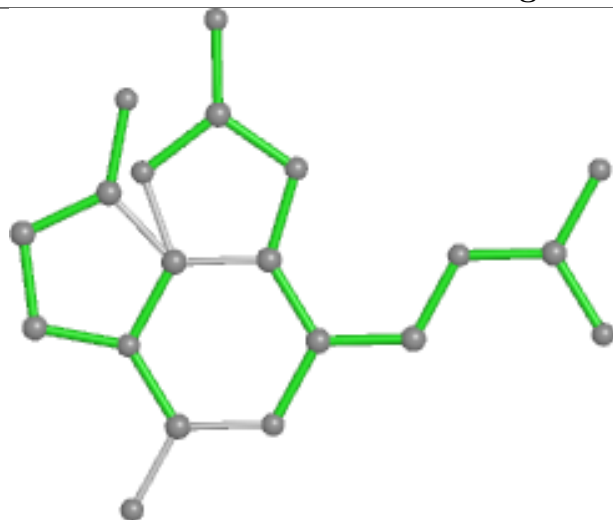
Torsions



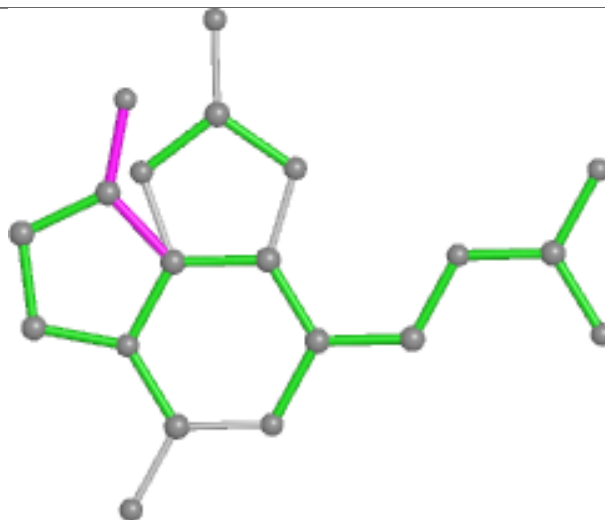
Rings



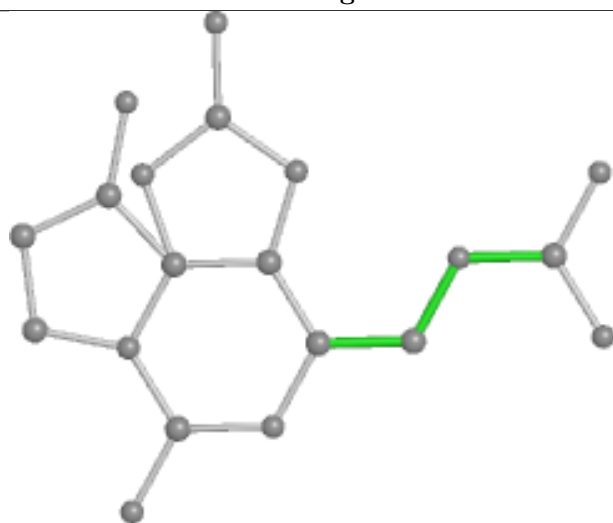
## Ligand D82 A 803



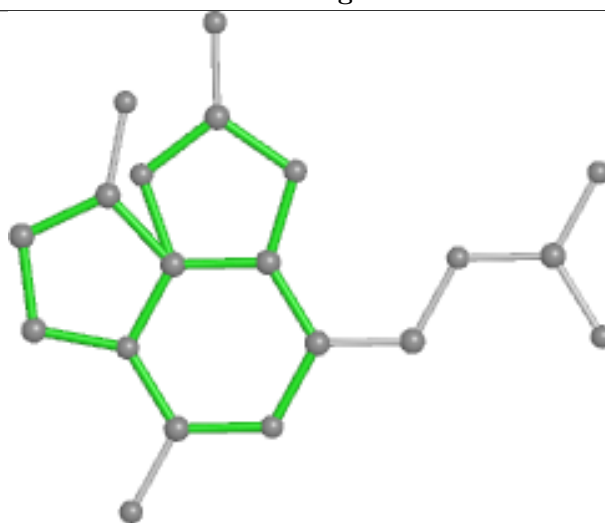
Bond lengths



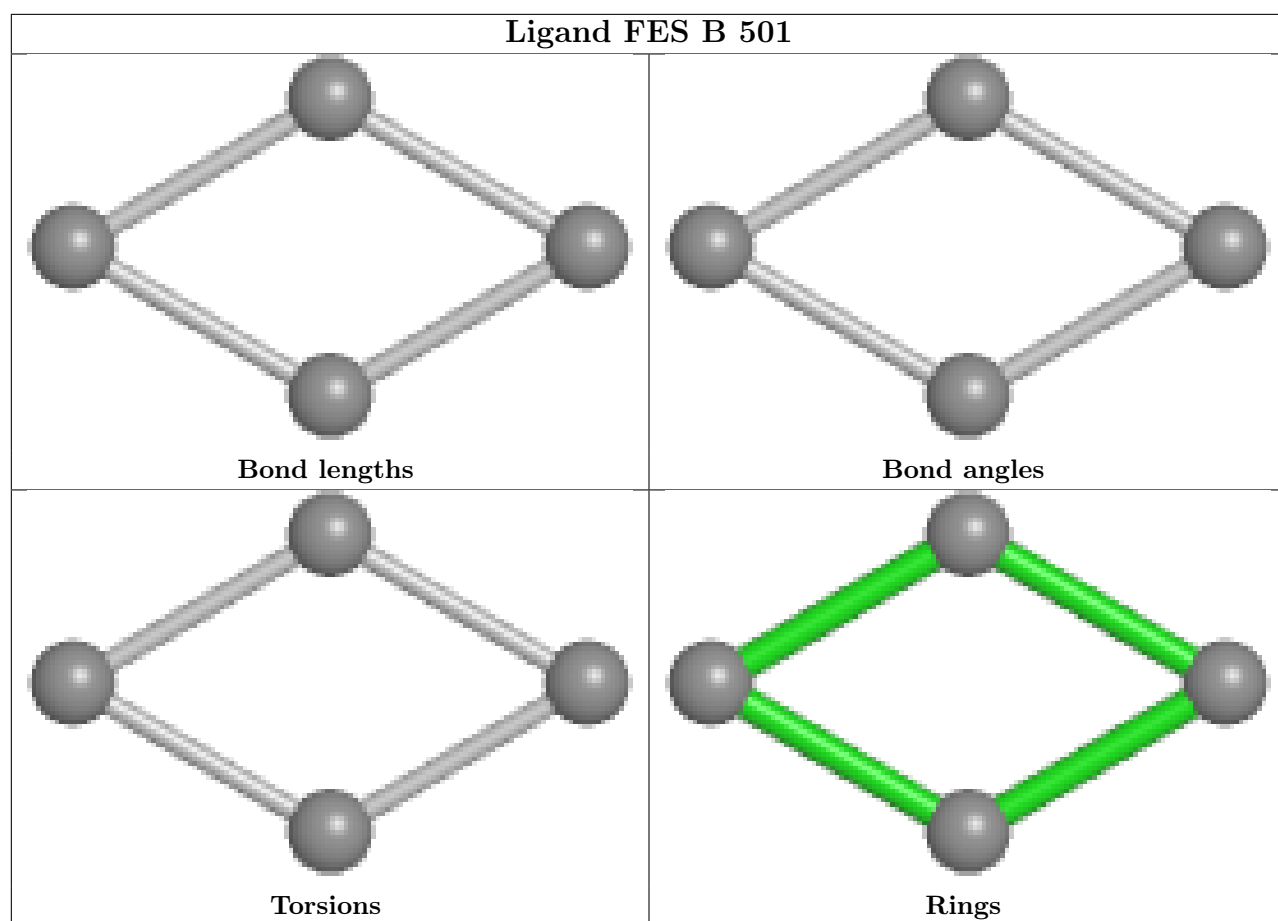
Bond angles

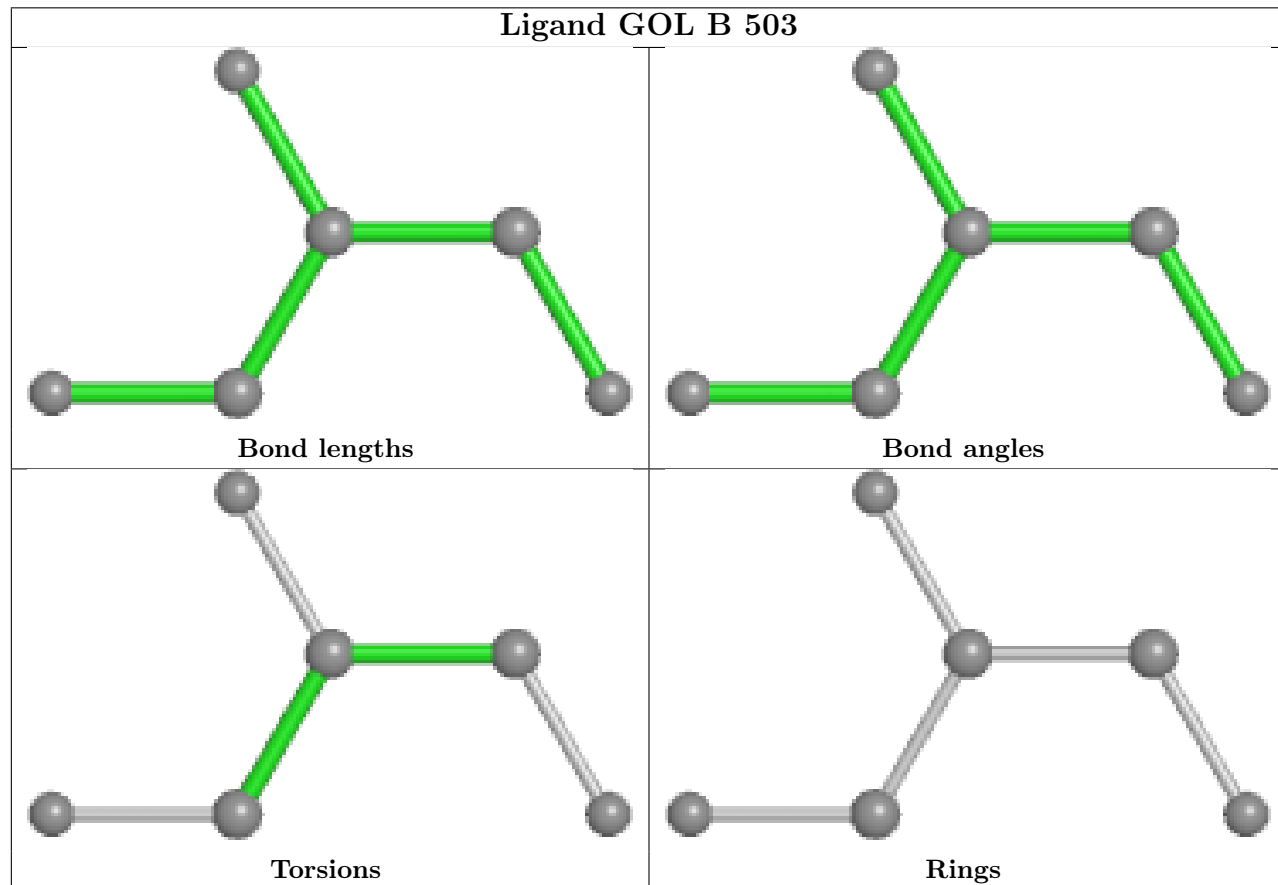
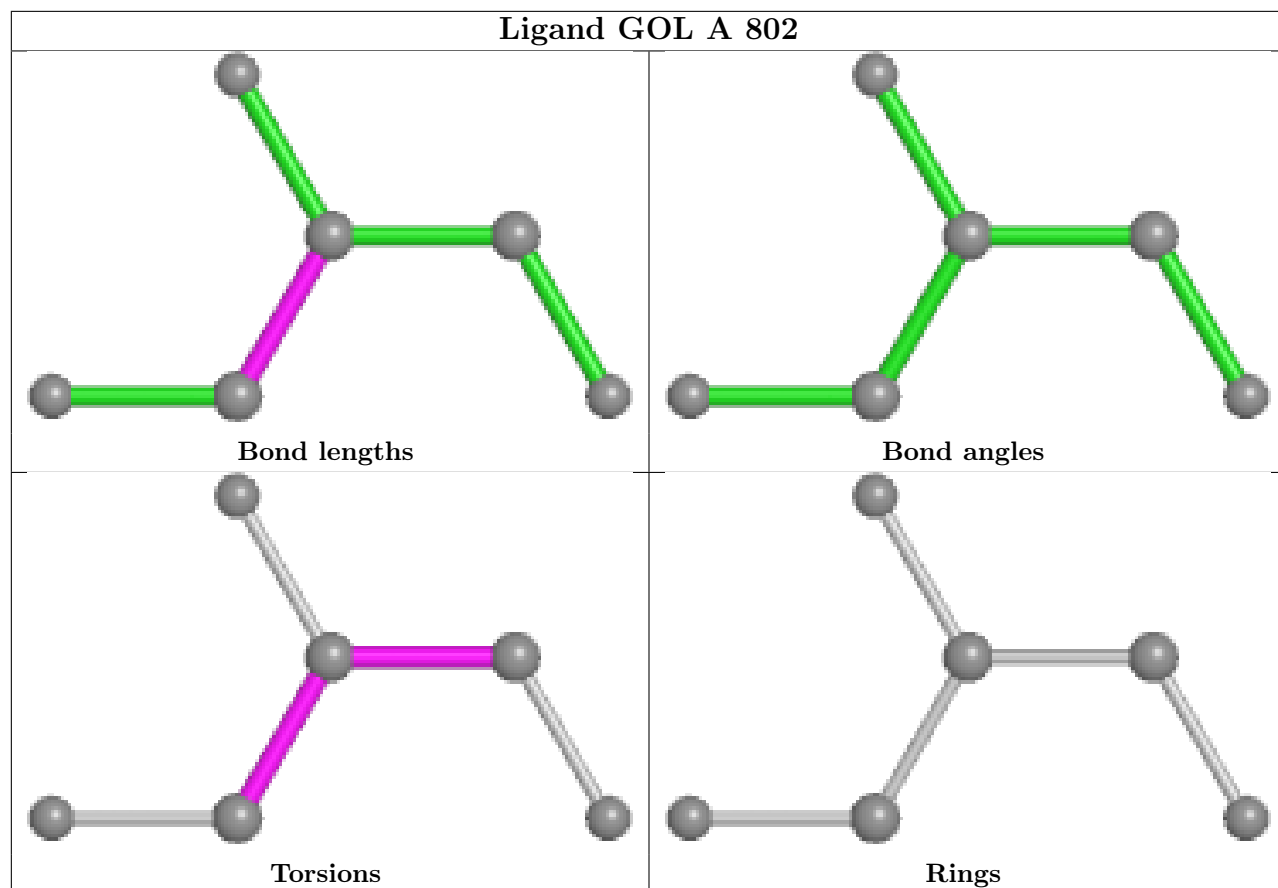


Torsions



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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	318/334 (95%)	-0.16	17 (5%) 26 21	17, 26, 51, 86	0
1	B	318/334 (95%)	-0.14	10 (3%) 49 43	18, 29, 57, 76	0
1	C	326/334 (97%)	-0.16	8 (2%) 57 52	16, 27, 52, 80	0
All	All	962/1002 (96%)	-0.16	35 (3%) 42 37	16, 27, 53, 86	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	PRO	7.4
1	A	305	LEU	5.8
1	A	212	ASP	5.0
1	A	203	SER	4.8
1	B	234	GLU	4.7
1	C	304	GLY	4.5
1	B	2	THR	4.4
1	C	177	ASN	4.4
1	A	234	GLU	4.4
1	A	233	SER	3.9
1	C	296	SER	3.8
1	B	211	ASP	3.7
1	B	202	THR	3.7
1	A	213	SER	3.6
1	A	202	THR	3.4
1	C	234	GLU	3.2
1	C	213	SER	3.0
1	A	44	GLN	2.9
1	A	178	HIS	2.9
1	A	2	THR	2.9
1	A	124	VAL	2.9
1	A	190	LYS	2.8
1	B	44	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	97	VAL	2.6
1	C	124	VAL	2.5
1	A	69	ASN	2.5
1	B	70	ASN	2.5
1	A	95	ASP	2.4
1	C	233	SER	2.3
1	B	190	LYS	2.3
1	B	201	HIS	2.1
1	C	2	THR	2.1
1	B	198	TYR	2.1
1	A	304	GLY	2.0
1	A	232	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	A	802	6/6	0.77	0.16	32,45,49,53	0
2	GOL	C	507	6/6	0.77	0.27	51,58,58,67	0
2	GOL	B	503	6/6	0.80	0.17	36,51,54,56	0
2	GOL	A	804	6/6	0.82	0.25	38,44,51,56	0
2	GOL	B	506	6/6	0.82	0.26	50,57,62,66	0
2	GOL	C	505	6/6	0.82	0.18	35,45,51,63	0
2	GOL	A	806	6/6	0.82	0.17	44,51,61,64	0
2	GOL	A	801	6/6	0.88	0.16	37,44,49,60	0
2	GOL	C	506	6/6	0.89	0.25	31,47,56,57	0
2	GOL	C	503	6/6	0.90	0.21	33,42,46,52	0
2	GOL	A	805	6/6	0.92	0.24	55,56,60,61	0

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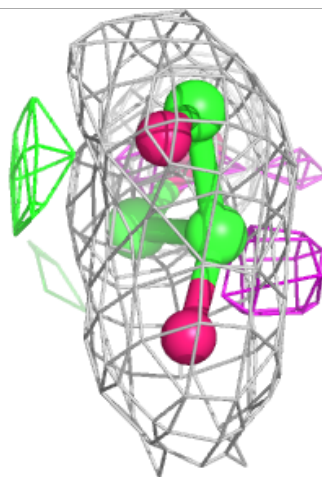
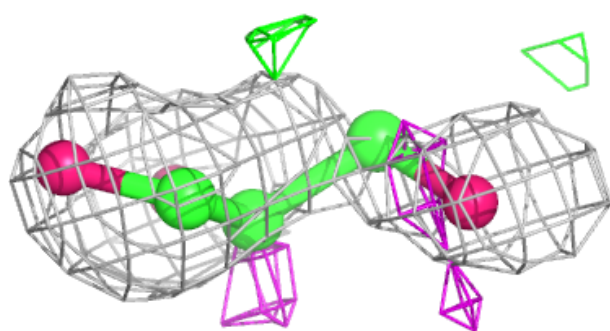
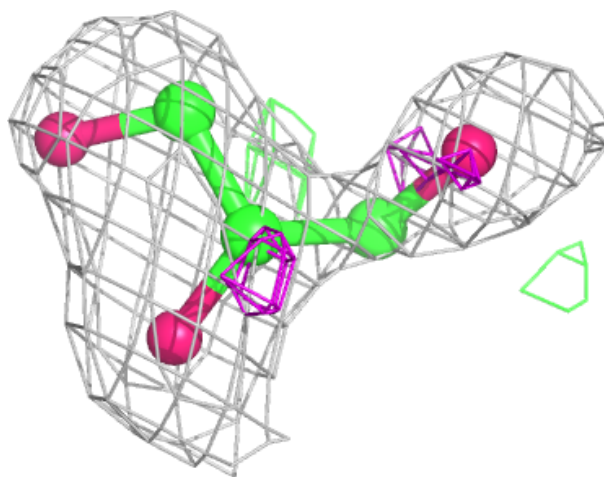
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	C	502	6/6	0.92	0.12	33,47,50,57	0
3	D82	B	505	20/20	0.93	0.07	21,28,37,40	0
6	CL	A	809	1/1	0.93	0.05	48,48,48,48	0
3	D82	C	504	20/20	0.94	0.07	24,30,45,46	0
2	GOL	B	504	6/6	0.94	0.09	46,49,54,60	0
3	D82	A	803	20/20	0.95	0.08	21,26,36,38	0
2	GOL	B	502	6/6	0.95	0.12	26,39,48,54	0
6	CL	A	810	1/1	0.96	0.04	43,43,43,43	0
6	CL	C	510	1/1	0.96	0.05	37,37,37,37	0
6	CL	B	508	1/1	0.97	0.03	50,50,50,50	0
6	CL	A	812	1/1	0.97	0.09	43,43,43,43	0
5	FES	A	808	4/4	0.99	0.08	21,22,22,24	0
5	FES	B	501	4/4	0.99	0.07	23,24,24,26	0
6	CL	C	509	1/1	0.99	0.08	28,28,28,28	0
6	CL	A	811	1/1	0.99	0.05	29,29,29,29	0
5	FES	C	501	4/4	1.00	0.09	17,18,18,19	0
4	FE	C	508	1/1	1.00	0.10	22,22,22,22	0
4	FE	A	807	1/1	1.00	0.09	18,18,18,18	0
4	FE	B	507	1/1	1.00	0.10	20,20,20,20	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.

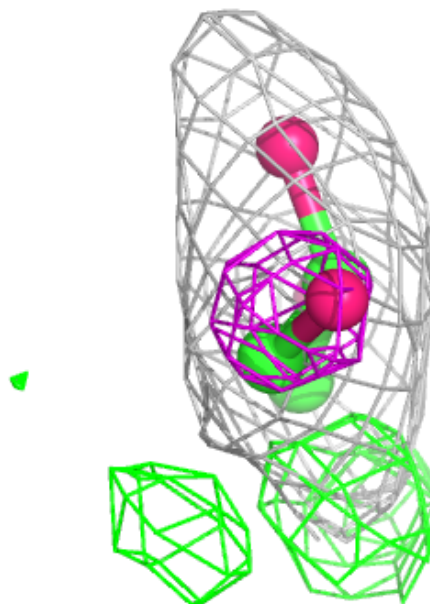
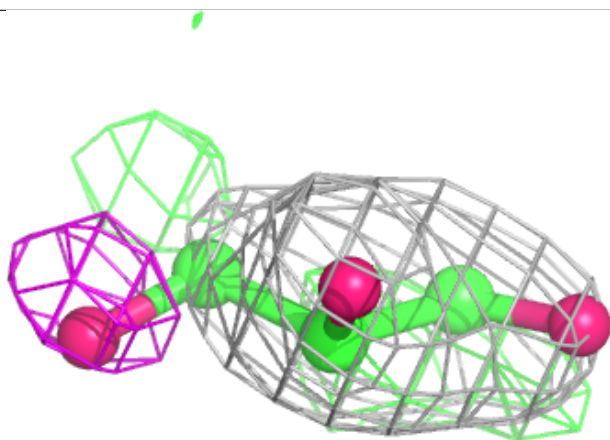
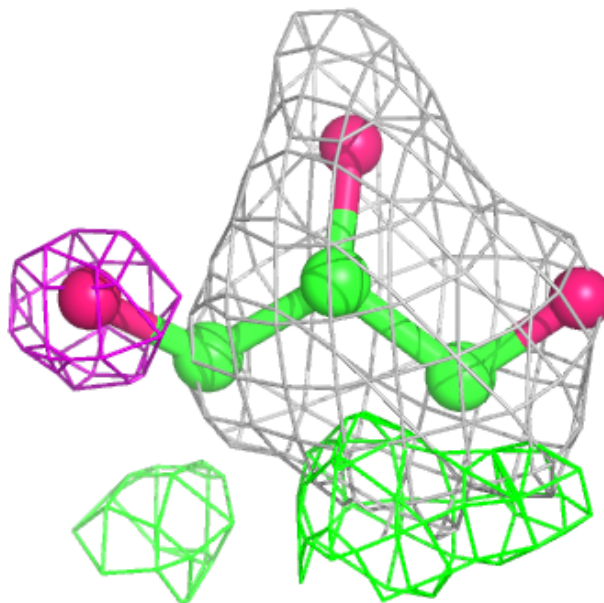
**Electron density around GOL A 802:**

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



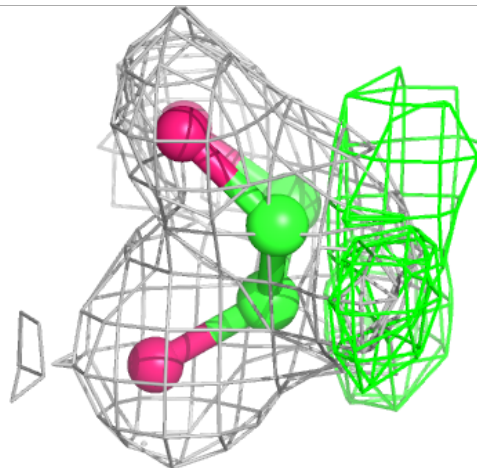
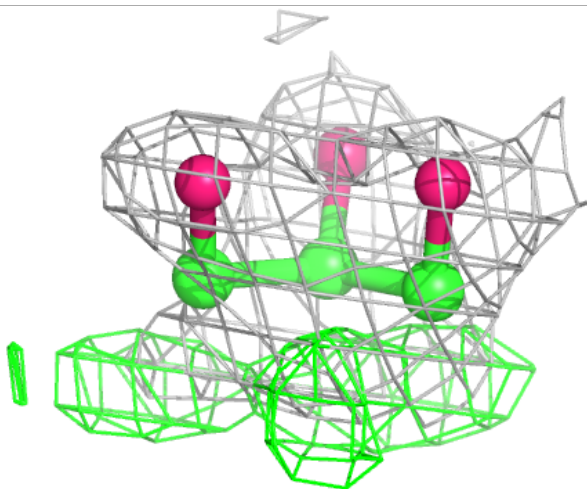
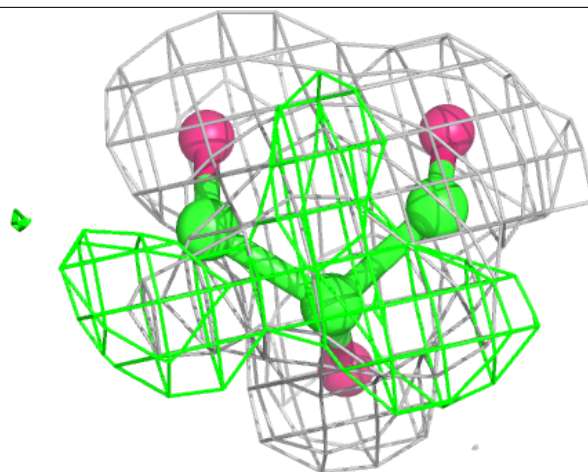
**Electron density around GOL C 507:**

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



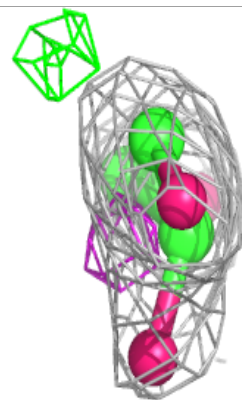
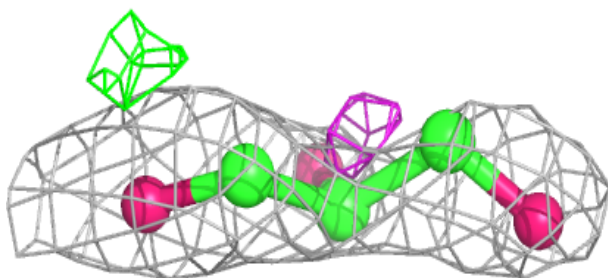
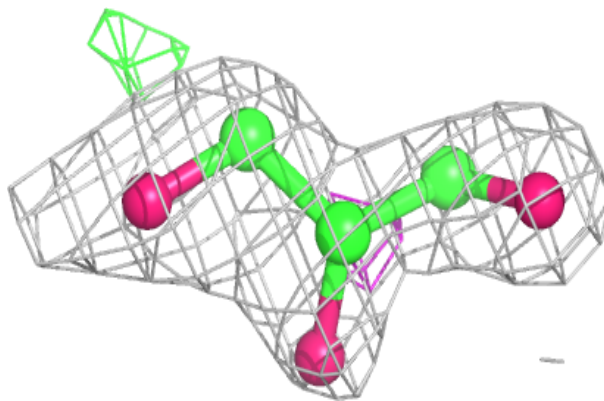
**Electron density around GOL B 503:**

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



**Electron density around GOL A 804:**

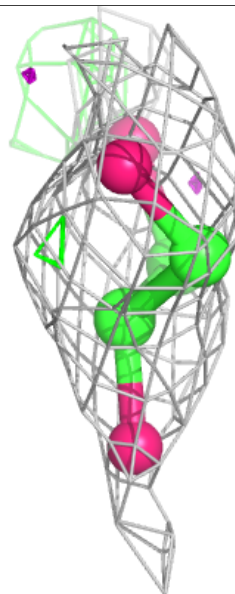
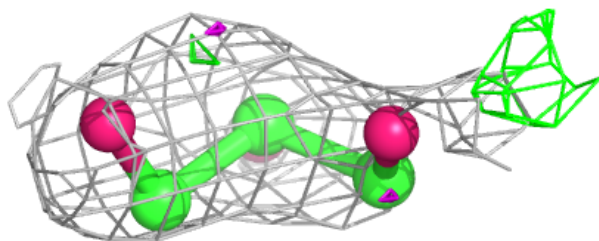
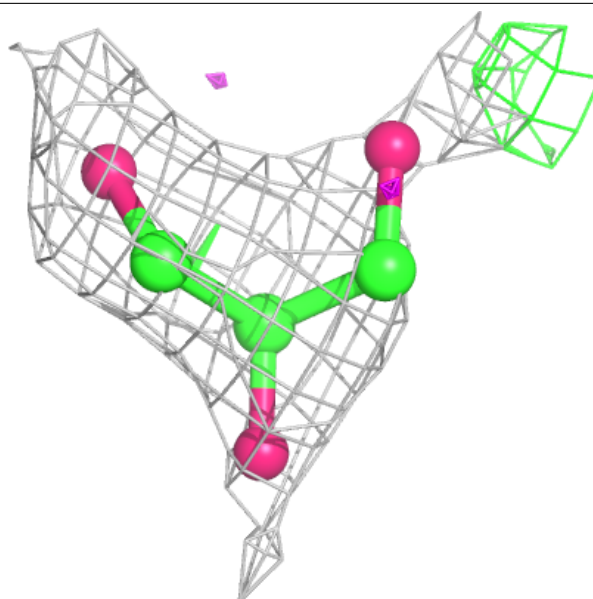
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around GOL B 506:**

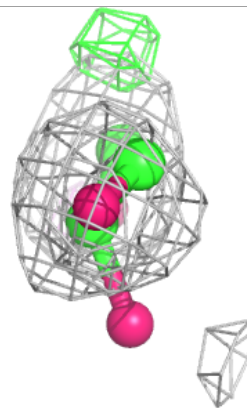
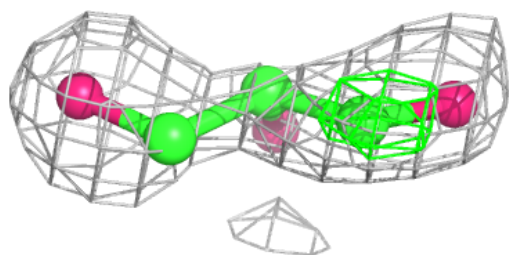
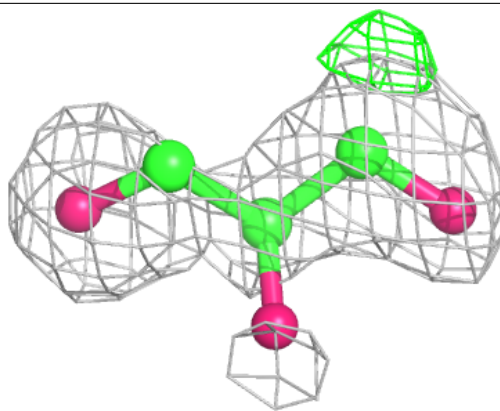
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





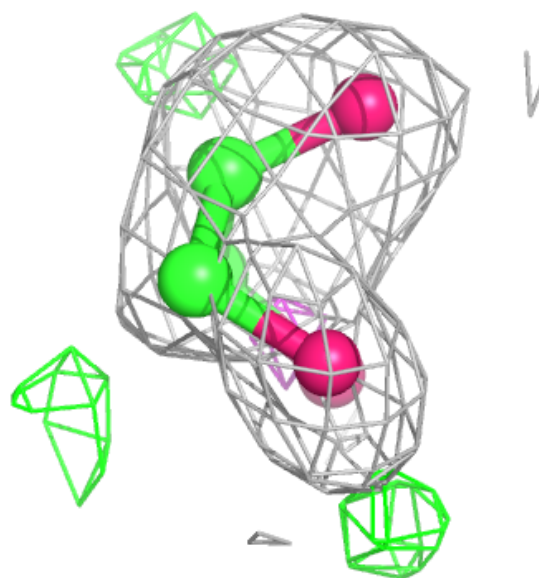
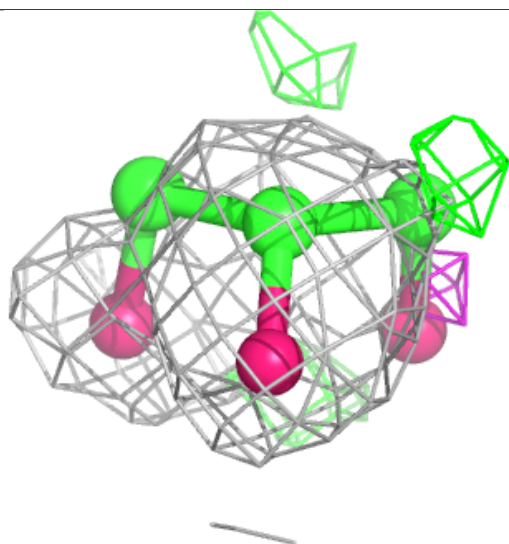
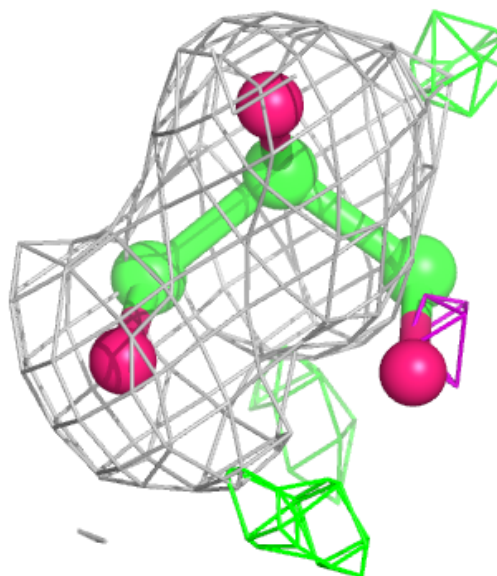
**Electron density around GOL C 505:**

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



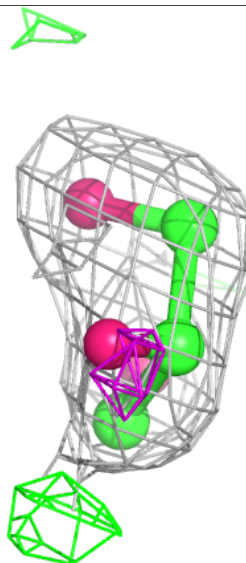
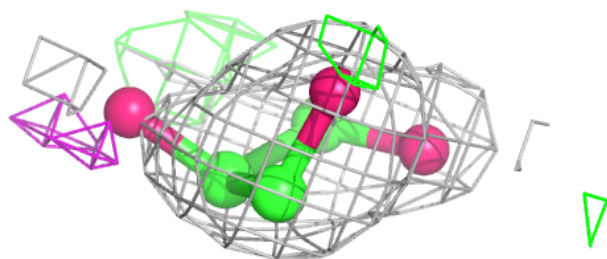
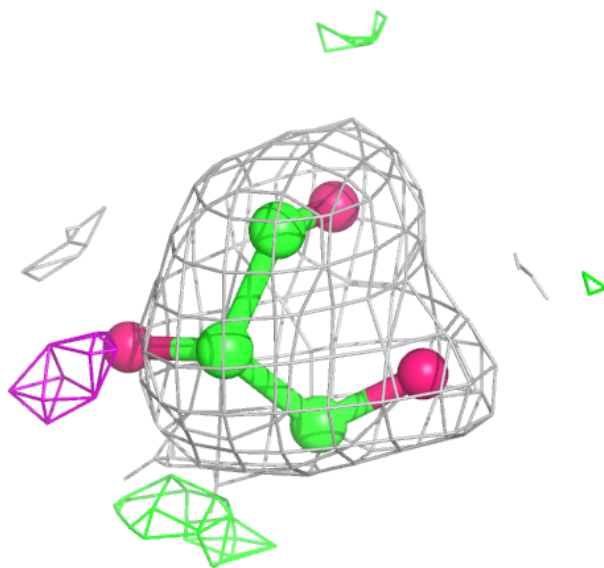
**Electron density around GOL A 806:**

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



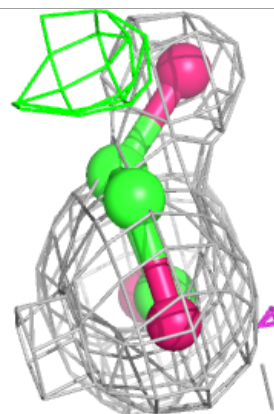
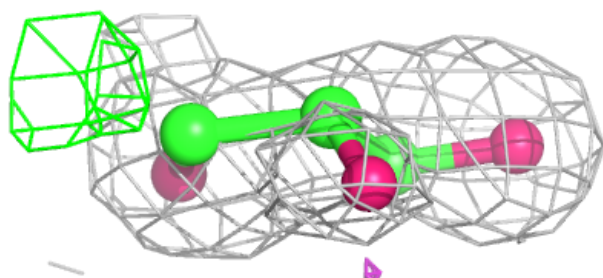
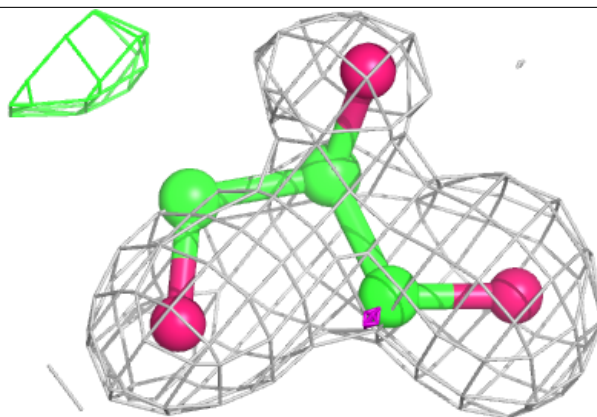
**Electron density around GOL A 801:**

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



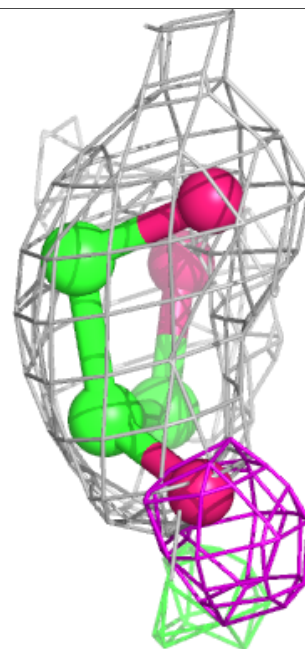
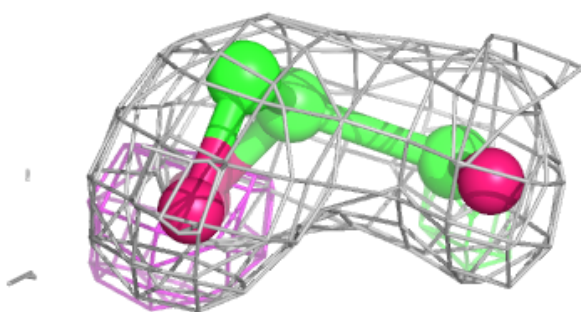
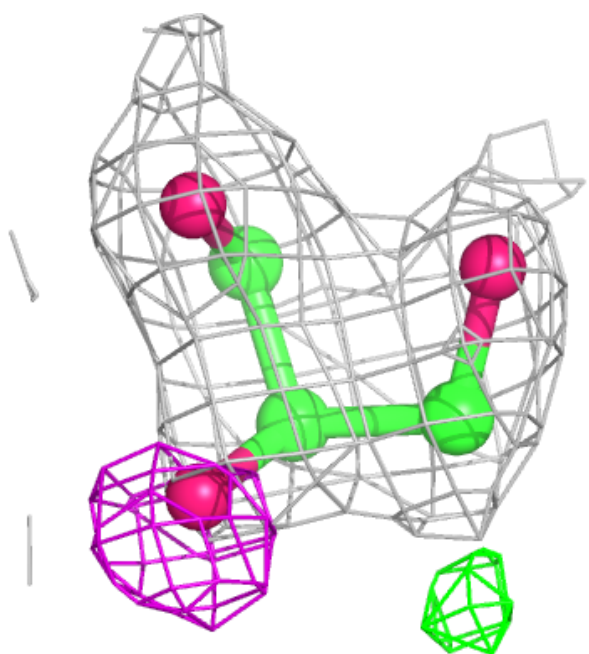
**Electron density around GOL C 506:**

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



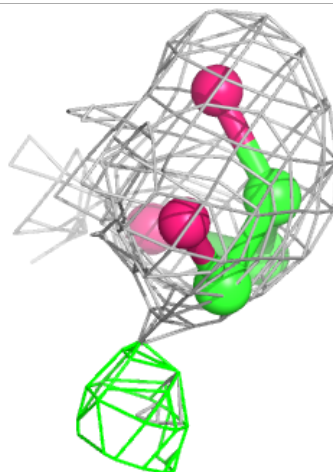
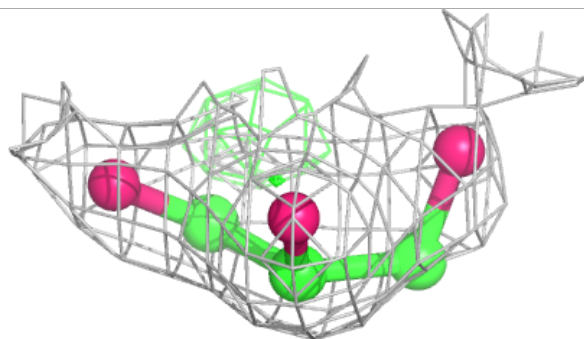
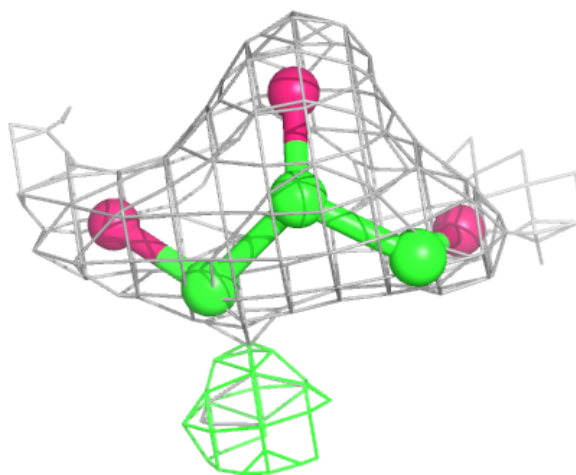
**Electron density around GOL C 503:**

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



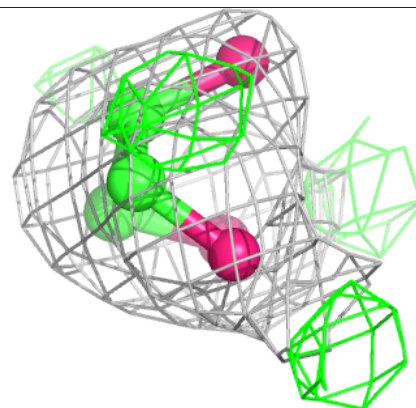
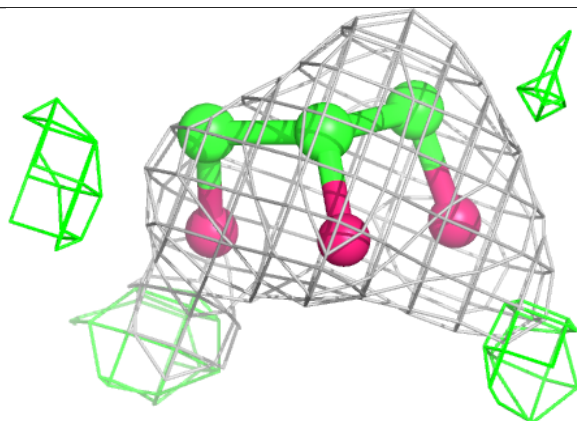
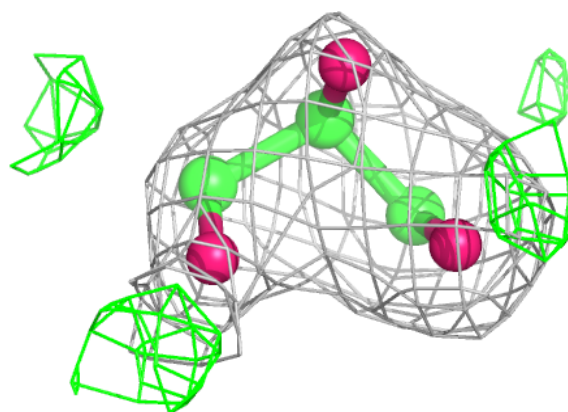
**Electron density around GOL A 805:**

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



**Electron density around GOL C 502:**

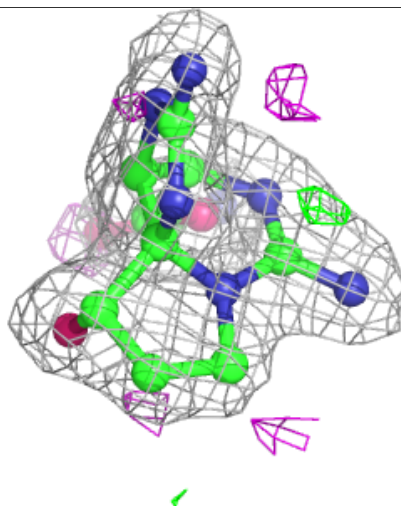
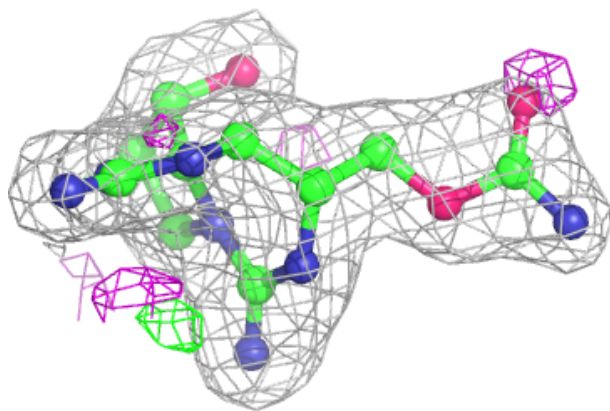
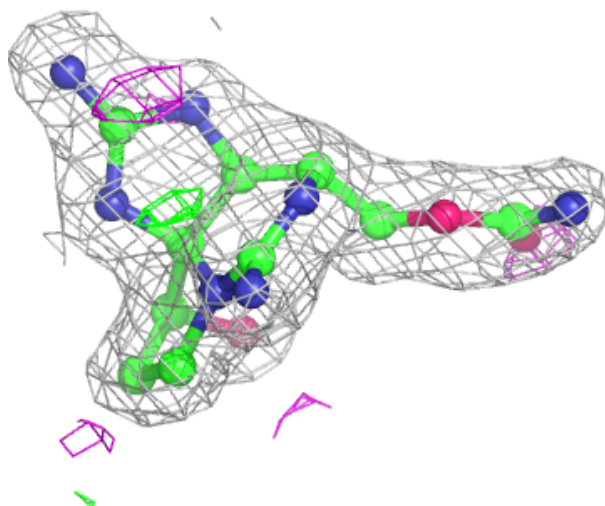
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around D82 B 505:**

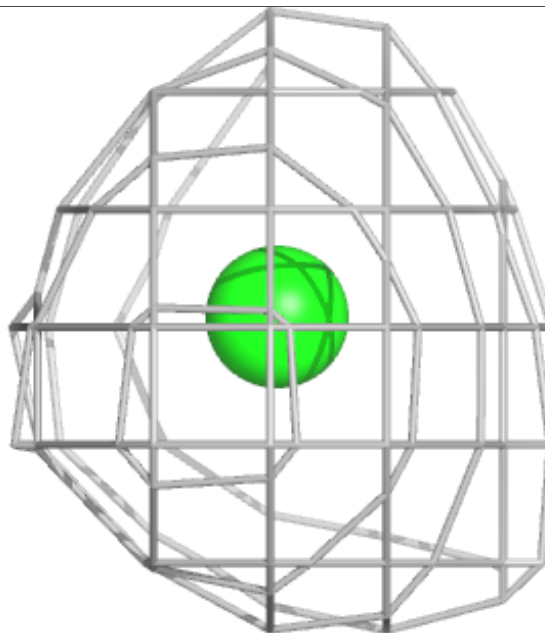
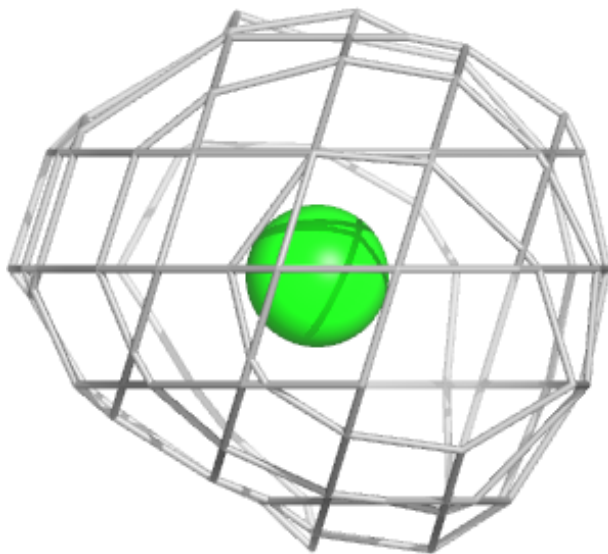
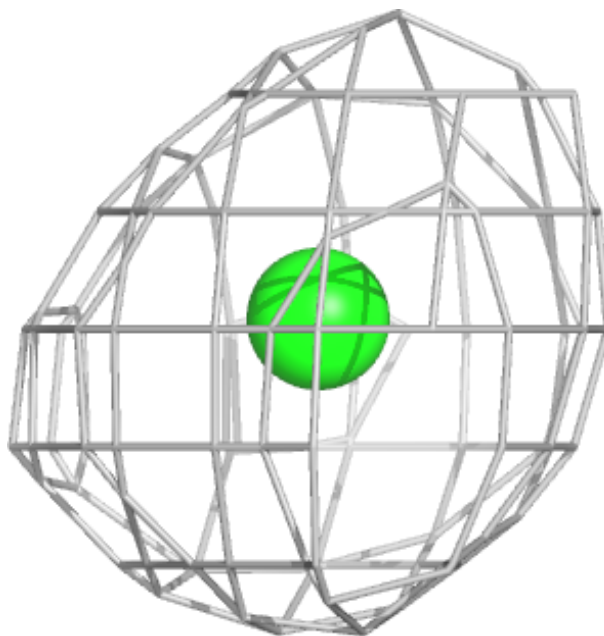
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





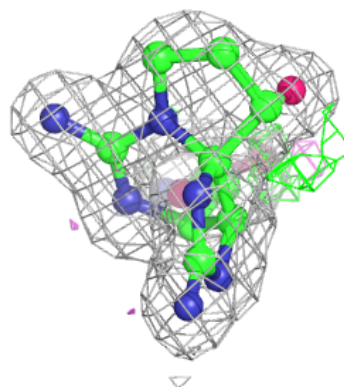
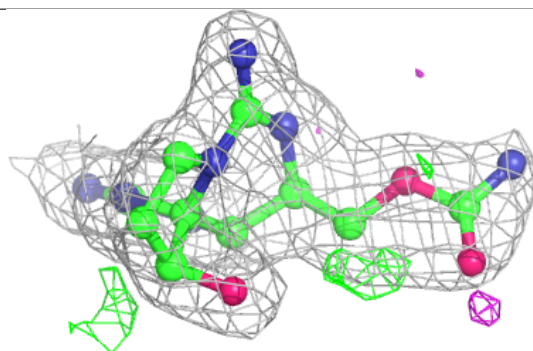
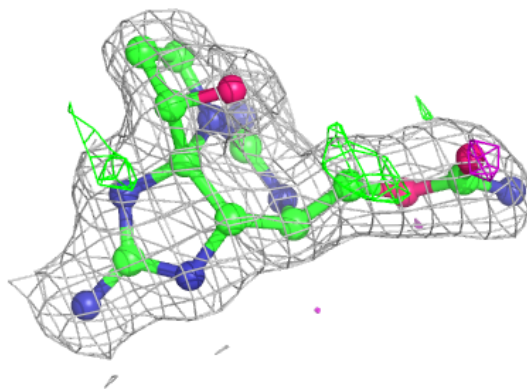
**Electron density around CL A 809:**

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

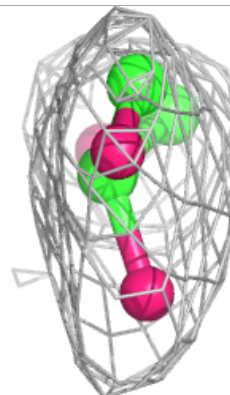
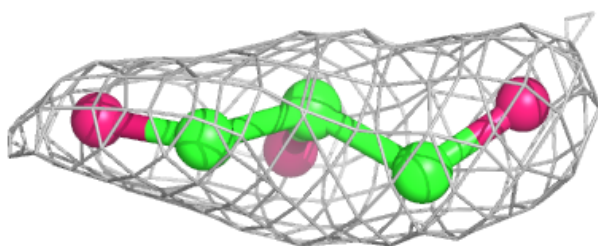
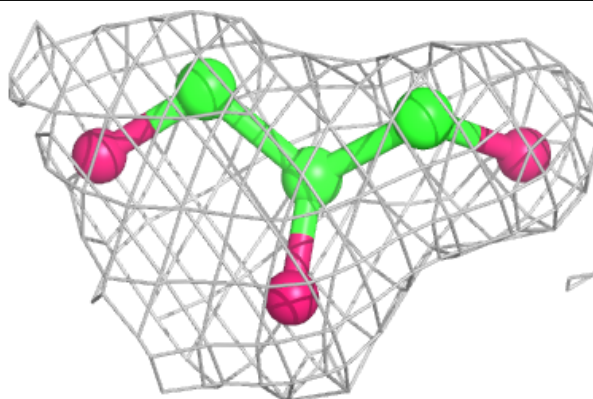


**Electron density around D82 C 504:**

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

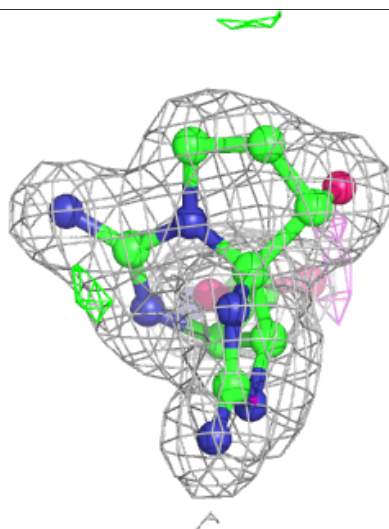
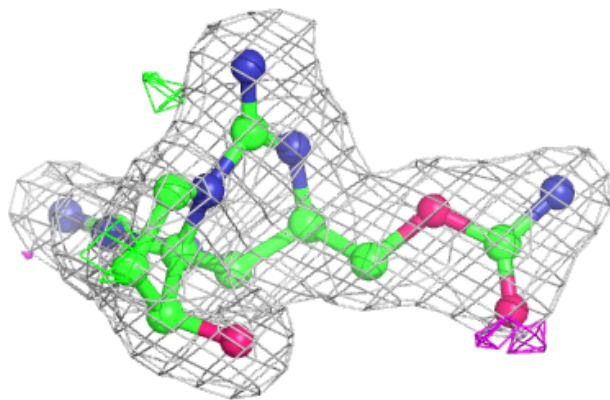
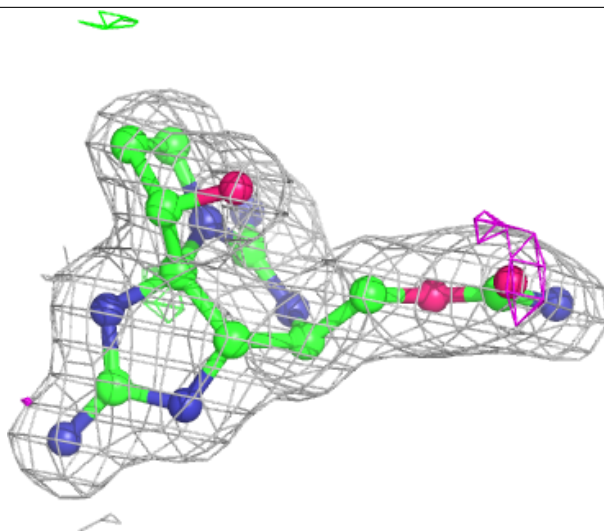
**Electron density around GOL B 504:**

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



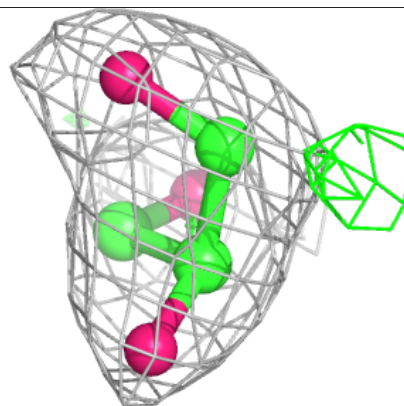
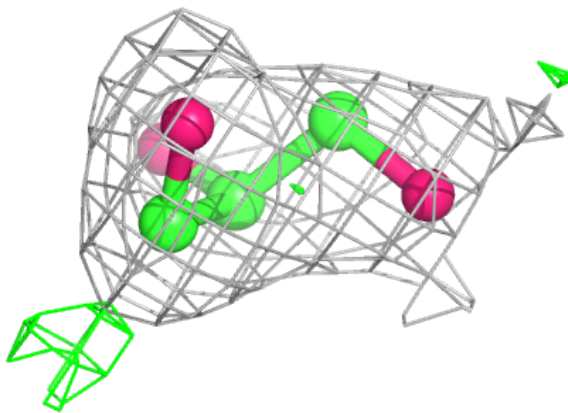
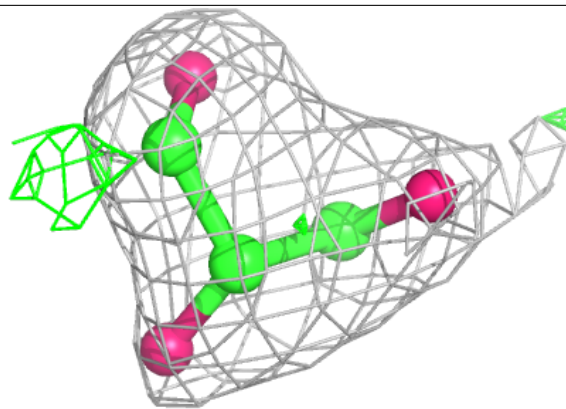
**Electron density around D82 A 803:**

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



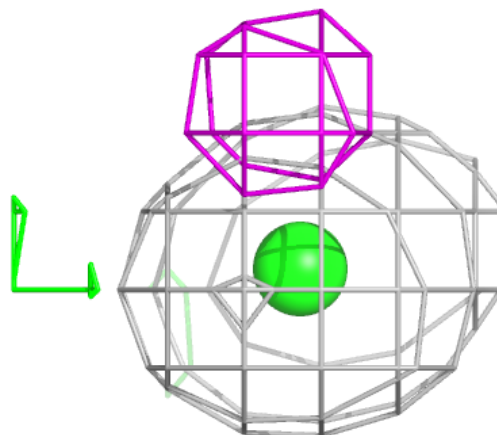
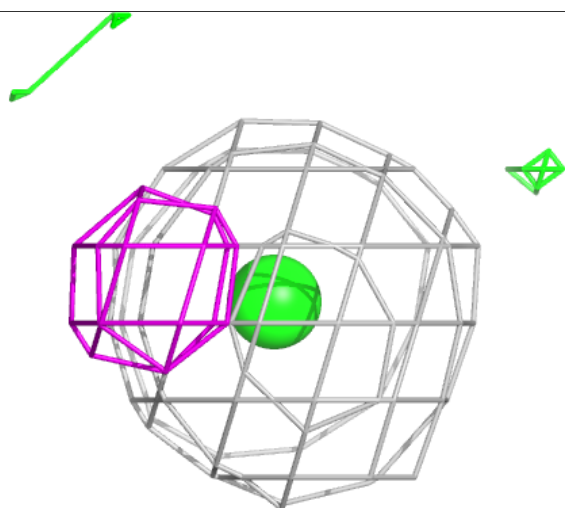
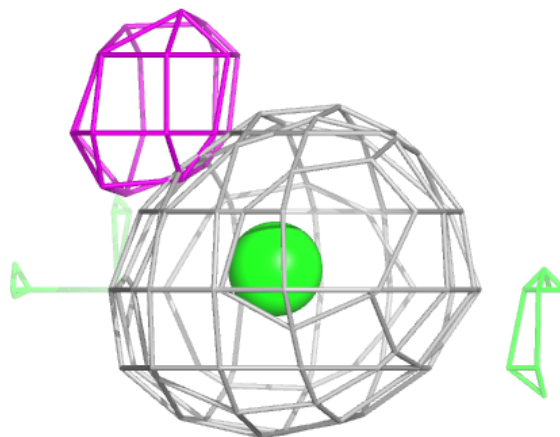
**Electron density around GOL B 502:**

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



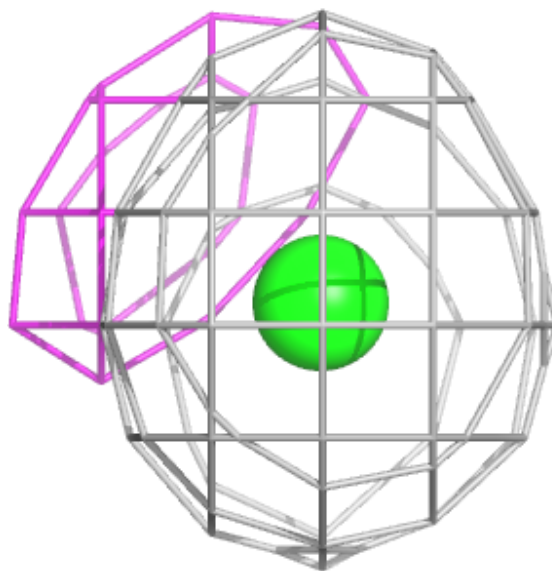
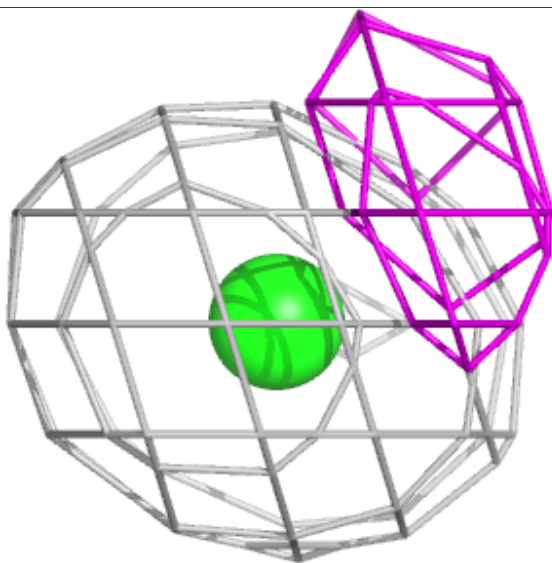
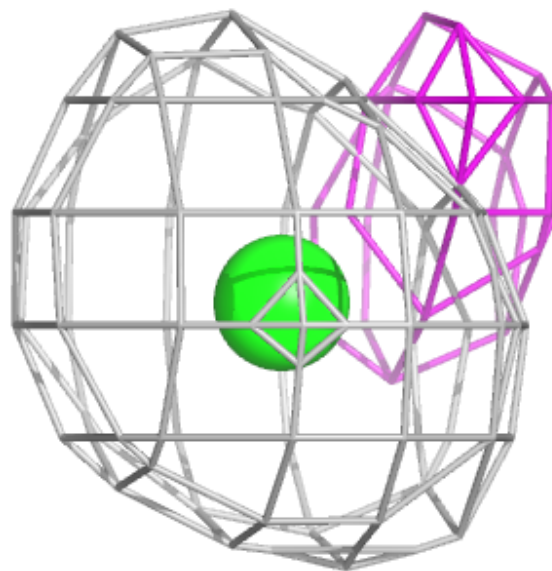
**Electron density around CL A 810:**

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



**Electron density around CL C 510:**

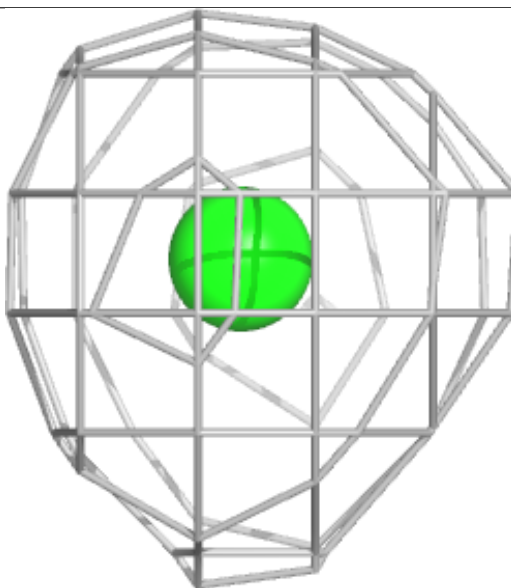
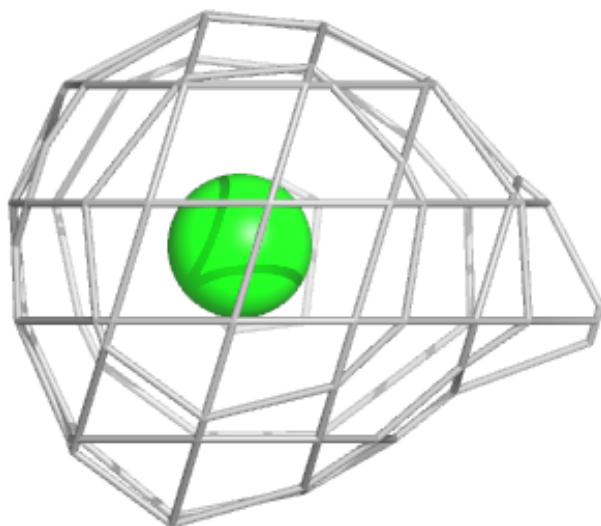
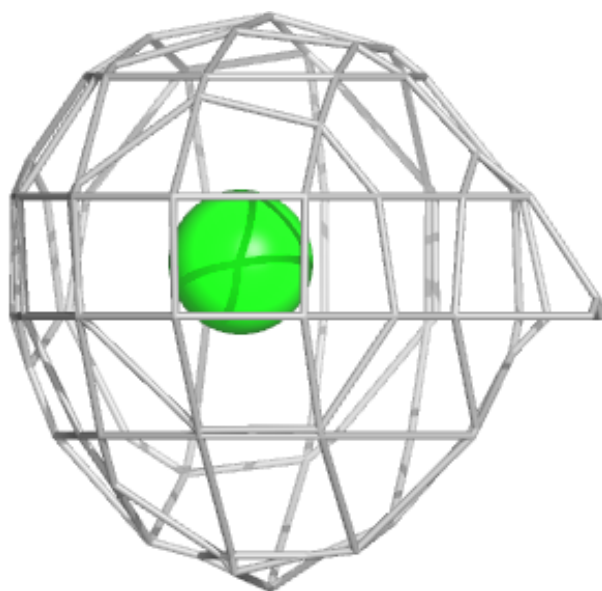
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





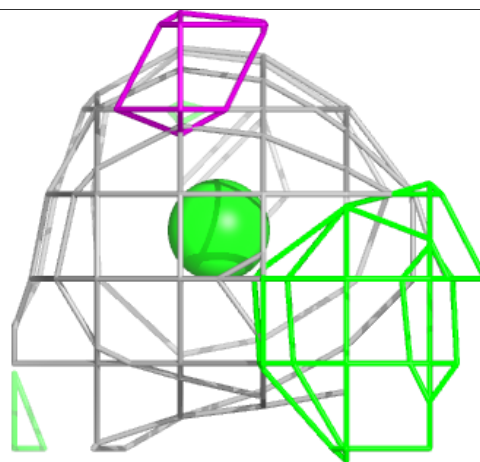
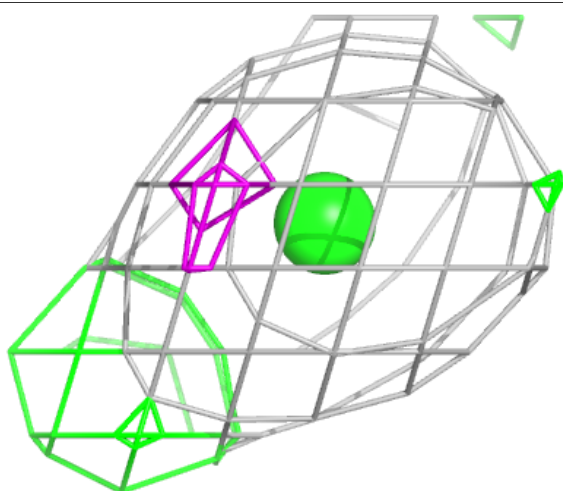
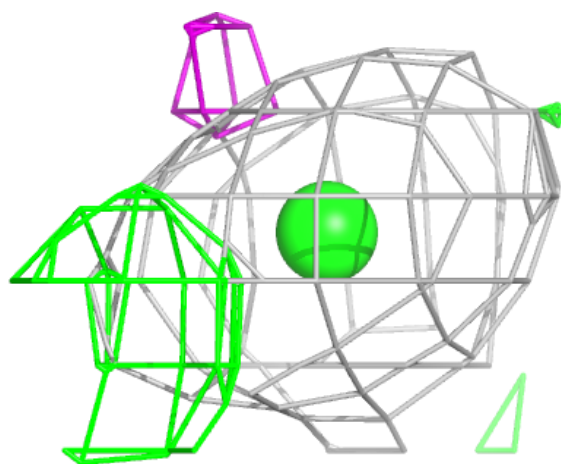
**Electron density around CL B 508:**

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



**Electron density around CL A 812:**

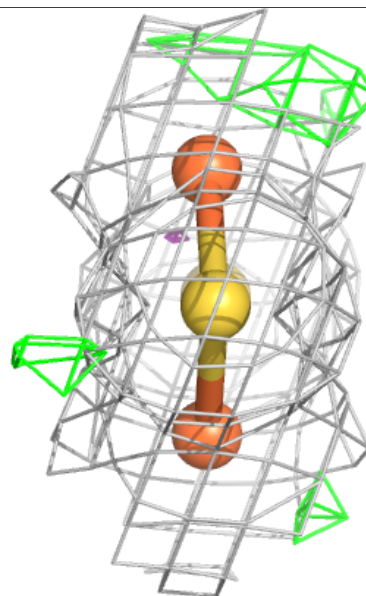
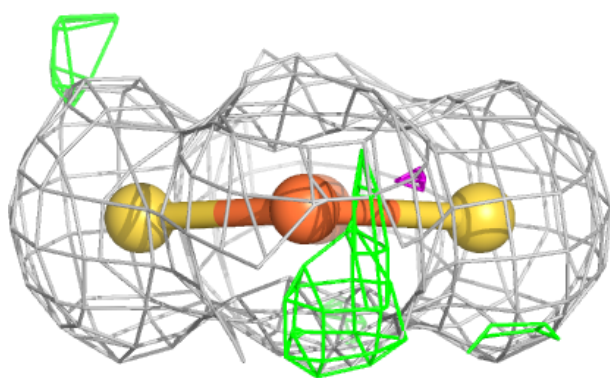
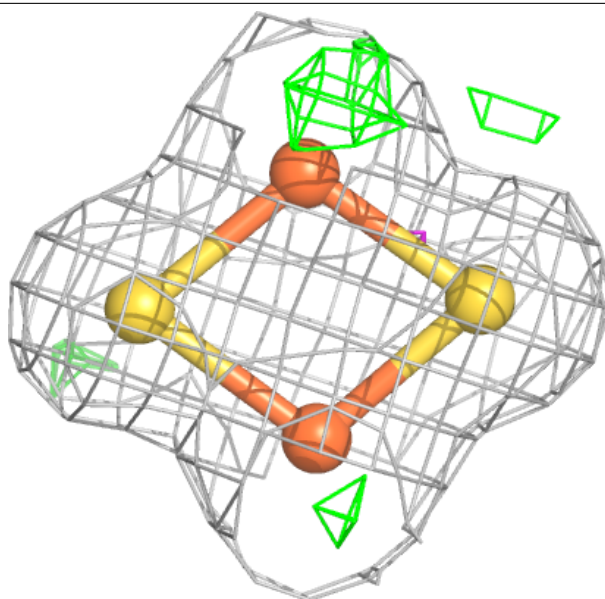
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





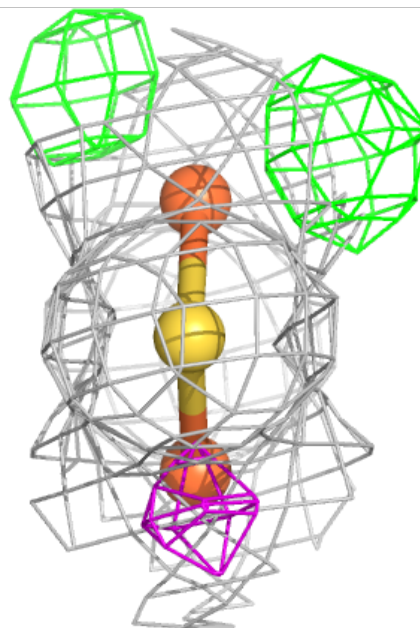
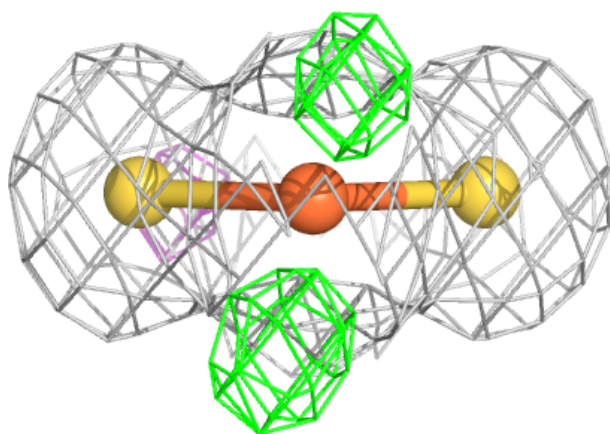
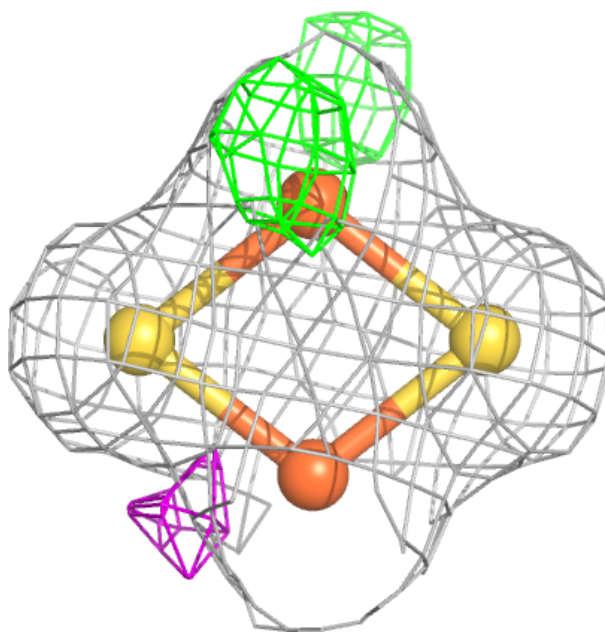
**Electron density around FES A 808:**

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



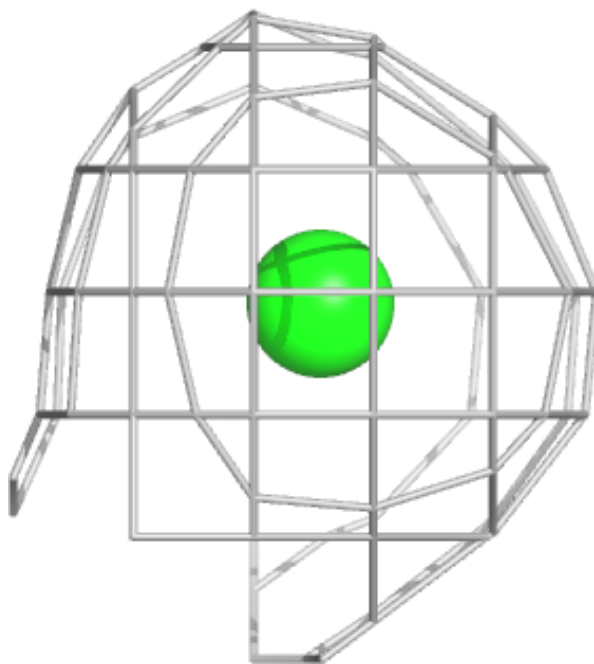
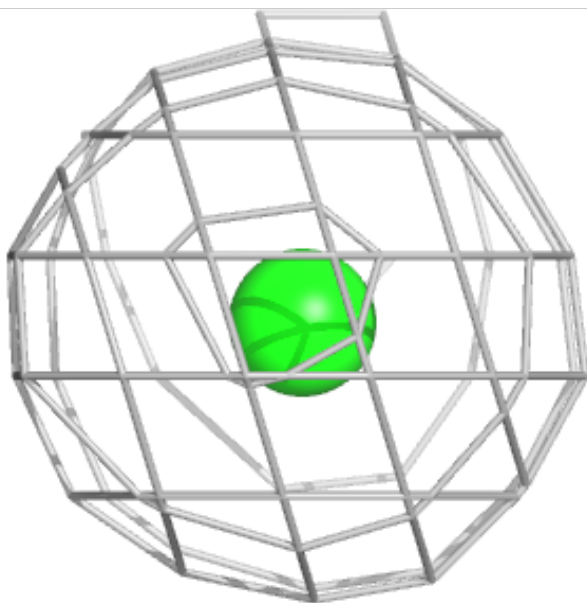
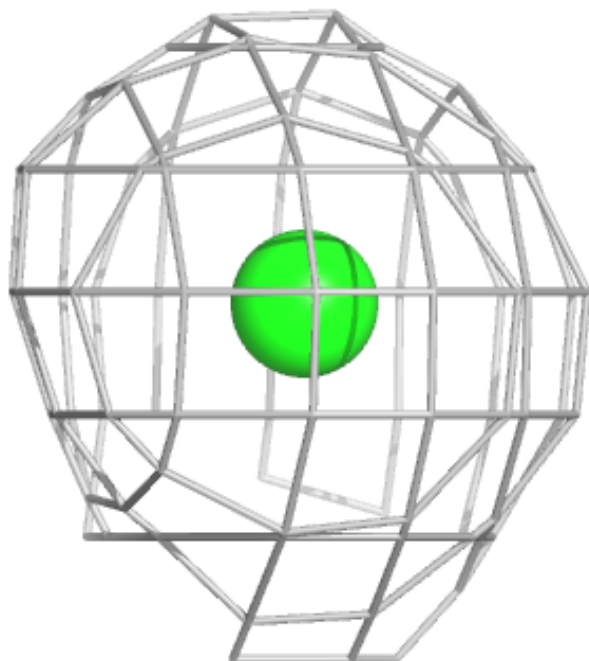
**Electron density around FES B 501:**

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



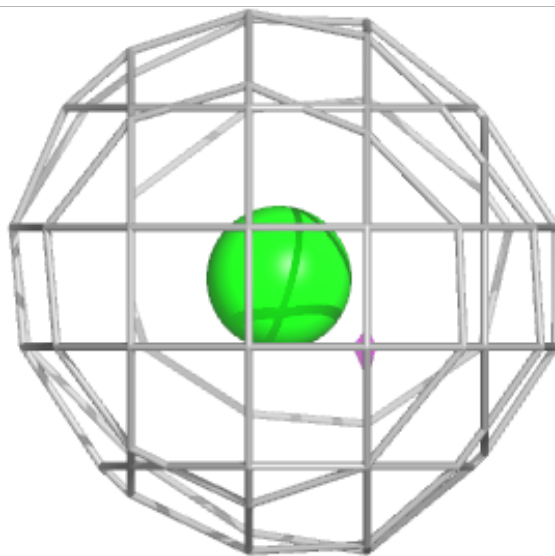
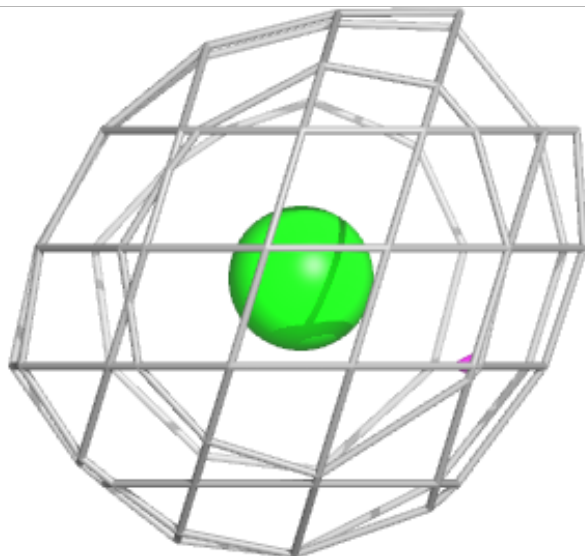
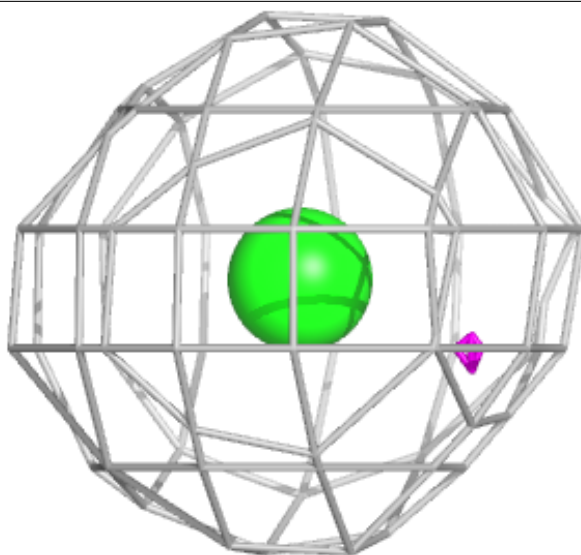
**Electron density around CL C 509:**

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



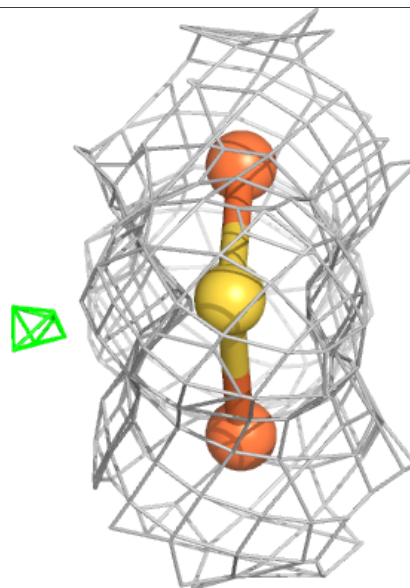
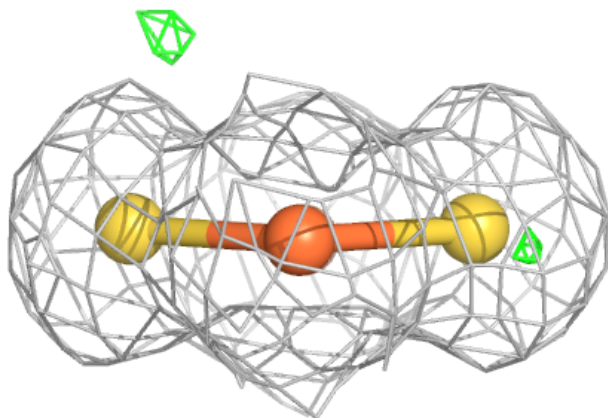
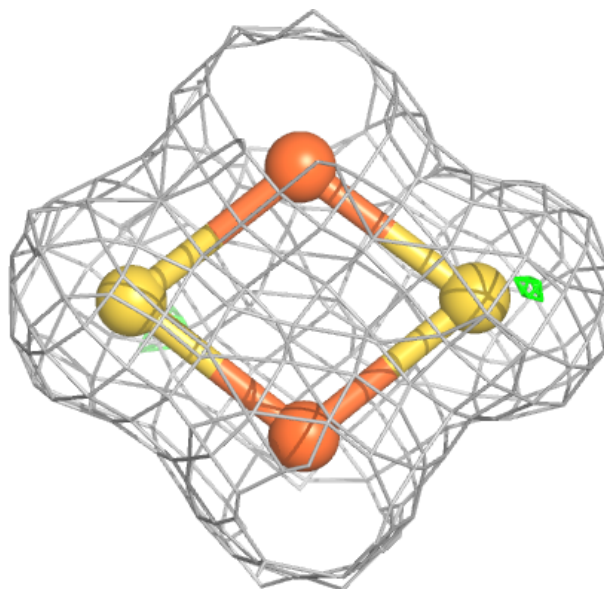
**Electron density around CL A 811:**

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



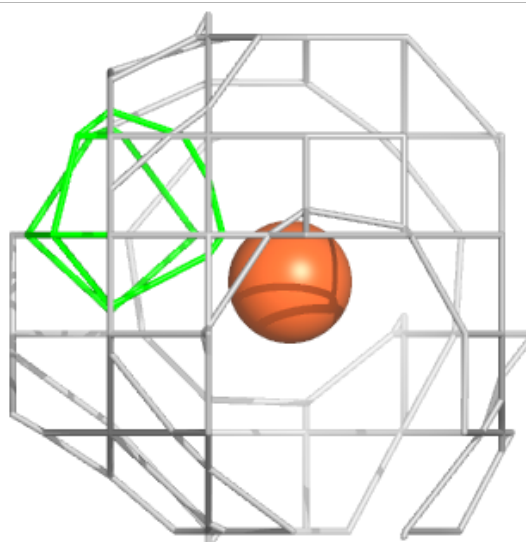
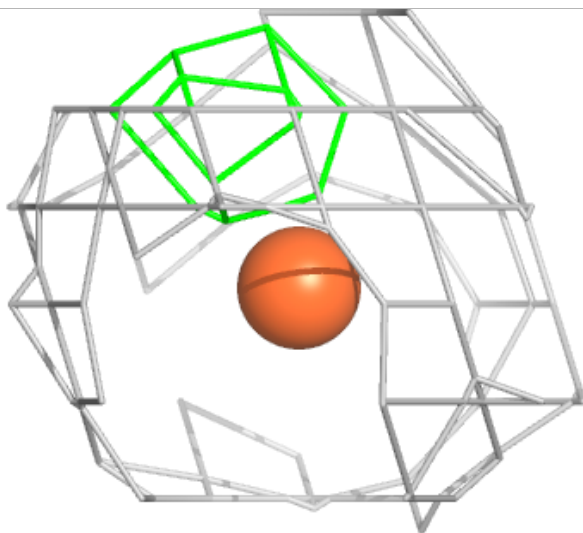
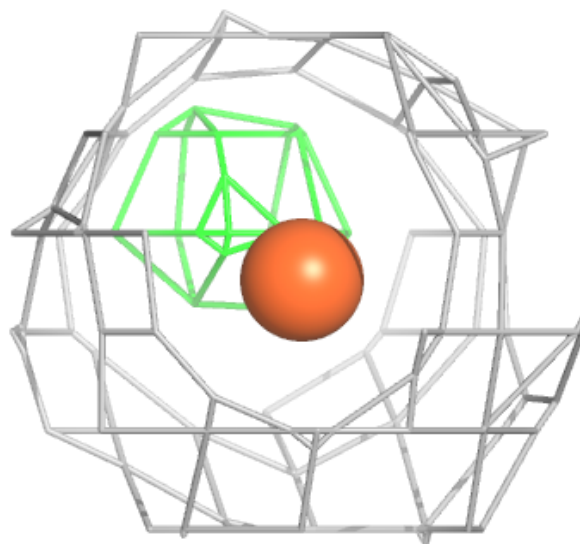
**Electron density around FES C 501:**

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



**Electron density around FE C 508:**

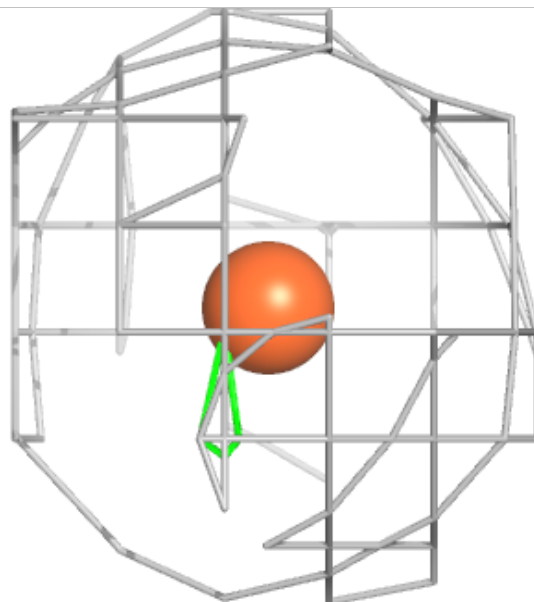
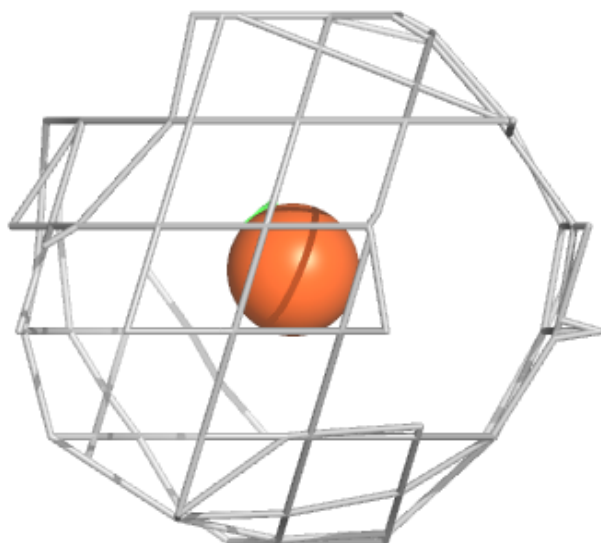
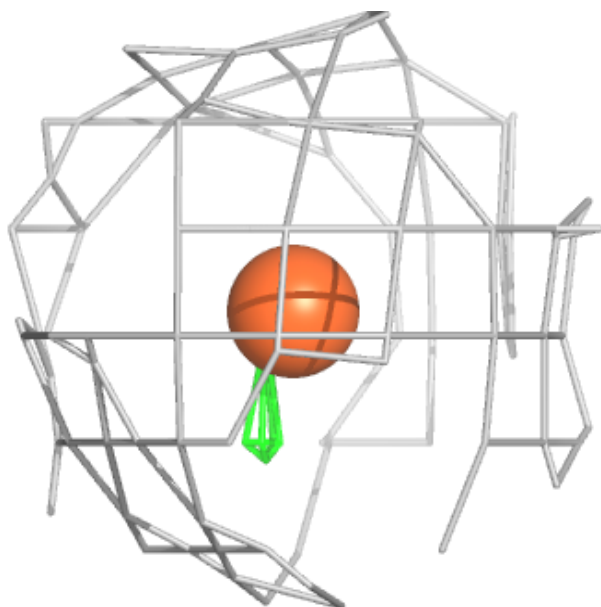
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

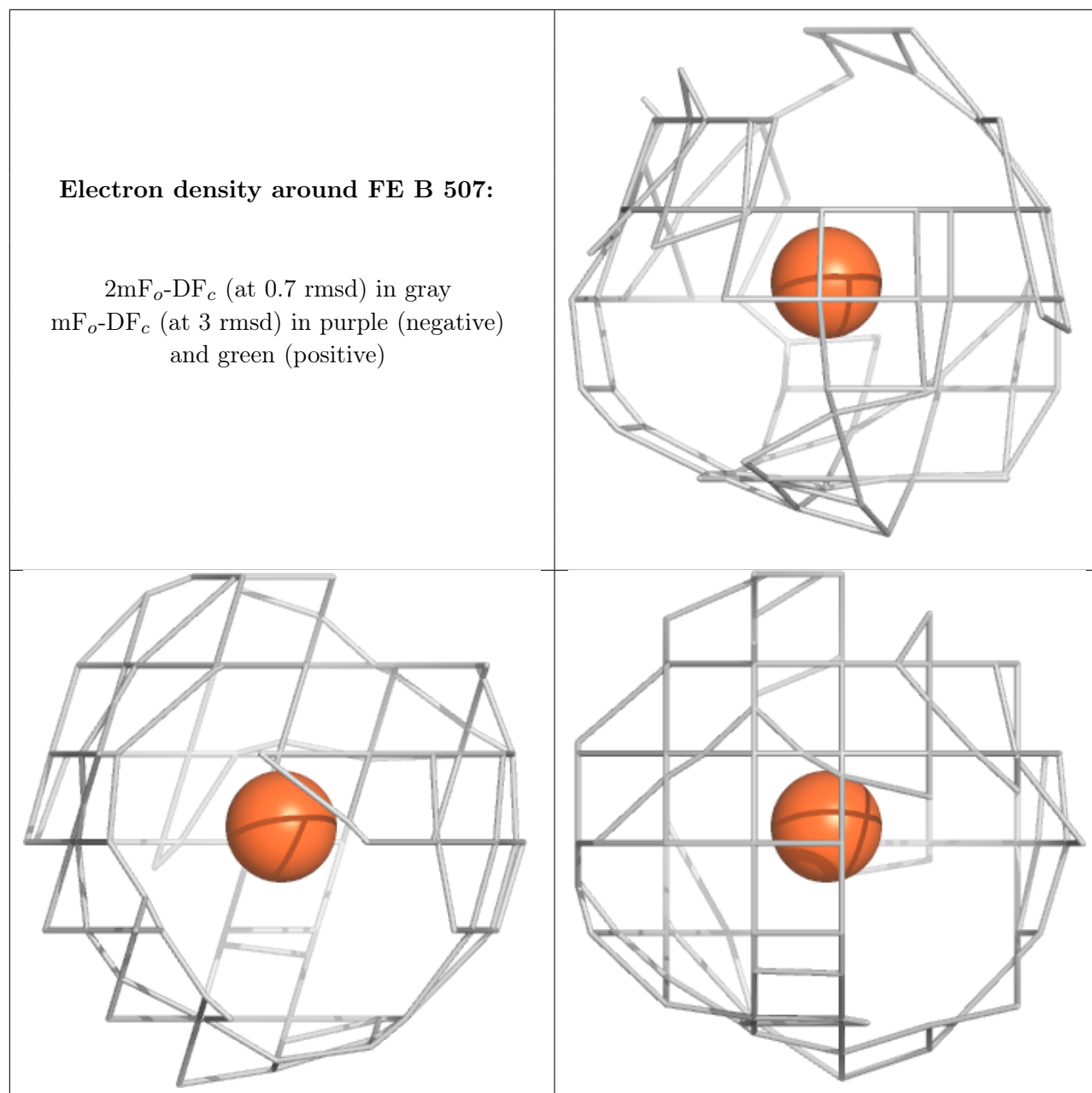




**Electron density around FE A 807:**

$2mF_o-DF_c$  (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.