Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 02:39 AM EDT

PDB ID	:	7SZH
Title	:	Structure of the Rieske Non-heme Iron Oxygenase SxtT 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*
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:

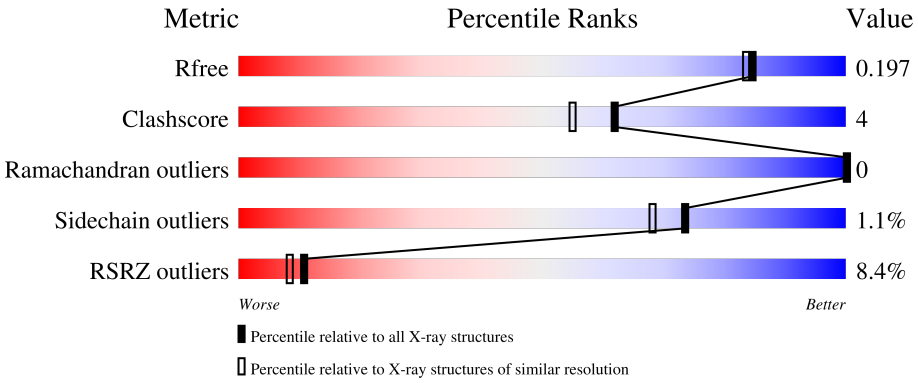
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.79 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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	7% 90% 7% .
1	B	334	12% 90% 8% .
1	C	334	6% 86% 10% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	1209	-	-	X	-

2 Entry composition

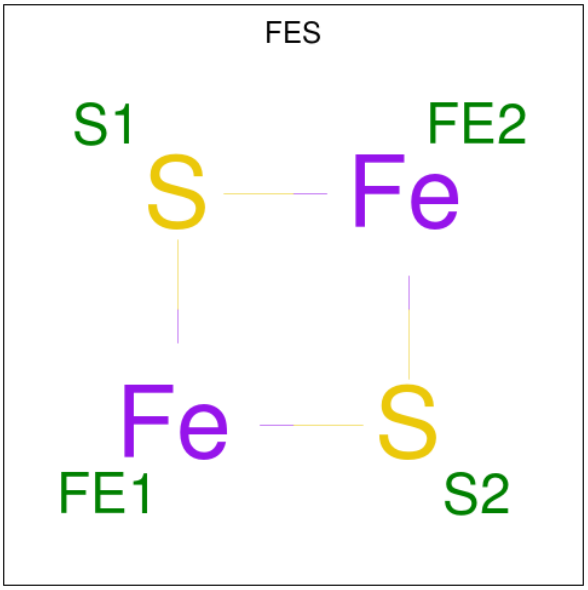
There are 8 unique types of molecules in this entry. The entry contains 9141 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SxtT.

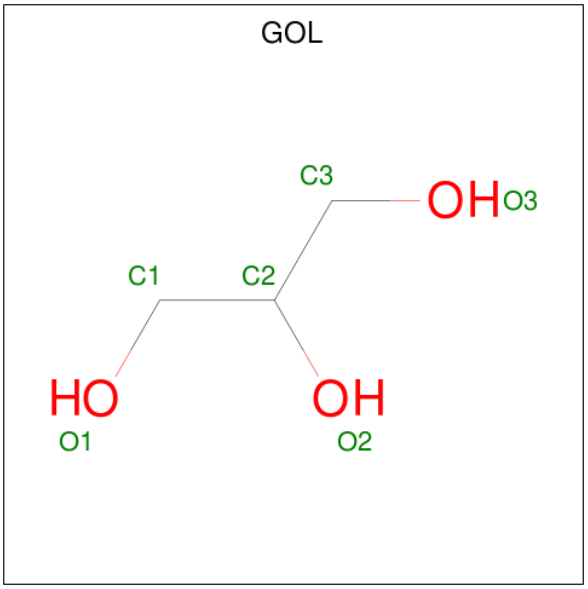
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	5	0
			2648	1682	452	491	23			
1	B	327	Total	C	N	O	S	0	19	0
			2779	1757	474	522	26			
1	C	319	Total	C	N	O	S	0	11	0
			2646	1680	453	490	23			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is GLYCEROL (three-letter code: 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	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

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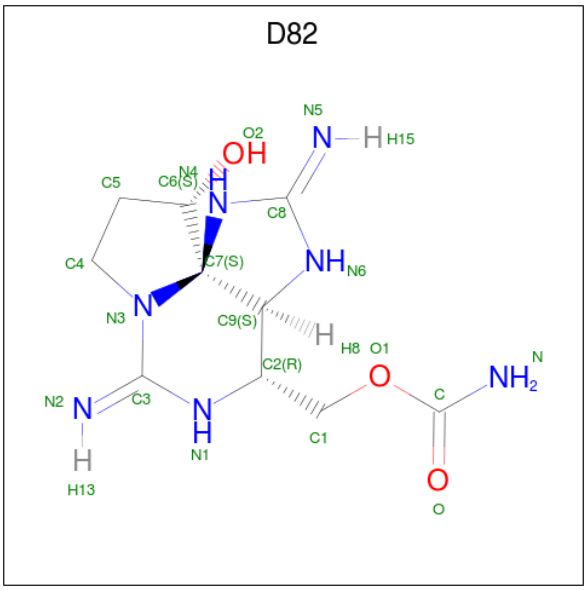
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

- Molecule 4 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
4	A	1	Total C N O 20 10 7 3	0	0

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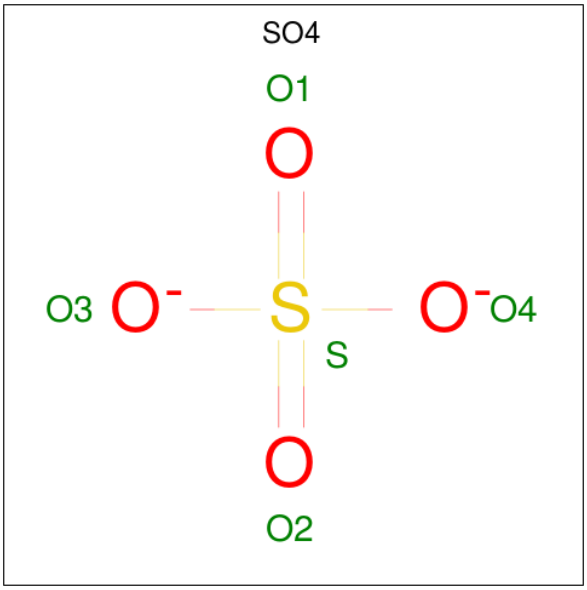
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 20 10 7 3	0	0
4	C	1	Total C N O 20 10 7 3	0	0

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Cl 2 2	0	0

- Molecule 8 is water.

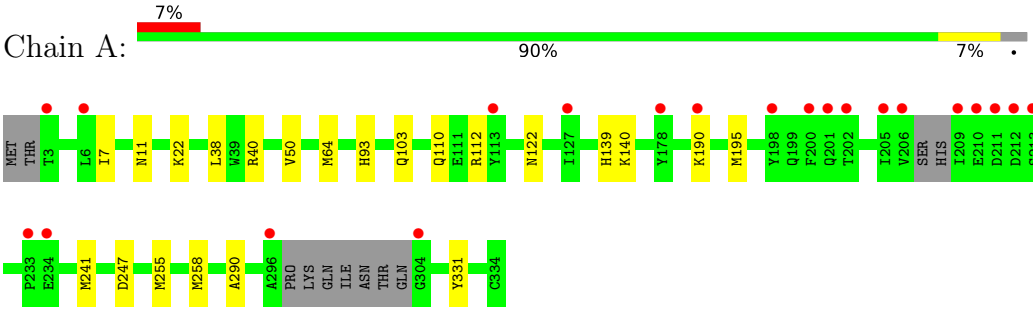
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	269	Total O 269 269	0	0
8	B	329	Total O 329 329	0	5
8	C	231	Total O 231 231	0	1

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.

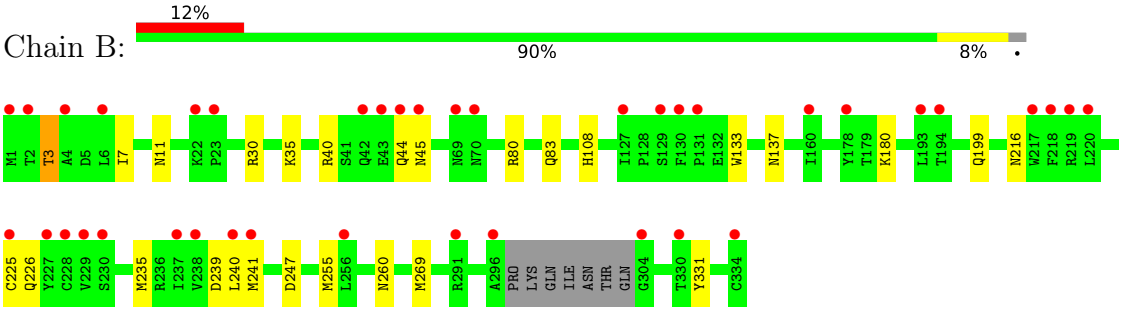
• Molecule 1: SxtT

Chain A:



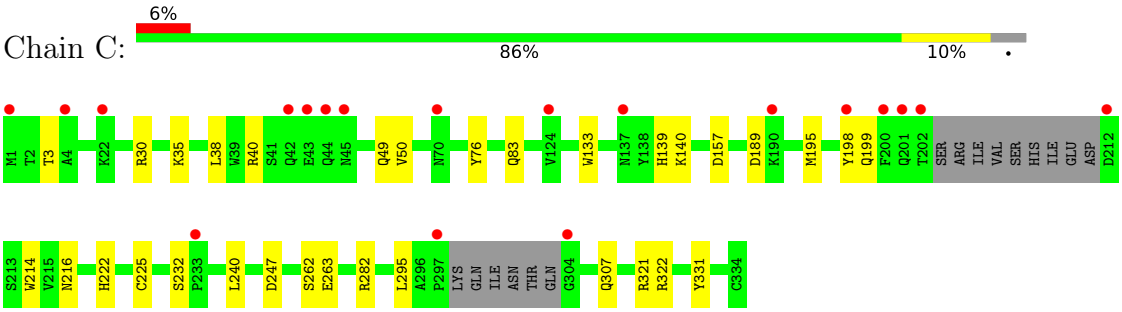
• Molecule 1: SxtT

Chain B:



• Molecule 1: SxtT

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	153.28Å 158.47Å 115.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.63 – 1.79 48.63 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.63-1.79) 98.6 (48.63-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.171 , 0.199 0.169 , 0.197	Depositor DCC
R_{free} test set	6494 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9141	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, D82, CL, SO4, FE, FES

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	0.40	0/2724	0.56	0/3713
1	B	0.38	0/2860	0.58	0/3898
1	C	0.37	0/2729	0.56	0/3722
All	All	0.38	0/8313	0.57	0/11333

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2648	0	2553	18	0
1	B	2779	0	2667	23	0
1	C	2646	0	2554	22	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
3	A	24	0	32	7	0
3	B	60	0	80	12	0
3	C	48	0	64	7	0
4	A	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	20	0	0	5	0
4	C	20	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	5	0	0	0	0
6	B	15	0	0	0	0
6	C	10	0	0	0	0
7	A	2	0	0	2	0
8	A	269	0	0	9	0
8	B	329	0	0	7	0
8	C	231	0	0	6	0
All	All	9141	0	7950	72	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 4.

All (72) 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)
4:B:1212:D82:C4	8:B:1434[B]:HOH:O	1.94	1.16
3:C:508:GOL:H32	8:C:776:HOH:O	1.66	0.93
7:A:509:CL:CL	8:A:784:HOH:O	2.30	0.85
1:B:226:GLN:OE1	8:B:1302[B]:HOH:O	1.96	0.84
7:A:510:CL:CL	8:A:839:HOH:O	2.42	0.74
4:B:1212:D82:N4	8:B:1303:HOH:O	2.20	0.73
1:C:282[B]:ARG:NH1	8:C:602:HOH:O	2.22	0.71
1:B:133:TRP:HE1	3:B:1207:GOL:H31	1.57	0.70
1:B:108:HIS:HA	3:B:1204:GOL:H11	1.73	0.69
1:B:216:ASN:HD21	4:B:1212:D82:C	2.08	0.67
1:B:3:THR:HB	1:B:331:TYR:CD1	2.30	0.66
1:A:40:ARG:HH22	3:A:502:GOL:H2	1.63	0.64
1:A:140:LYS:HG2	3:A:503:GOL:H31	1.80	0.63
1:A:112:ARG:HH12	3:A:504:GOL:H11	1.63	0.63
1:C:295:LEU:HD12	1:C:322:ARG:HG3	1.81	0.63
1:A:93:HIS:HD1	3:A:505:GOL:H32	1.64	0.62
1:C:3:THR:HB	1:C:331:TYR:CD1	2.33	0.62
1:A:228[A]:CYS:SG	8:A:796:HOH:O	2.56	0.61
1:A:228[B]:CYS:SG	8:A:796:HOH:O	2.56	0.61
1:A:122:ASN:ND2	8:A:602:HOH:O	2.26	0.59
4:A:506:D82:N4	8:A:607:HOH:O	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:LYS:HG2	3:C:504:GOL:H12	1.85	0.58
1:C:133:TRP:HE1	3:C:503:GOL:H31	1.68	0.58
1:B:137:ASN:ND2	8:B:1304:HOH:O	2.21	0.57
1:C:30:ARG:HH12	1:C:35:LYS:HE2	1.68	0.57
4:C:506:D82:N4	8:C:611:HOH:O	2.32	0.57
1:C:38:LEU:HG	1:C:50:VAL:HG22	1.87	0.56
1:C:83:GLN:NE2	8:C:610:HOH:O	2.31	0.56
1:C:30:ARG:NH1	1:C:35:LYS:HE2	2.22	0.54
1:B:241[A]:MET:HG3	1:B:255[A]:MET:HG2	1.88	0.54
1:A:64:MET:HG2	3:B:1201:GOL:H2	1.90	0.53
1:C:157:ASP:OD1	1:C:321:ARG:NH1	2.41	0.52
1:C:198:TYR:CE1	1:C:216:ASN:HB2	2.45	0.52
1:B:44:GLN:HA	3:B:1209:GOL:H32	1.93	0.51
1:B:260[B]:ASN:ND2	8:B:1322:HOH:O	2.43	0.50
1:B:30:ARG:HH22	3:B:1211:GOL:H2	1.76	0.49
1:B:239:ASP:OD2	4:B:1212:D82:N1	2.45	0.49
1:B:45:ASN:H	3:B:1209:GOL:H32	1.77	0.49
1:C:282[A]:ARG:HD3	8:C:701:HOH:O	2.13	0.49
3:A:505:GOL:H11	1:B:180:LYS:HE3	1.94	0.49
1:C:40:ARG:HH22	3:C:509:GOL:H32	1.77	0.48
1:C:262:SER:HA	3:C:502:GOL:H32	1.94	0.48
1:C:225[B]:CYS:SG	1:C:240:LEU:HD11	2.54	0.48
1:A:93:HIS:HD1	3:A:505:GOL:C3	2.27	0.48
1:A:241[A]:MET:HG3	1:A:255:MET:HG2	1.96	0.48
1:C:222:HIS:HB3	1:C:225[B]:CYS:HB3	1.97	0.47
1:B:225[B]:CYS:SG	1:B:240:LEU:HD11	2.55	0.46
1:A:38:LEU:HG	1:A:50:VAL:HG22	1.98	0.45
1:B:199:GLN:NE2	8:B:1312:HOH:O	2.50	0.45
1:A:110:GLN:HG2	8:A:643:HOH:O	2.17	0.45
1:C:214:TRP:CD2	1:C:232:SER:HB3	2.51	0.45
1:A:139:HIS:O	1:A:258:MET:HA	2.17	0.44
1:C:139:HIS:HA	3:C:504:GOL:H11	1.99	0.44
1:B:83:GLN:HB2	3:B:1203:GOL:H31	1.98	0.44
1:A:22:LYS:HD3	1:A:22:LYS:HA	1.80	0.44
1:A:290:ALA:O	8:A:601:HOH:O	2.21	0.44
1:B:45:ASN:HA	3:B:1209:GOL:H12	1.98	0.44
4:B:1212:D82:O2	4:B:1212:D82:O	2.35	0.44
1:A:247:ASP:HA	1:A:331:TYR:OH	2.17	0.44
1:B:269[B]:MET:HE2	1:B:269[B]:MET:HB3	1.91	0.44
1:B:40:ARG:HH22	3:B:1209:GOL:H2	1.82	0.44
1:B:80:ARG:HH12	3:B:1205:GOL:H2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:ASP:HA	1:C:331:TYR:OH	2.18	0.43
1:B:7:ILE:O	1:B:11:ASN:HB2	2.18	0.43
3:B:1210:GOL:H12	8:B:1307:HOH:O	2.19	0.43
1:C:263:GLU:H	3:C:502:GOL:H11	1.83	0.43
1:C:38:LEU:HA	1:C:49:GLN:O	2.19	0.42
1:A:112:ARG:HH22	3:A:504:GOL:H11	1.84	0.42
1:C:307:GLN:NE2	8:C:624:HOH:O	2.53	0.42
1:B:247:ASP:HA	1:B:331:TYR:OH	2.20	0.42
1:B:35:LYS:HD2	3:B:1211:GOL:H2	2.02	0.42
1:A:103:GLN:HB2	8:A:815:HOH:O	2.20	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	323/334 (97%)	314 (97%)	9 (3%)	0	100	100
1	B	343/334 (103%)	333 (97%)	10 (3%)	0	100	100
1	C	324/334 (97%)	314 (97%)	10 (3%)	0	100	100
All	All	990/1002 (99%)	961 (97%)	29 (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	298/303 (98%)	294 (99%)	4 (1%)	69 62
1	B	316/303 (104%)	314 (99%)	2 (1%)	86 84
1	C	299/303 (99%)	295 (99%)	4 (1%)	69 62
All	All	913/909 (100%)	903 (99%)	10 (1%)	73 68

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	11	ASN
1	A	190	LYS
1	A	195	MET
1	B	3	THR
1	B	235	MET
1	C	76	TYR
1	C	189	ASP
1	C	195	MET
1	C	199	GLN

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 39 ligands modelled in this entry, 5 are monoatomic - leaving 34 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	$\#\|Z\| > 2$
6	SO4	B	1214	-	4,4,4	0.16	0	6,6,6	0.07	0
3	GOL	B	1201	-	5,5,5	0.89	0	5,5,5	0.96	0
3	GOL	B	1203	-	5,5,5	0.86	0	5,5,5	1.13	1 (20%)
4	D82	B	1212	-	17,22,22	0.62	0	14,34,34	0.98	1 (7%)
6	SO4	B	1216	-	4,4,4	0.15	0	6,6,6	0.08	0
3	GOL	C	509	-	5,5,5	0.90	0	5,5,5	0.91	0
3	GOL	B	1204	-	5,5,5	0.89	0	5,5,5	0.99	0
6	SO4	C	512	-	4,4,4	0.15	0	6,6,6	0.06	0
3	GOL	B	1208	-	5,5,5	0.83	0	5,5,5	0.95	0
3	GOL	B	1206	-	5,5,5	0.86	0	5,5,5	1.02	0
4	D82	A	506	-	17,22,22	0.56	0	14,34,34	0.80	0
3	GOL	C	507	-	5,5,5	0.83	0	5,5,5	0.95	0
4	D82	C	506	-	17,22,22	0.57	0	14,34,34	1.00	1 (7%)
3	GOL	C	510	-	5,5,5	0.87	0	5,5,5	0.99	0
3	GOL	C	508	-	5,5,5	0.08	0	5,5,5	0.32	0
3	GOL	A	504	-	5,5,5	0.96	0	5,5,5	0.98	0
2	FES	B	1202	1	0,4,4	-	-	-		
2	FES	C	501	1	0,4,4	-	-	-		
3	GOL	A	505	-	5,5,5	0.91	0	5,5,5	0.89	0
3	GOL	C	505	-	5,5,5	0.95	0	5,5,5	0.98	0
3	GOL	B	1210	-	5,5,5	0.89	0	5,5,5	0.75	0
3	GOL	B	1207	-	5,5,5	0.11	0	5,5,5	0.34	0
3	GOL	C	504	-	5,5,5	0.82	0	5,5,5	1.08	0
3	GOL	B	1205	-	5,5,5	0.88	0	5,5,5	0.96	0
3	GOL	A	502	-	5,5,5	0.85	0	5,5,5	1.03	0
3	GOL	C	502	-	5,5,5	0.80	0	5,5,5	1.05	0
3	GOL	A	503	-	5,5,5	0.96	0	5,5,5	0.95	0
3	GOL	C	503	-	5,5,5	0.93	0	5,5,5	1.15	0
6	SO4	B	1215	-	4,4,4	0.13	0	6,6,6	0.09	0
6	SO4	A	508	-	4,4,4	0.13	0	6,6,6	0.07	0
6	SO4	C	513	-	4,4,4	0.15	0	6,6,6	0.05	0
3	GOL	B	1211	-	5,5,5	0.91	0	5,5,5	0.97	0
3	GOL	B	1209	-	5,5,5	0.83	0	5,5,5	1.04	0
2	FES	A	501	1	0,4,4	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	1201	-	-	0/4/4/4	-
3	GOL	B	1203	-	-	4/4/4/4	-
4	D82	B	1212	-	-	1/5/49/49	0/3/3/3
3	GOL	C	509	-	-	4/4/4/4	-
3	GOL	B	1204	-	-	4/4/4/4	-
3	GOL	B	1208	-	-	2/4/4/4	-
3	GOL	B	1206	-	-	1/4/4/4	-
4	D82	A	506	-	-	0/5/49/49	0/3/3/3
3	GOL	C	507	-	-	1/4/4/4	-
4	D82	C	506	-	-	0/5/49/49	0/3/3/3
3	GOL	C	510	-	-	0/4/4/4	-
3	GOL	C	508	-	-	4/4/4/4	-
3	GOL	A	504	-	-	0/4/4/4	-
2	FES	B	1202	1	-	-	0/1/1/1
2	FES	C	501	1	-	-	0/1/1/1
3	GOL	A	505	-	-	4/4/4/4	-
3	GOL	C	505	-	-	2/4/4/4	-
3	GOL	C	504	-	-	2/4/4/4	-
3	GOL	B	1210	-	-	0/4/4/4	-
3	GOL	B	1207	-	-	2/4/4/4	-
3	GOL	B	1205	-	-	0/4/4/4	-
3	GOL	A	502	-	-	4/4/4/4	-
3	GOL	C	502	-	-	2/4/4/4	-
3	GOL	A	503	-	-	3/4/4/4	-
3	GOL	C	503	-	-	2/4/4/4	-
3	GOL	B	1211	-	-	0/4/4/4	-
3	GOL	B	1209	-	-	0/4/4/4	-
2	FES	A	501	1	-	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1212	D82	O2-C6-C7	-2.85	103.00	110.50
4	C	506	D82	O2-C6-C7	-2.72	103.35	110.50
3	B	1203	GOL	C3-C2-C1	-2.14	103.40	111.70

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	505	GOL	O1-C1-C2-C3
3	A	505	GOL	C1-C2-C3-O3
3	B	1203	GOL	C1-C2-C3-O3
3	B	1204	GOL	O1-C1-C2-O2
3	B	1204	GOL	O1-C1-C2-C3
3	B	1207	GOL	C1-C2-C3-O3
3	C	502	GOL	C1-C2-C3-O3
3	C	503	GOL	O1-C1-C2-O2
3	C	504	GOL	O1-C1-C2-C3
3	C	505	GOL	C1-C2-C3-O3
3	C	508	GOL	O1-C1-C2-C3
3	C	508	GOL	C1-C2-C3-O3
3	C	508	GOL	O2-C2-C3-O3
3	C	509	GOL	O1-C1-C2-O2
3	C	509	GOL	O1-C1-C2-C3
3	A	502	GOL	O1-C1-C2-O2
3	B	1203	GOL	O2-C2-C3-O3
3	C	509	GOL	O2-C2-C3-O3
3	A	502	GOL	O1-C1-C2-C3
3	A	503	GOL	O1-C1-C2-C3
3	A	503	GOL	C1-C2-C3-O3
3	B	1203	GOL	O1-C1-C2-C3
3	B	1204	GOL	C1-C2-C3-O3
3	B	1208	GOL	O1-C1-C2-C3
3	C	503	GOL	O1-C1-C2-C3
3	C	507	GOL	C1-C2-C3-O3
3	C	509	GOL	C1-C2-C3-O3
3	A	505	GOL	O1-C1-C2-O2
3	A	505	GOL	O2-C2-C3-O3
3	B	1203	GOL	O1-C1-C2-O2
3	C	504	GOL	O1-C1-C2-O2
3	C	505	GOL	O2-C2-C3-O3
3	C	508	GOL	O1-C1-C2-O2
3	B	1207	GOL	O2-C2-C3-O3
3	B	1208	GOL	O1-C1-C2-O2
3	C	502	GOL	O2-C2-C3-O3
4	B	1212	D82	O1-C1-C2-C9
3	B	1204	GOL	O2-C2-C3-O3
3	A	502	GOL	C1-C2-C3-O3
3	A	503	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	1206	GOL	C1-C2-C3-O3
3	A	502	GOL	O2-C2-C3-O3

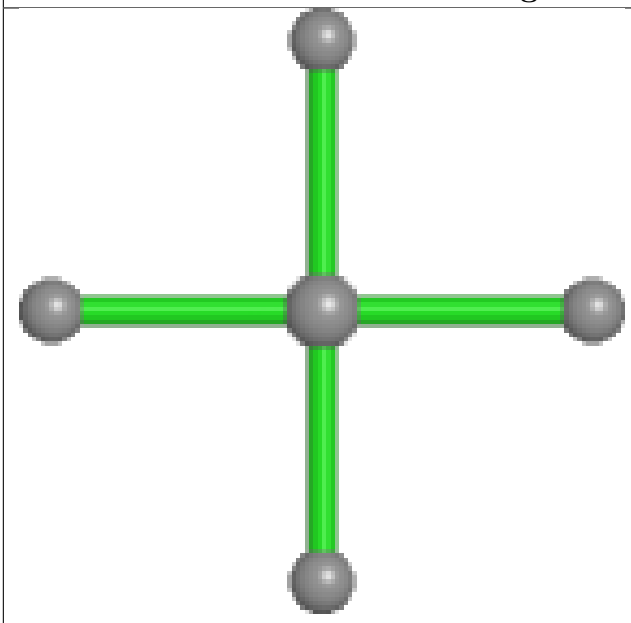
There are no ring outliers.

20 monomers are involved in 33 short contacts:

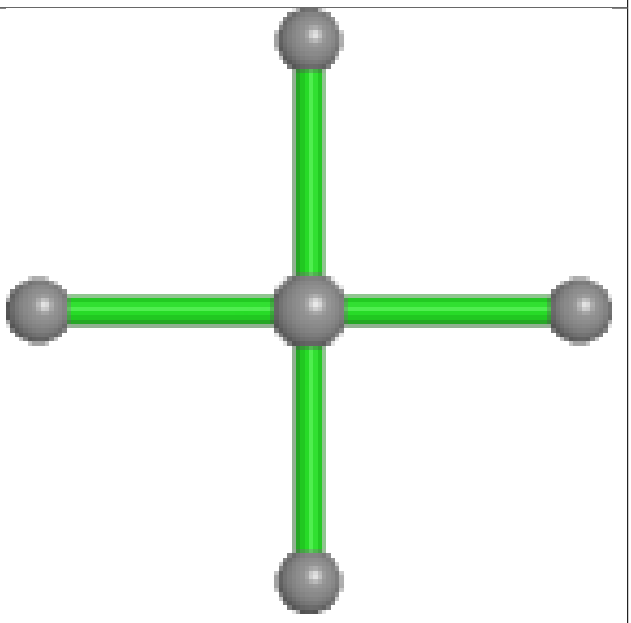
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1201	GOL	1	0
3	B	1203	GOL	1	0
4	B	1212	D82	5	0
3	C	509	GOL	1	0
3	B	1204	GOL	1	0
4	A	506	D82	1	0
4	C	506	D82	1	0
3	C	508	GOL	1	0
3	A	504	GOL	2	0
3	A	505	GOL	3	0
3	B	1210	GOL	1	0
3	B	1207	GOL	1	0
3	C	504	GOL	2	0
3	B	1205	GOL	1	0
3	A	502	GOL	1	0
3	C	502	GOL	2	0
3	A	503	GOL	1	0
3	C	503	GOL	1	0
3	B	1211	GOL	2	0
3	B	1209	GOL	4	0

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

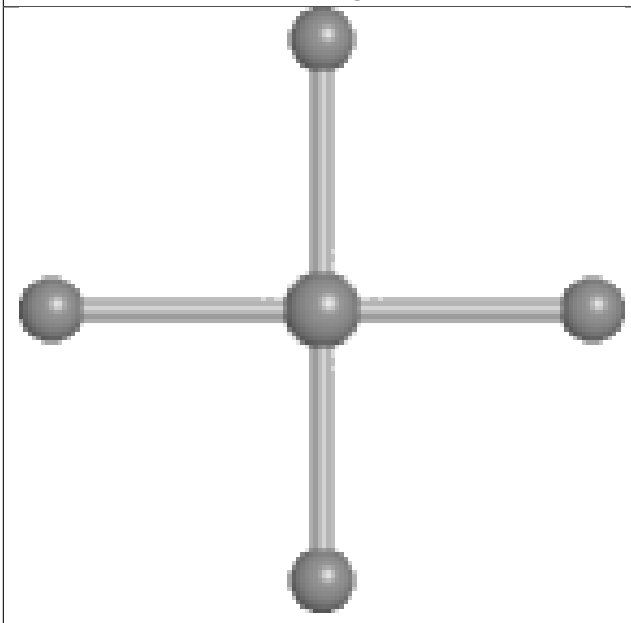
Ligand SO4 B 1214



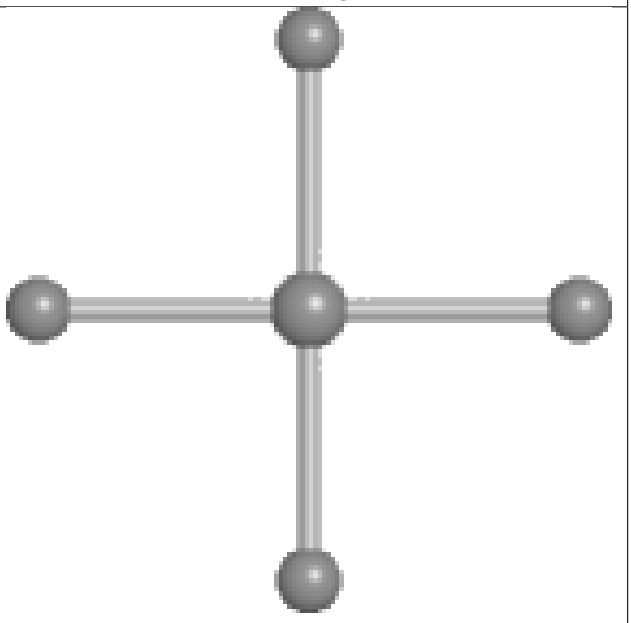
Bond lengths



Bond angles

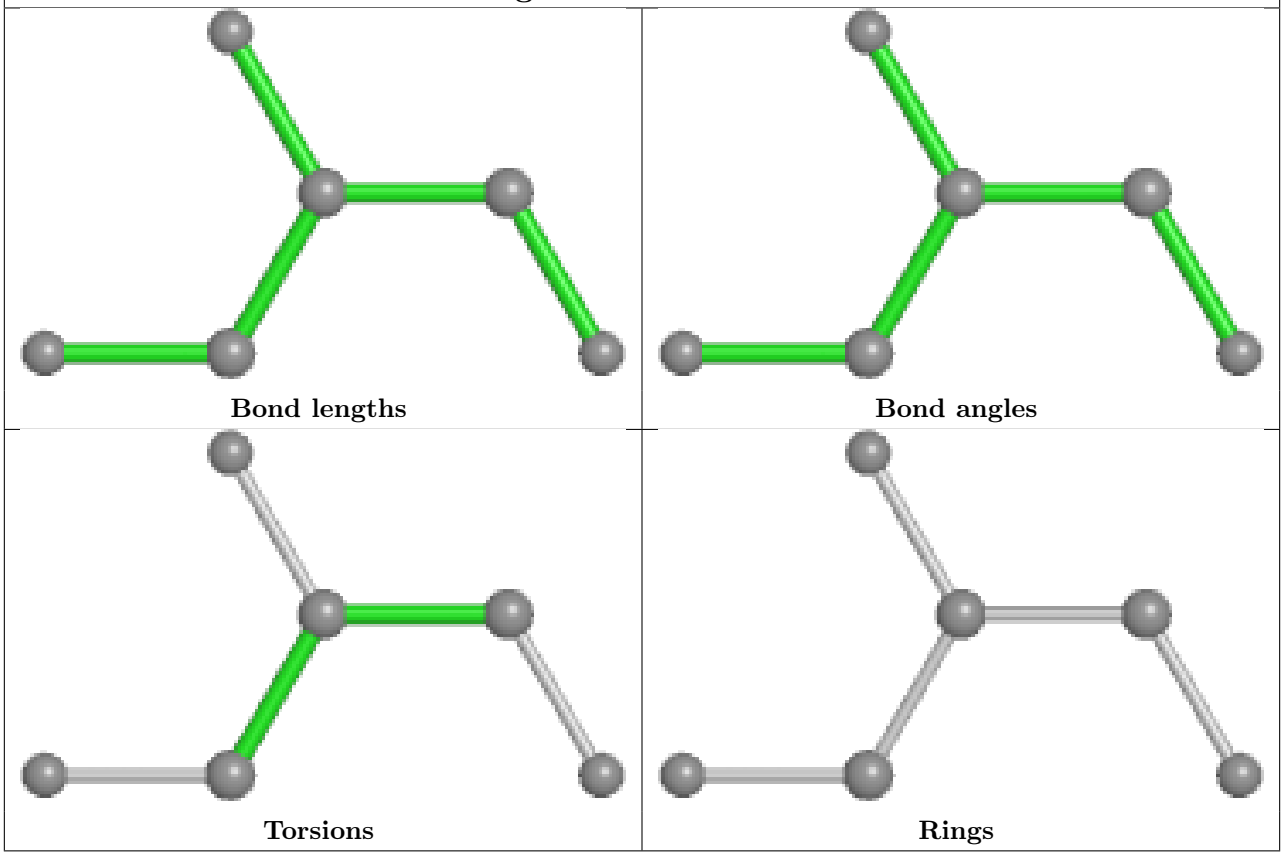


Torsions

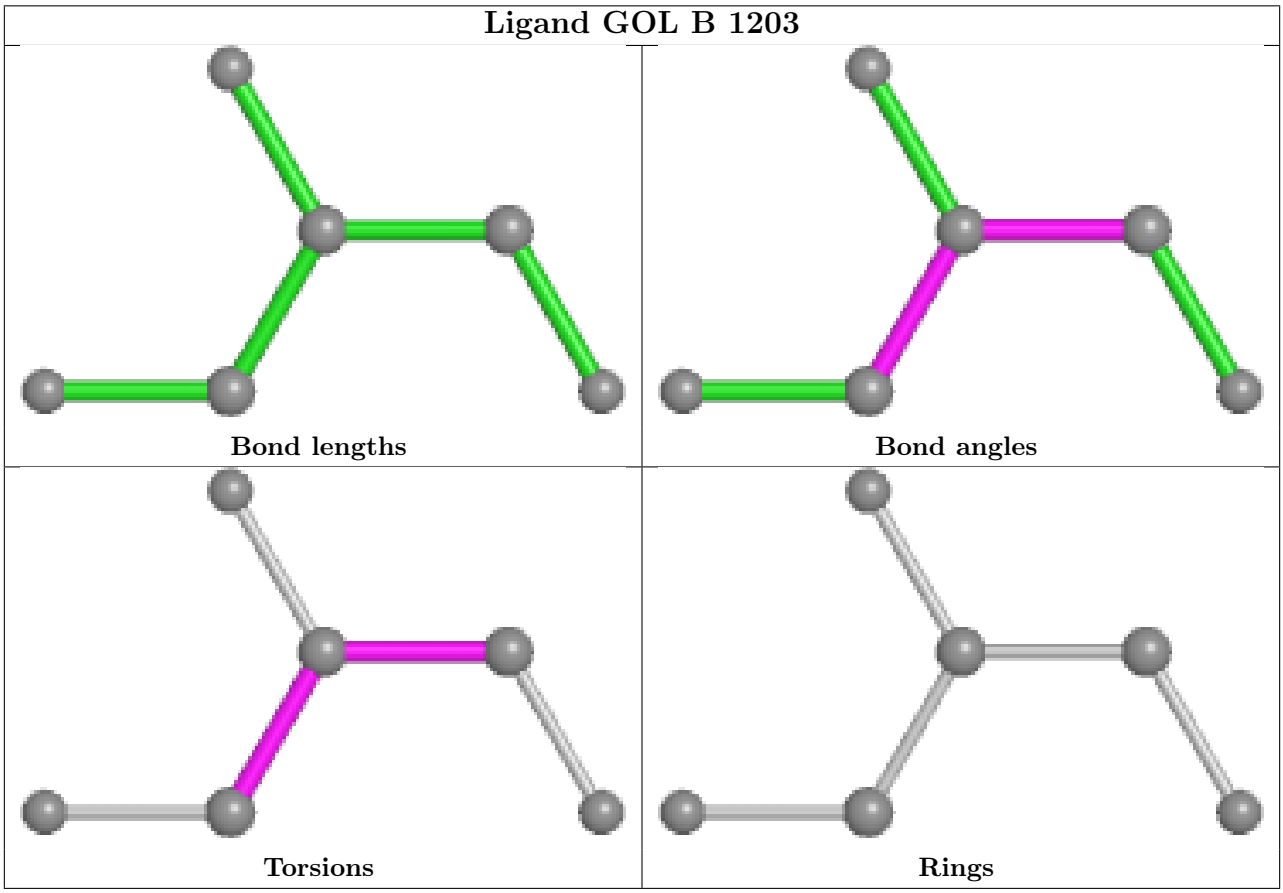


Rings

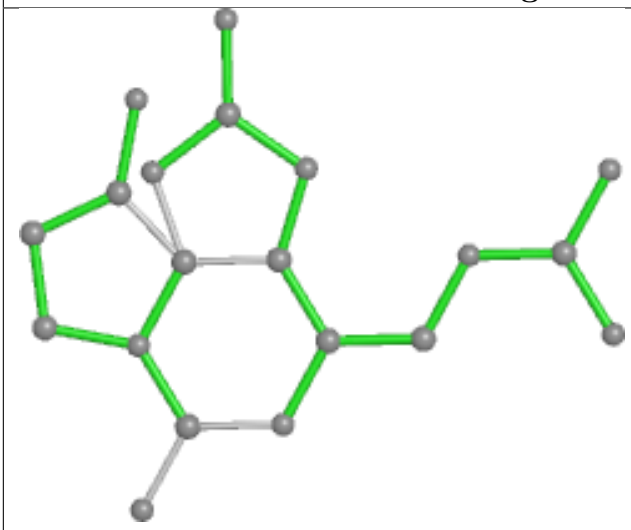
Ligand GOL B 1201



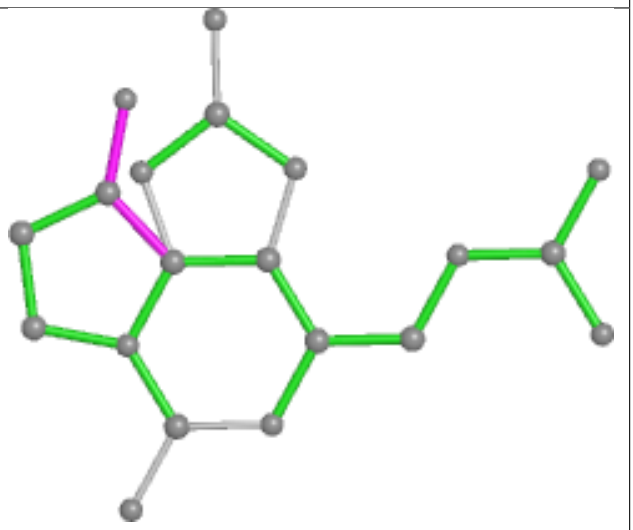
Ligand GOL B 1203



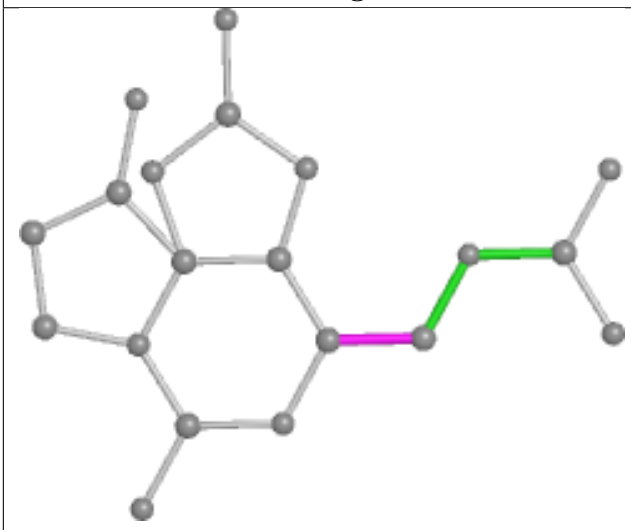
Ligand D82 B 1212



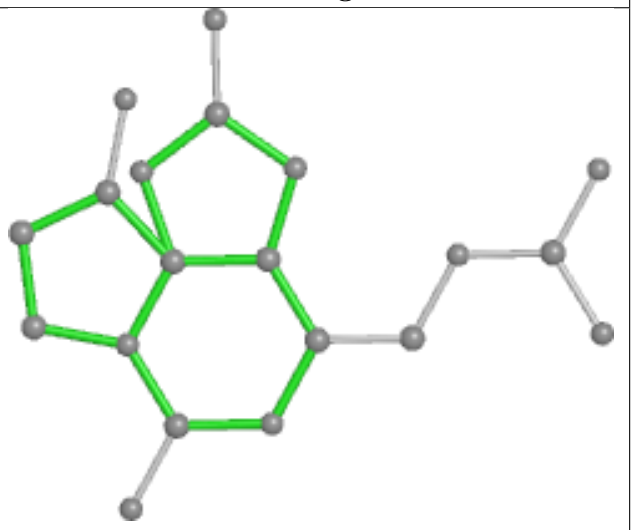
Bond lengths



Bond angles

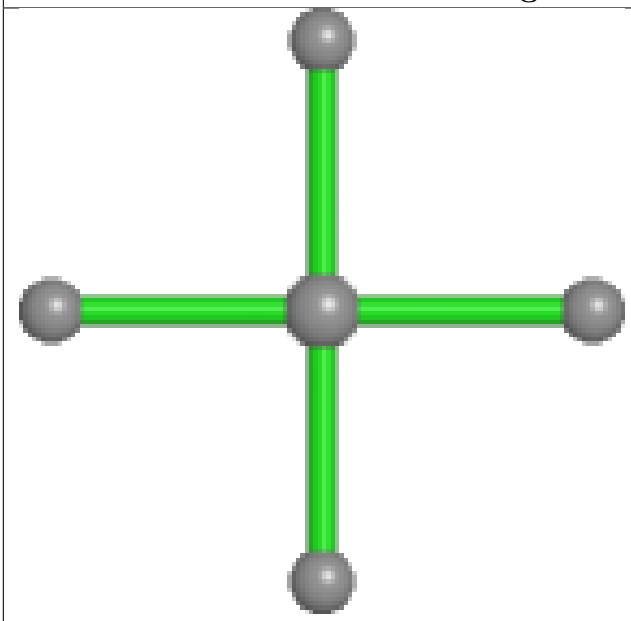


Torsions

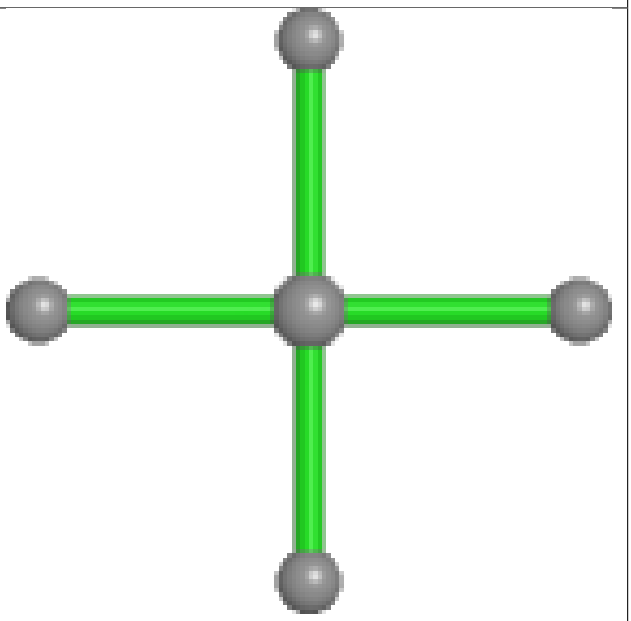


Rings

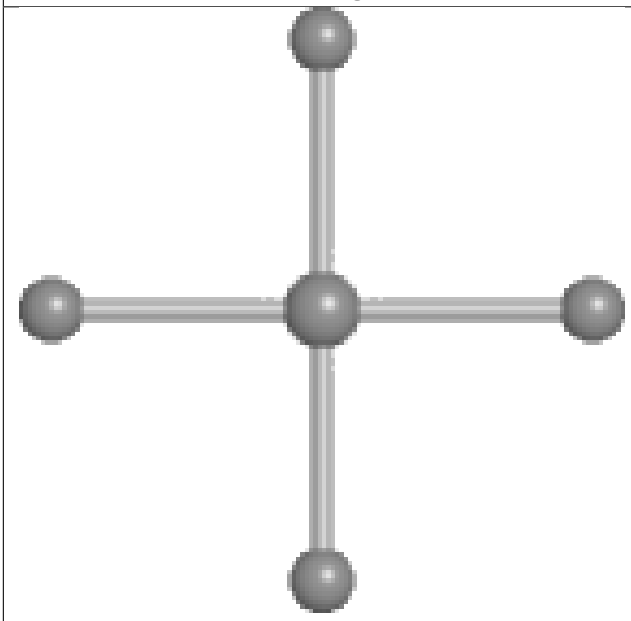
Ligand SO4 B 1216



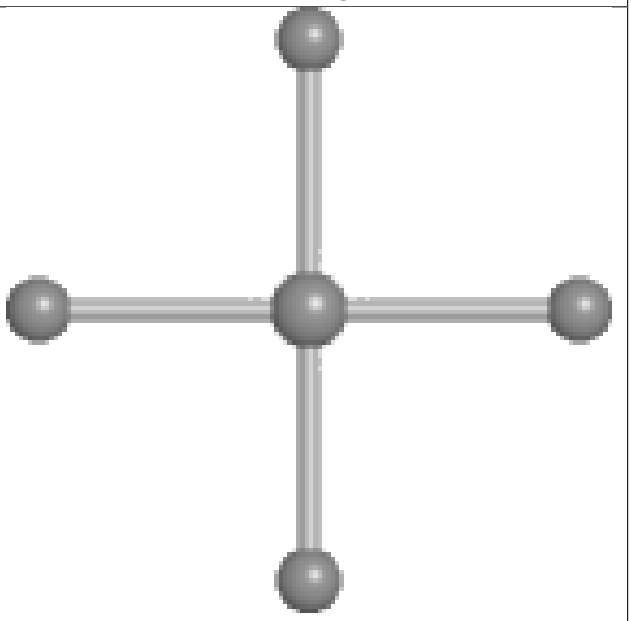
Bond lengths



Bond angles

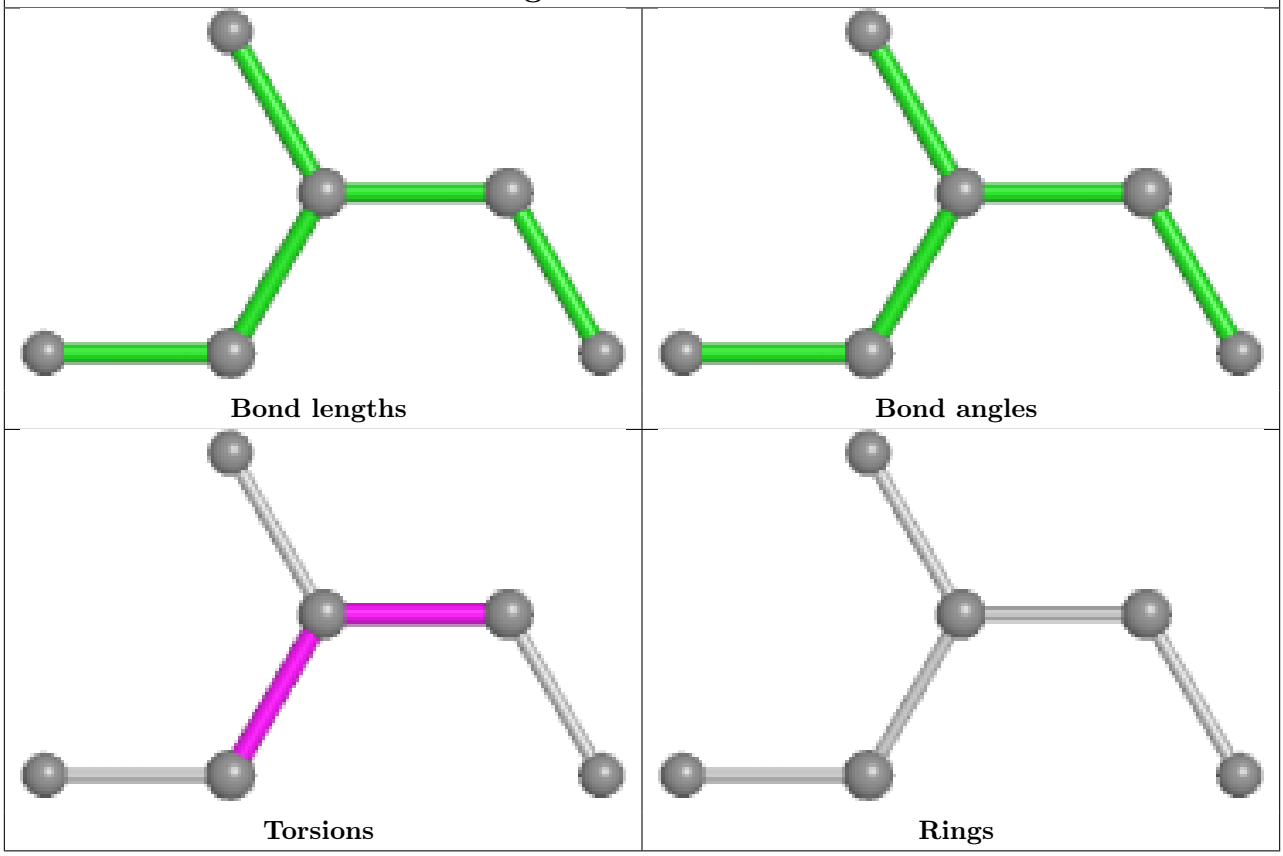


Torsions

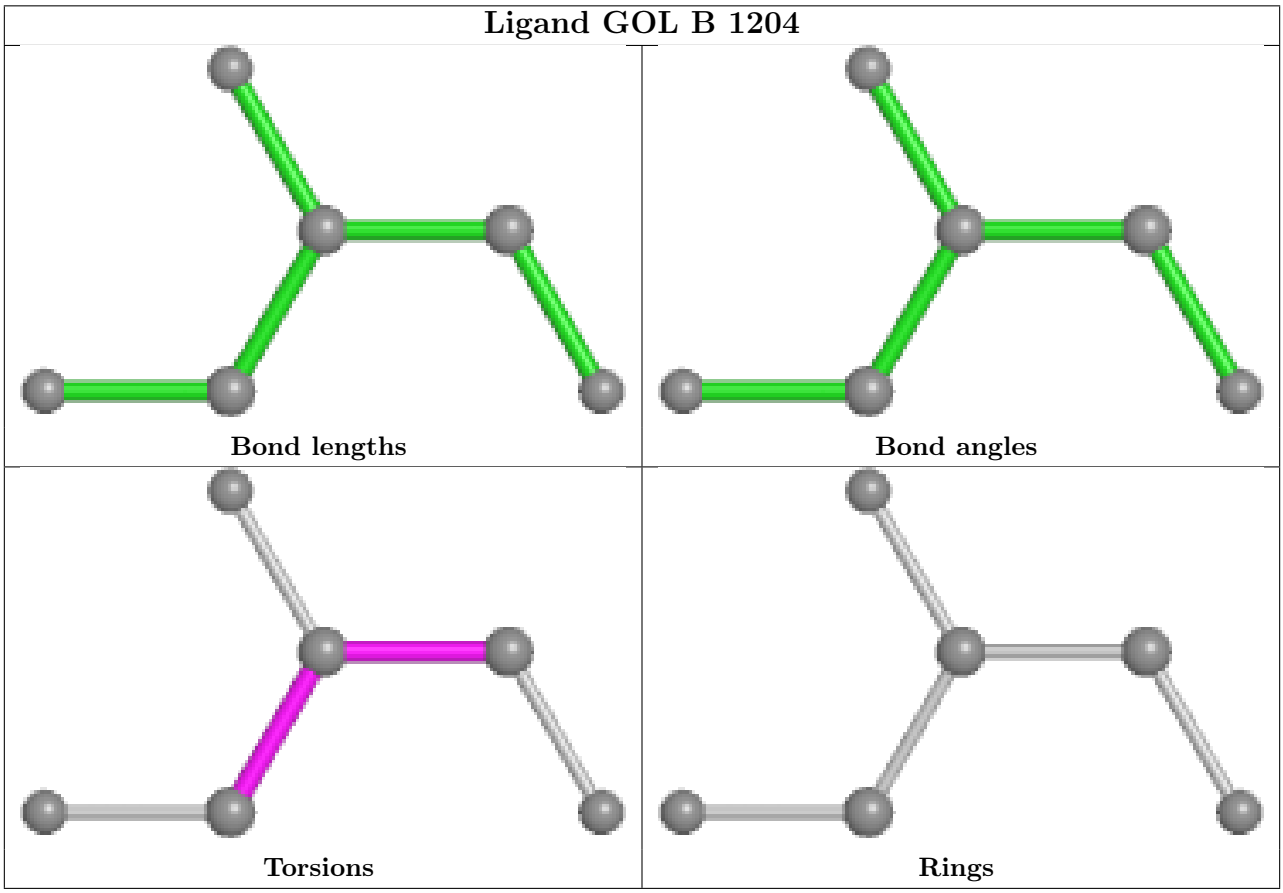


Rings

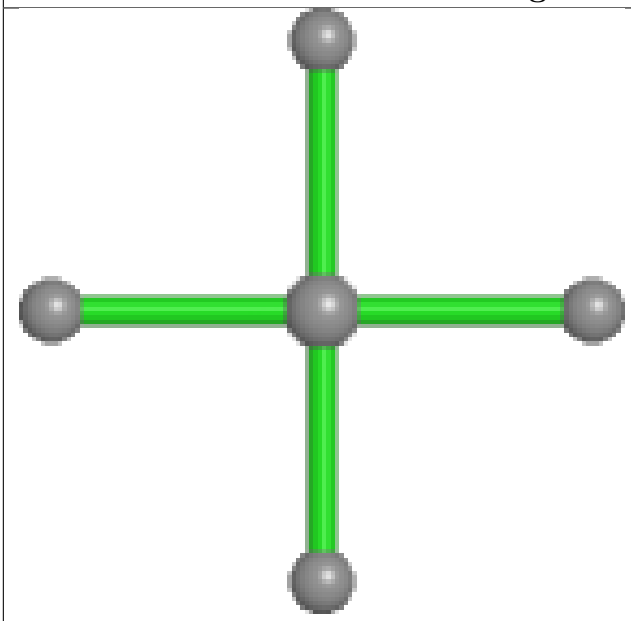
Ligand GOL C 509



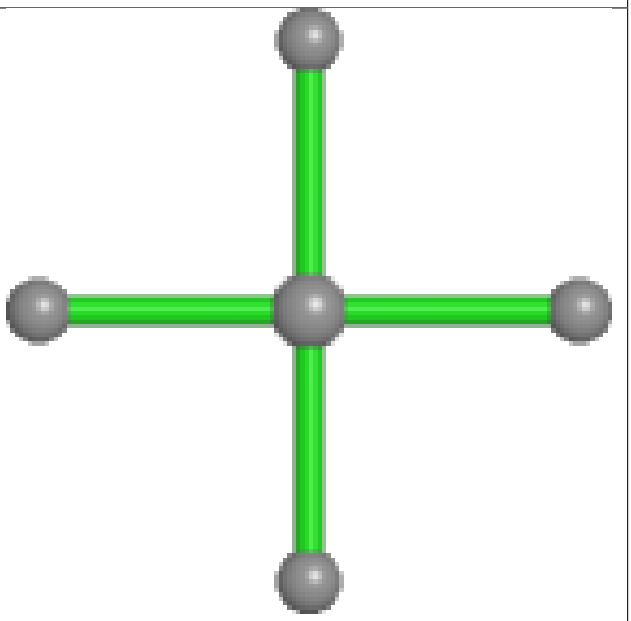
Ligand GOL B 1204



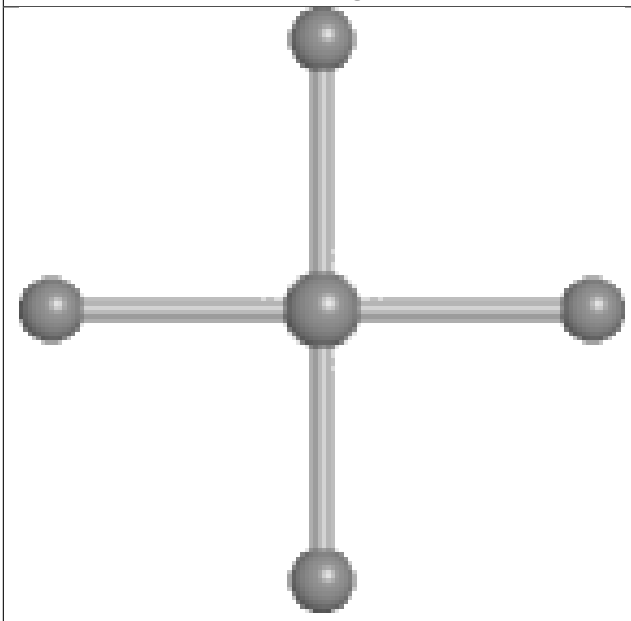
Ligand SO4 C 512



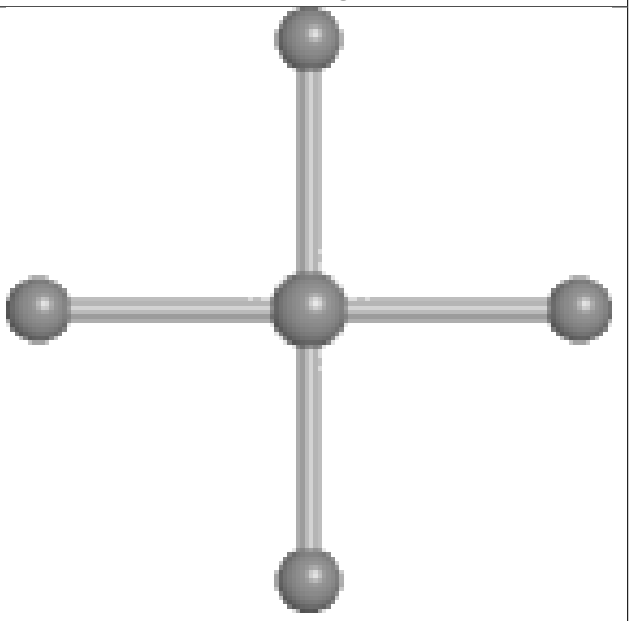
Bond lengths



Bond angles

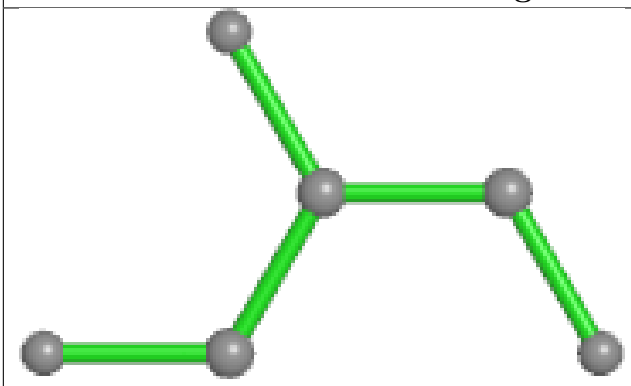


Torsions

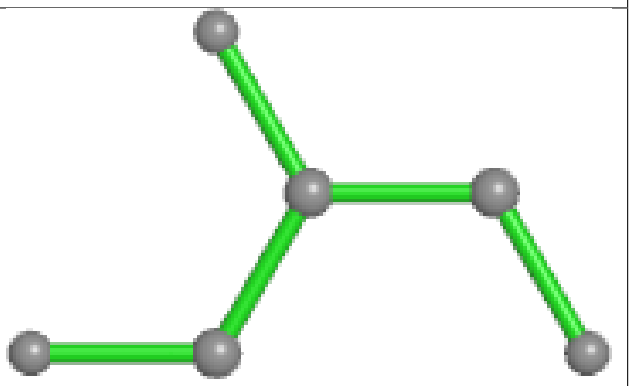


Rings

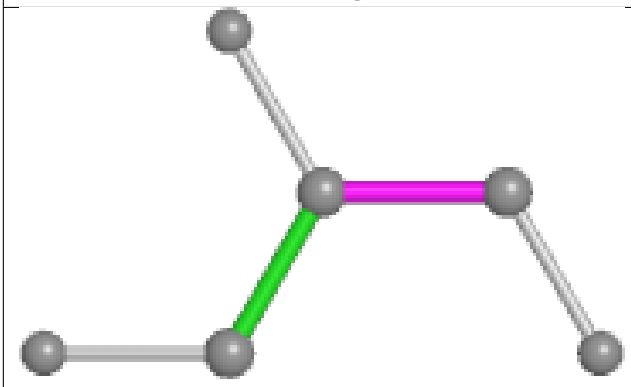
Ligand GOL B 1208



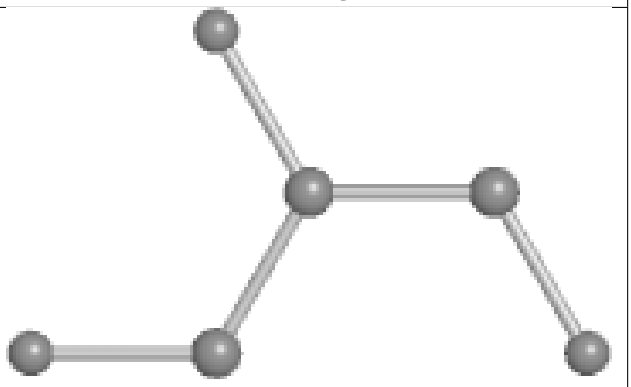
Bond lengths



Bond angles

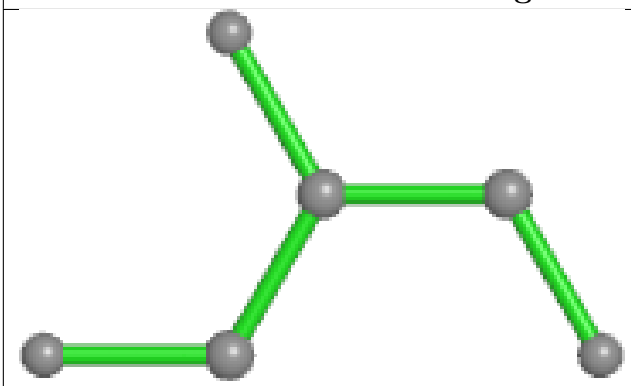


Torsions

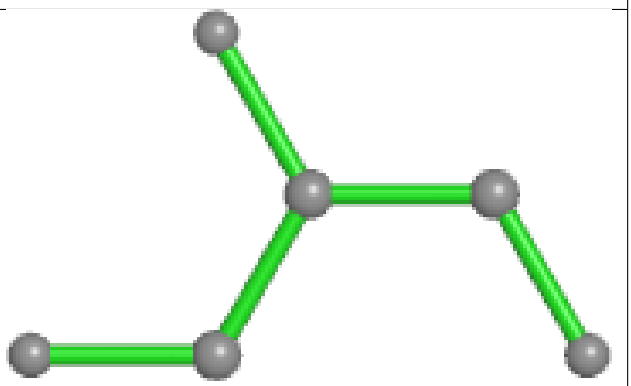


Rings

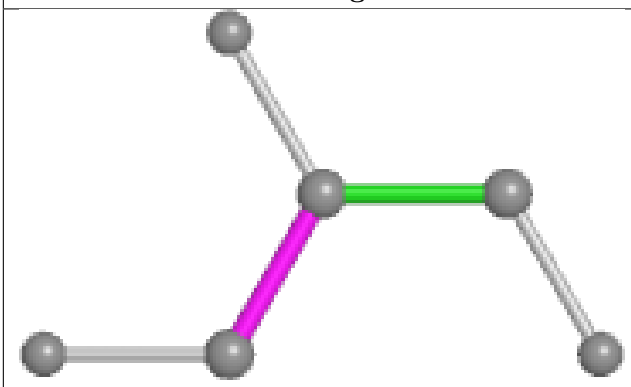
Ligand GOL B 1206



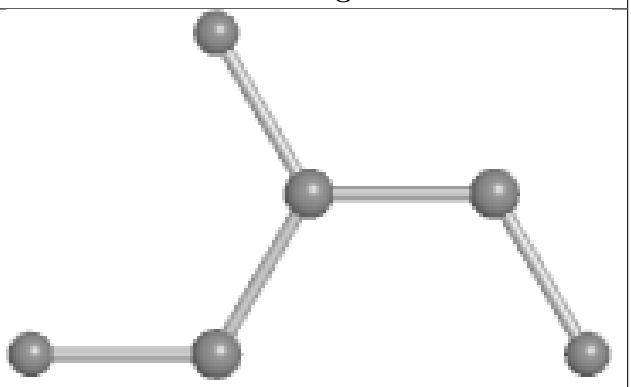
Bond lengths



Bond angles

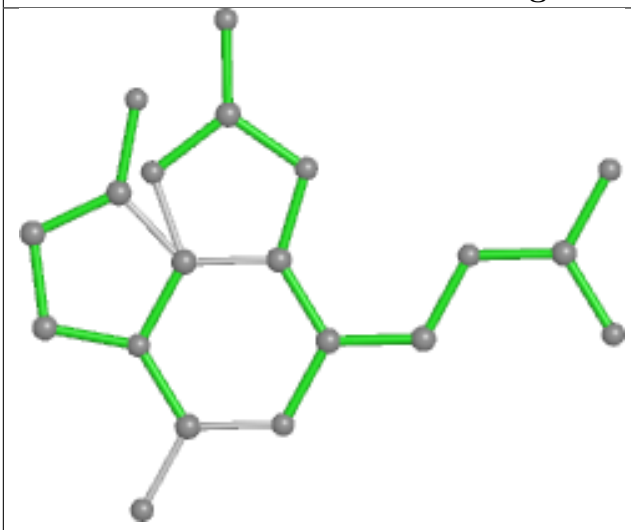


Torsions

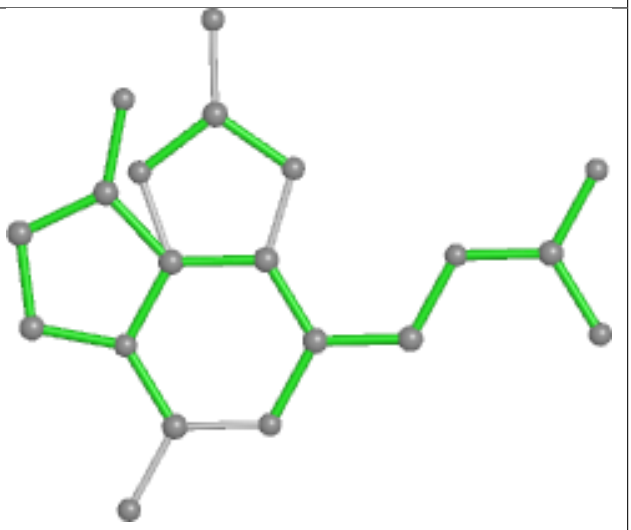


Rings

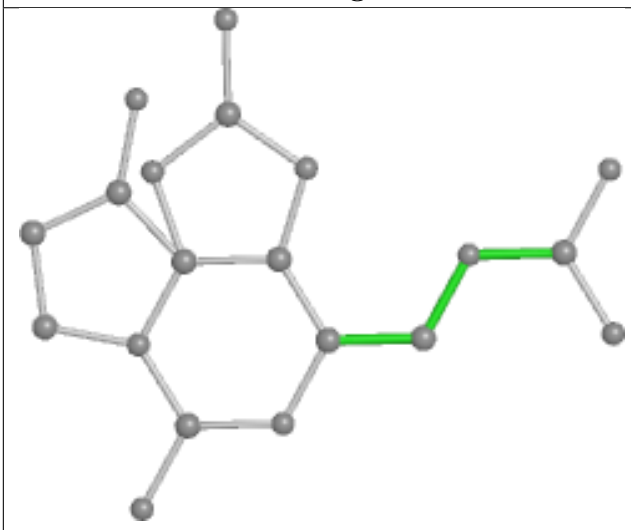
Ligand D82 A 506



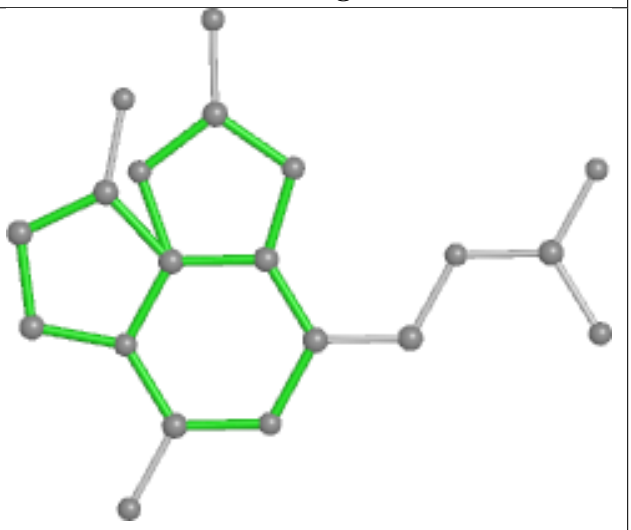
Bond lengths



Bond angles

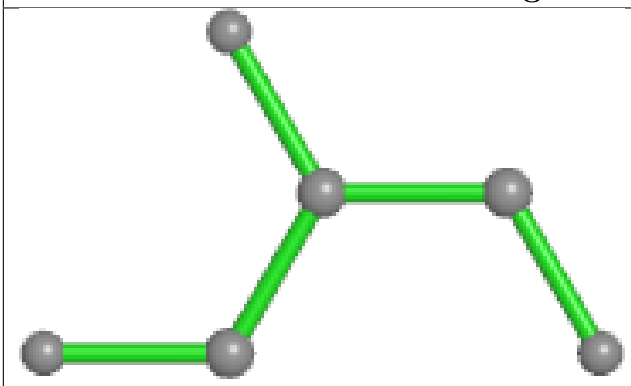


Torsions

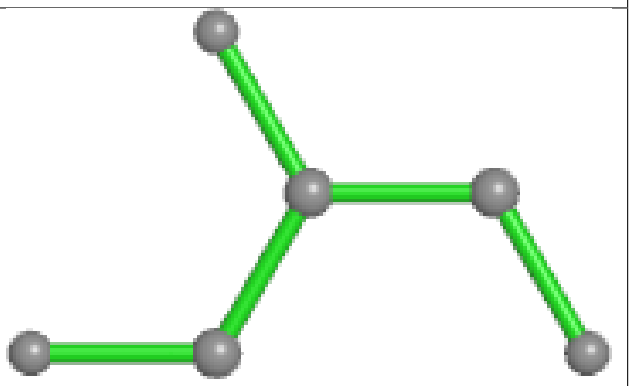


Rings

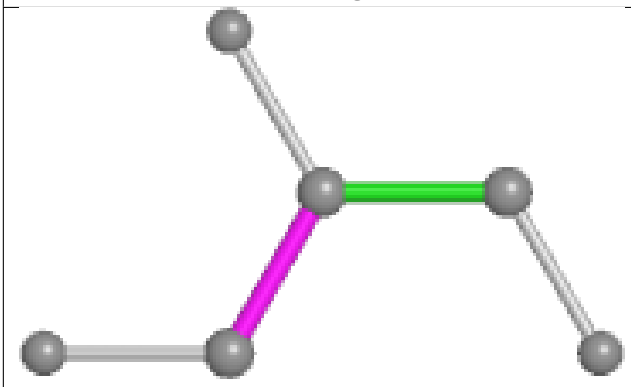
Ligand GOL C 507



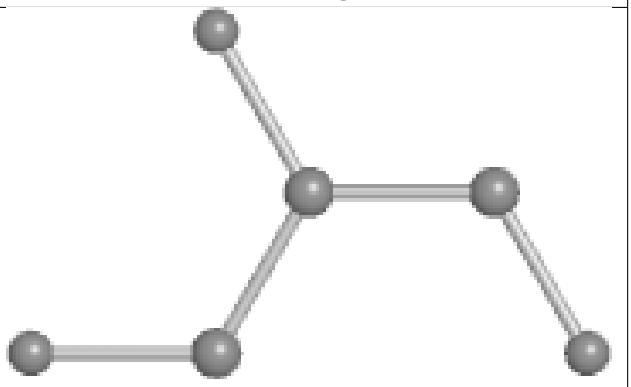
Bond lengths



Bond angles

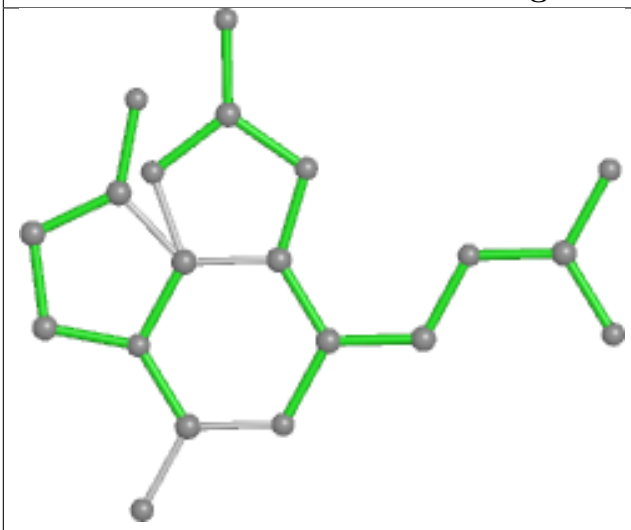


Torsions

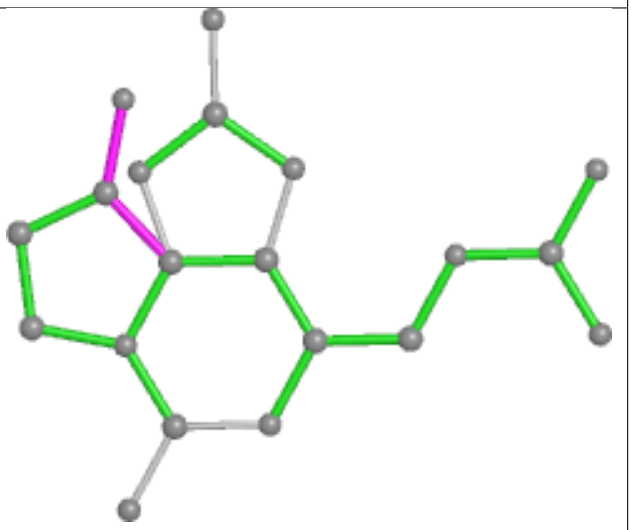


Rings

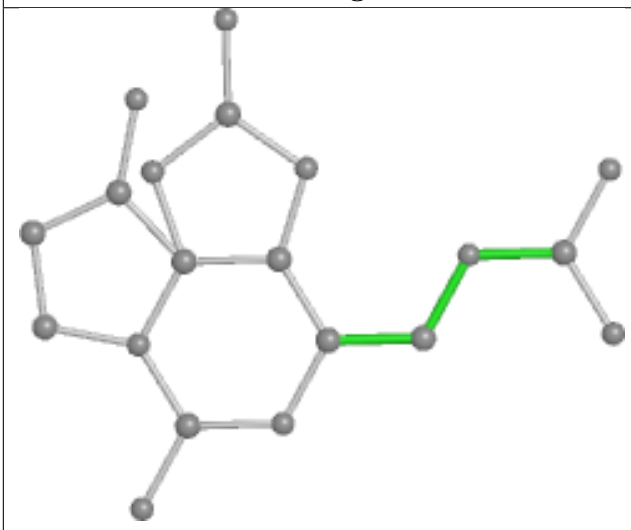
Ligand D82 C 506



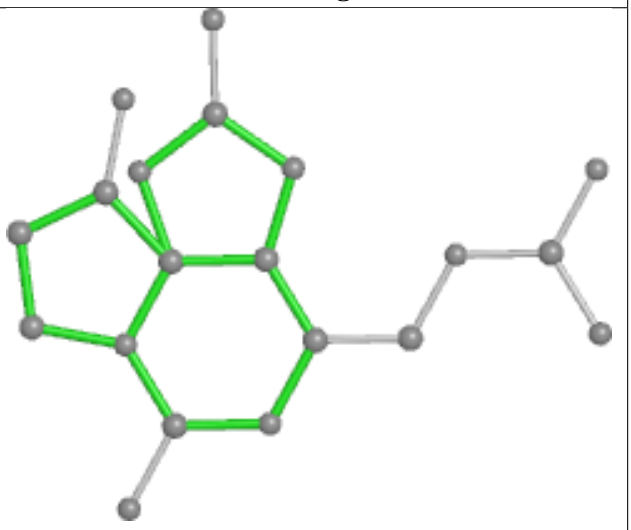
Bond lengths



Bond angles

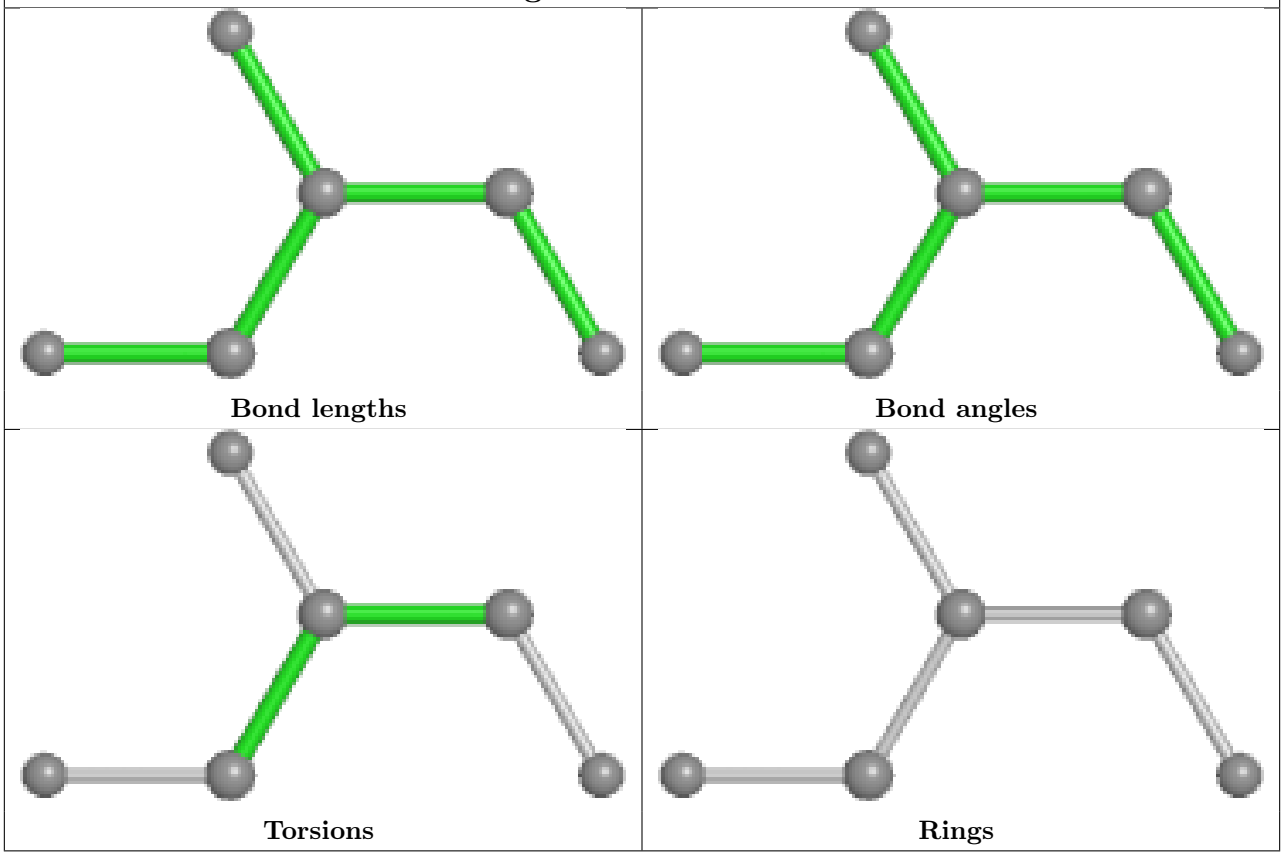


Torsions

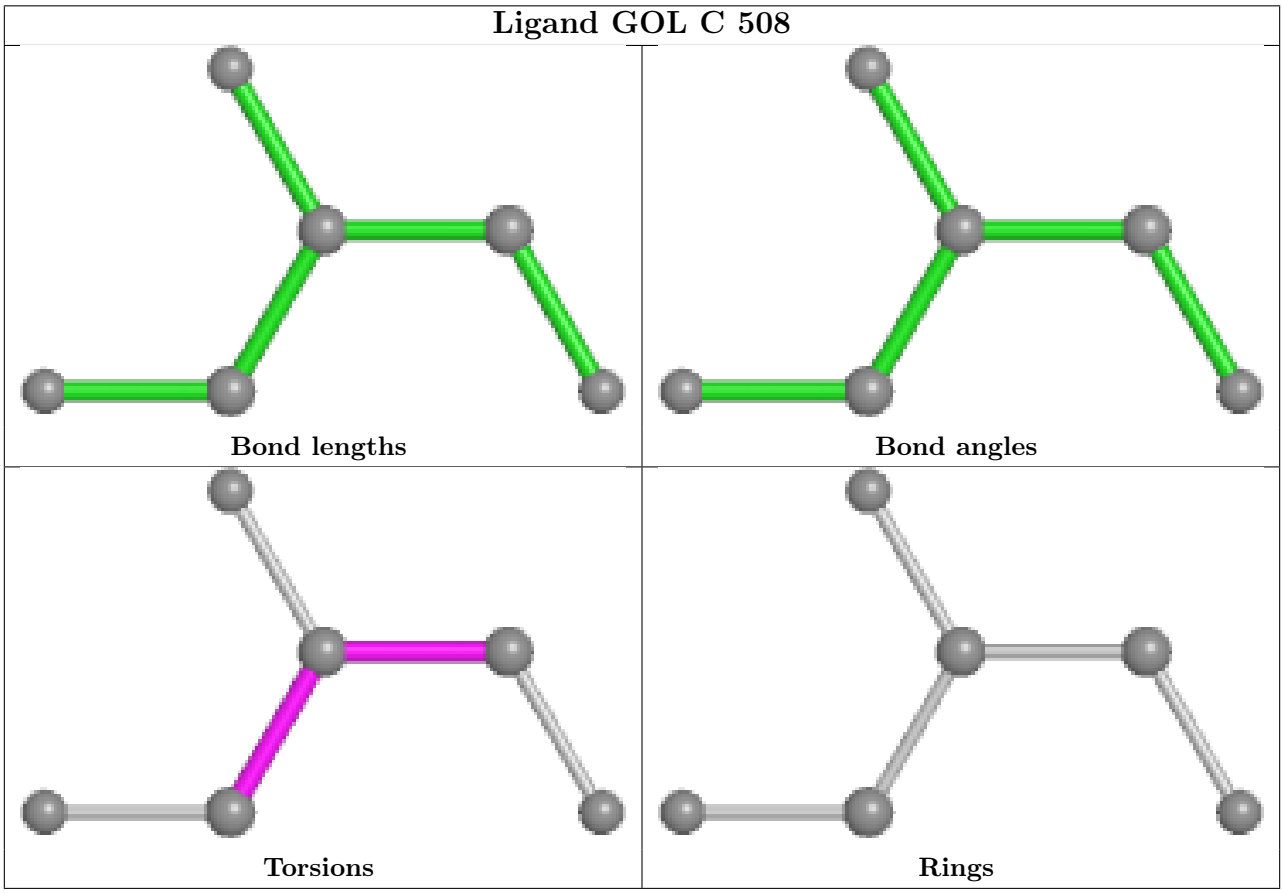


Rings

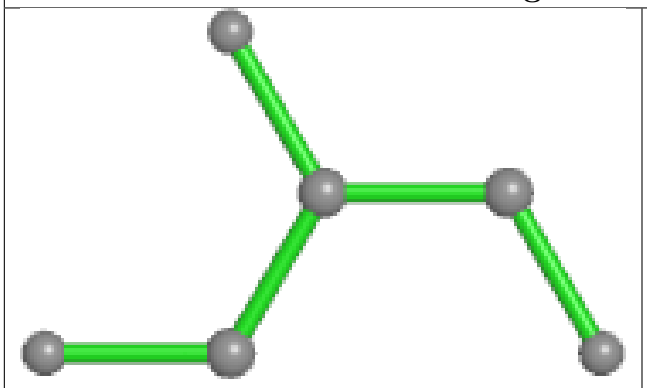
Ligand GOL C 510



Ligand GOL C 508



Ligand GOL A 504



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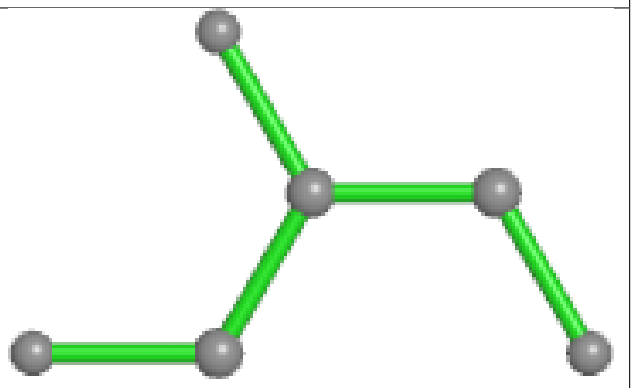
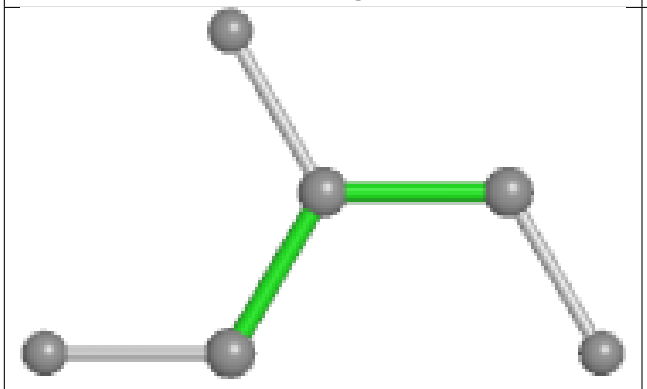
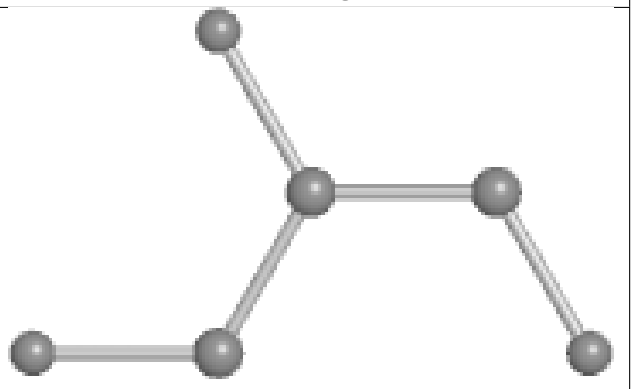


Bond angles

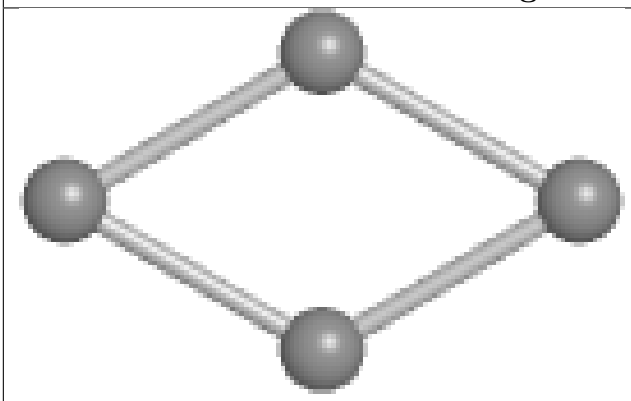


Torsions

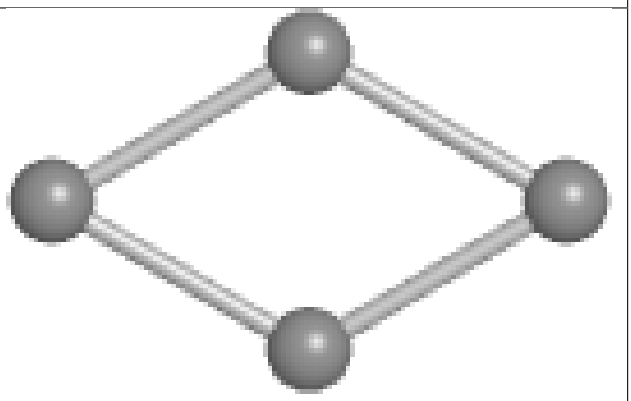


Rings

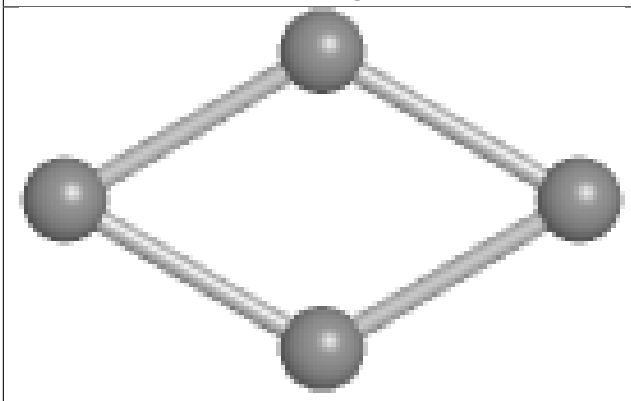
Ligand FES B 1202



Bond lengths



Bond angles



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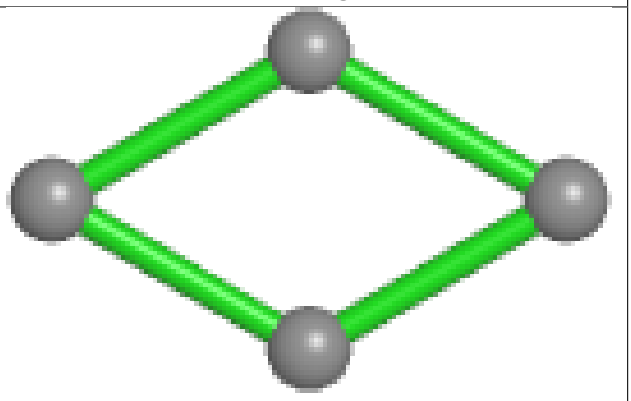
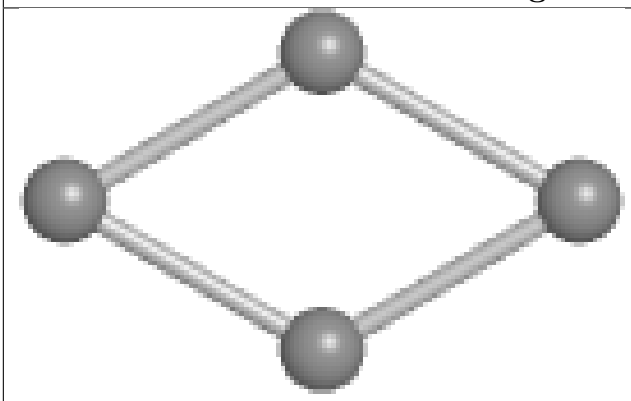
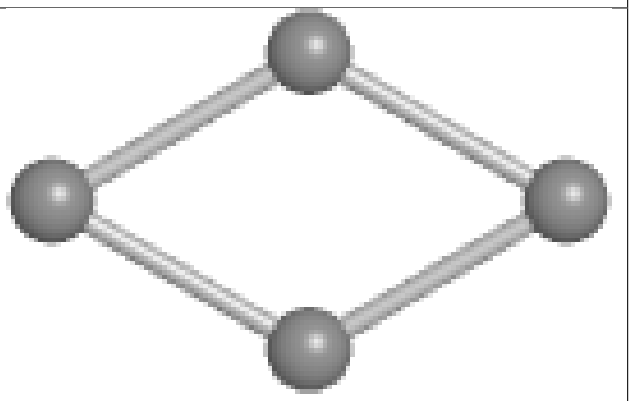


Rings

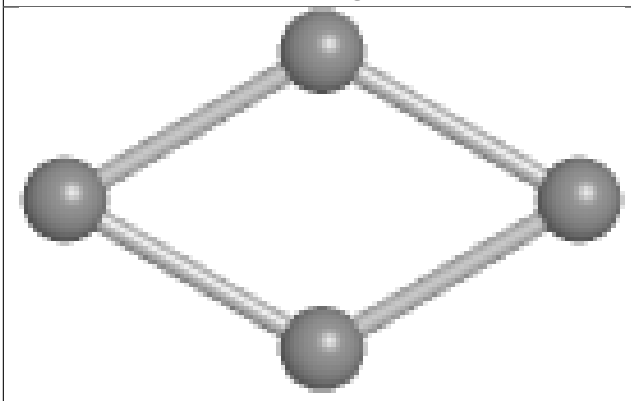
Ligand FES C 501



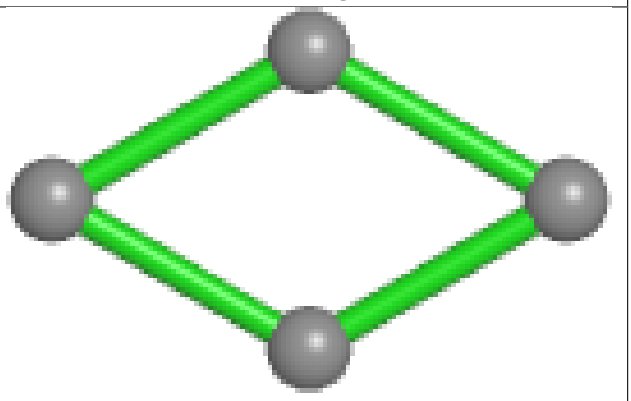
Bond lengths



Bond angles

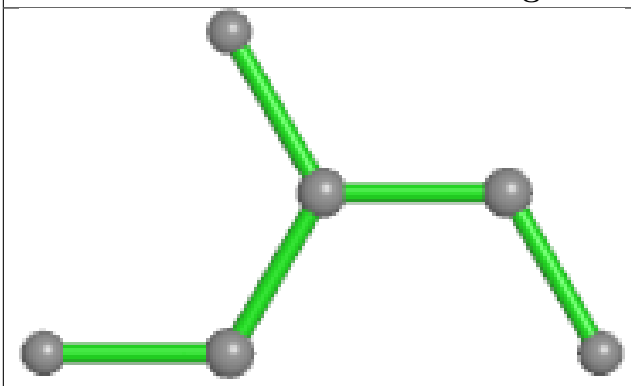


Torsions

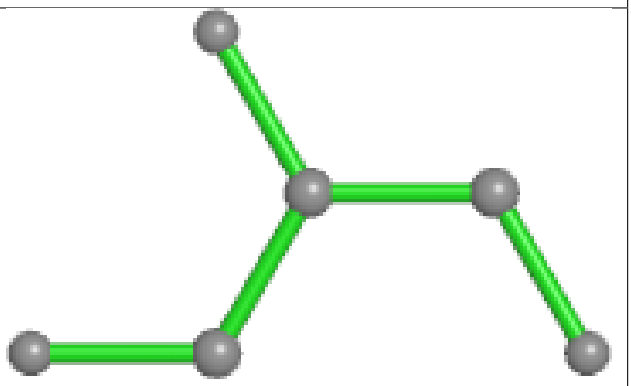


Rings

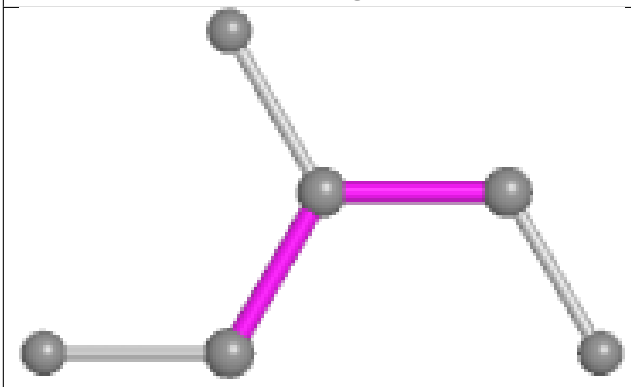
Ligand GOL A 505



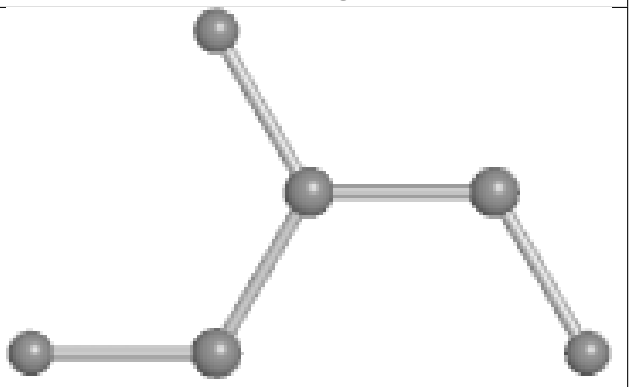
Bond lengths



Bond angles

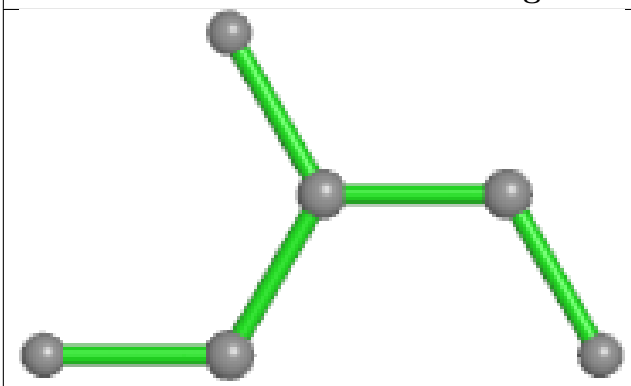


Torsions

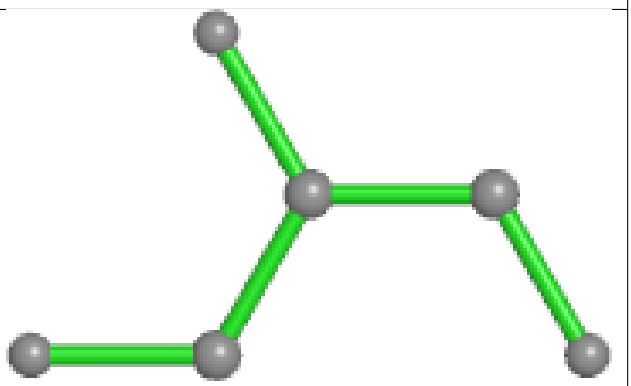


Rings

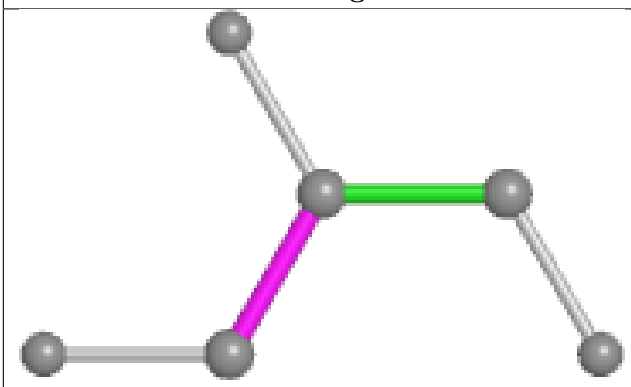
Ligand GOL C 505



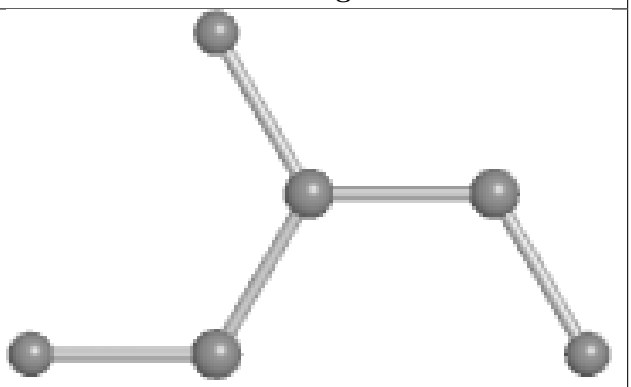
Bond lengths



Bond angles

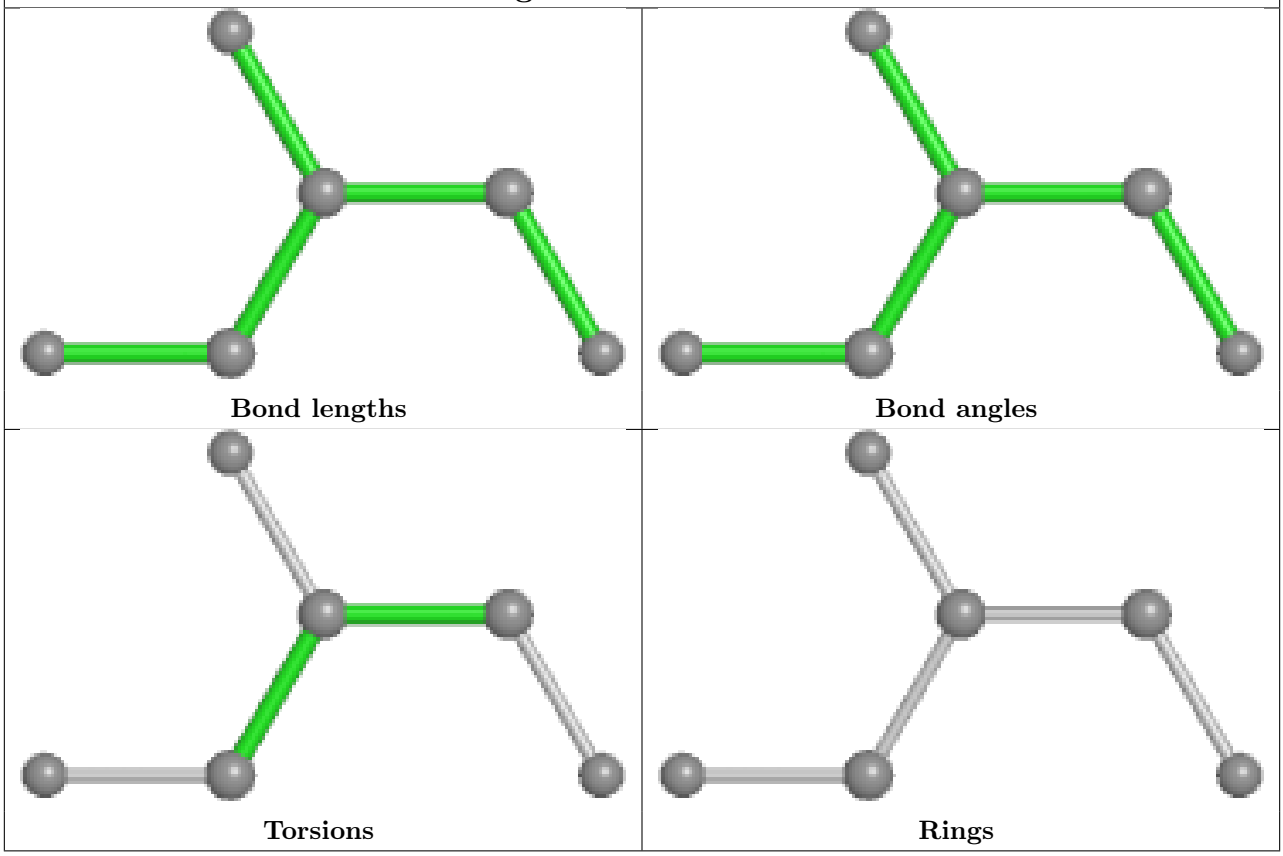


Torsions

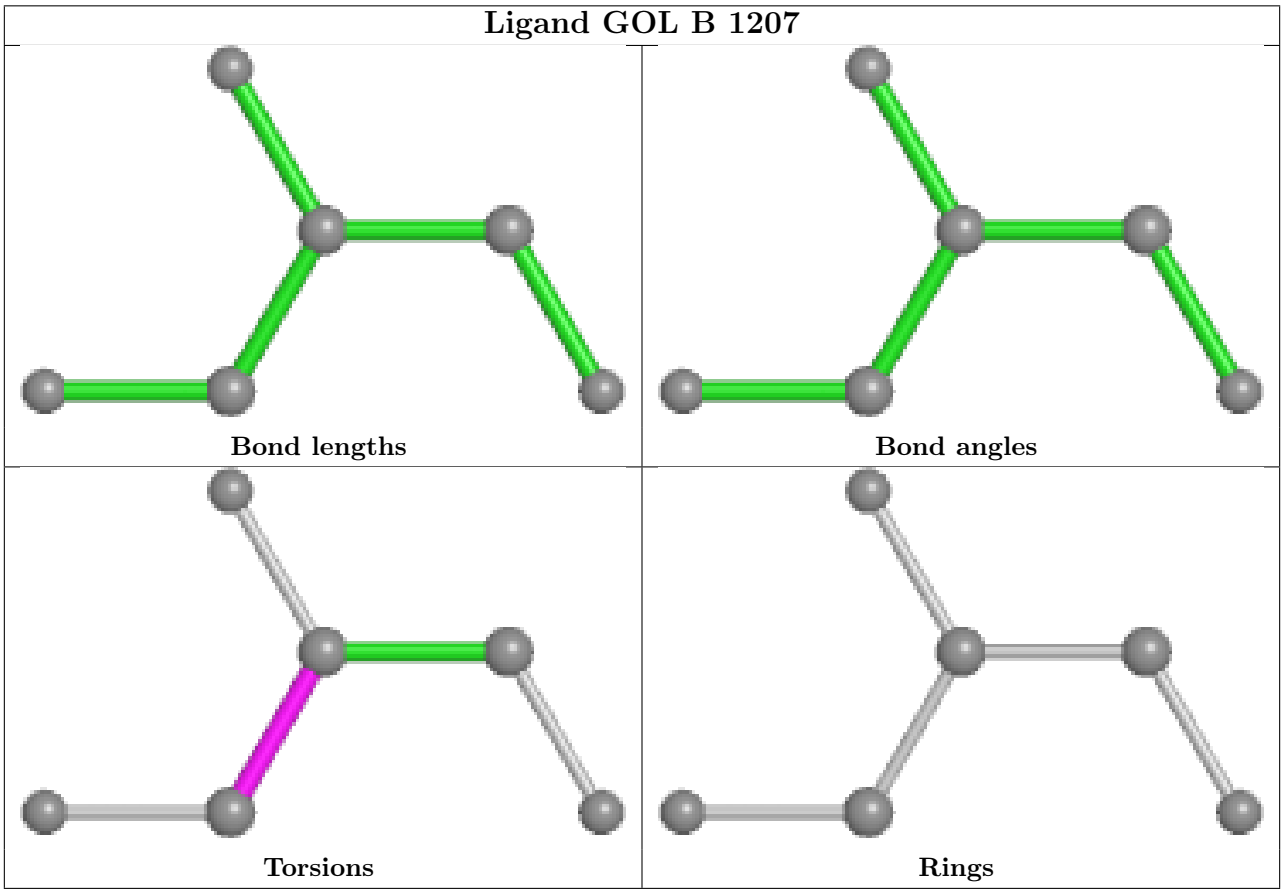


Rings

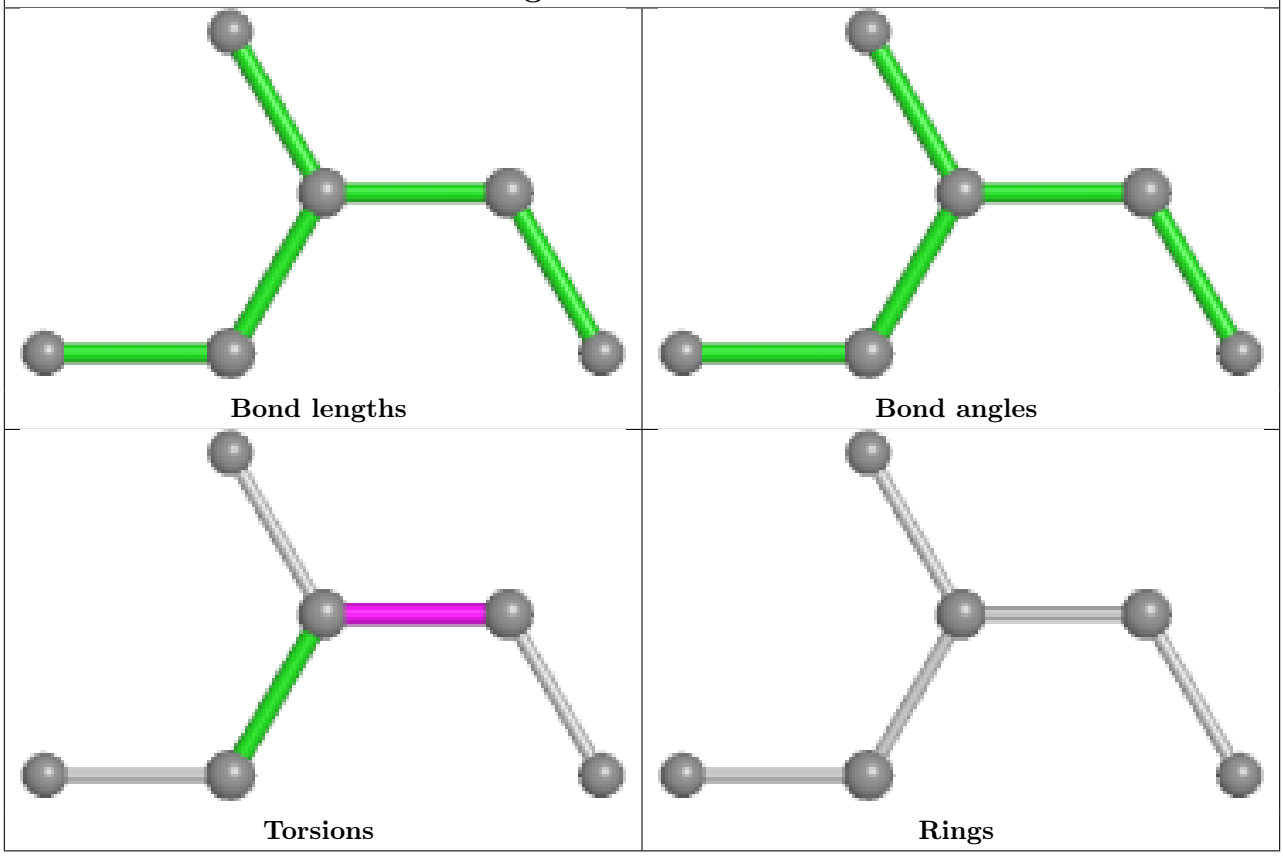
Ligand GOL B 1210



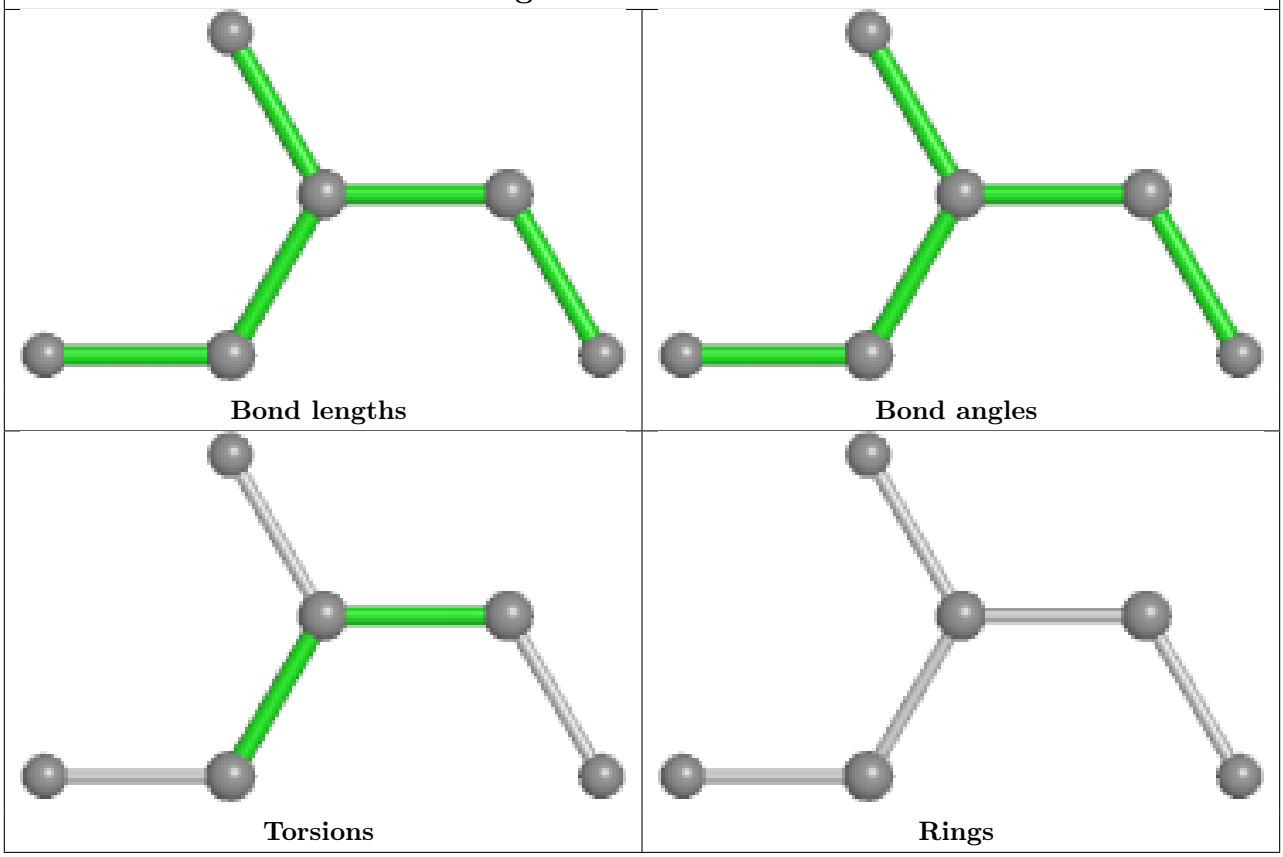
Ligand GOL B 1207



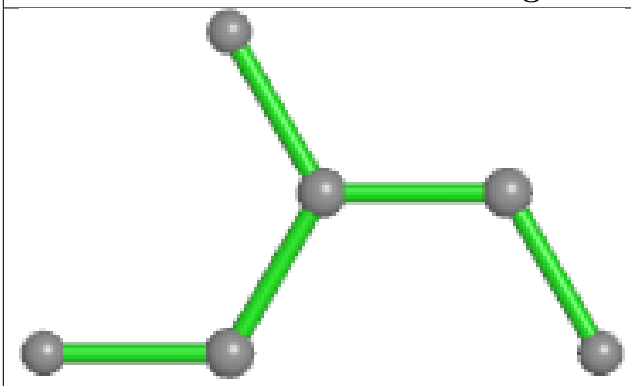
Ligand GOL C 504



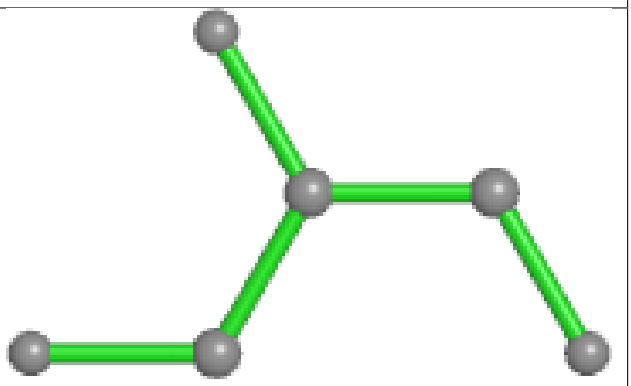
Ligand GOL B 1205



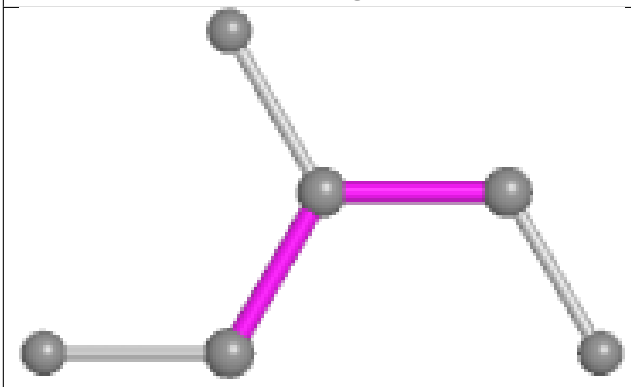
Ligand GOL A 502



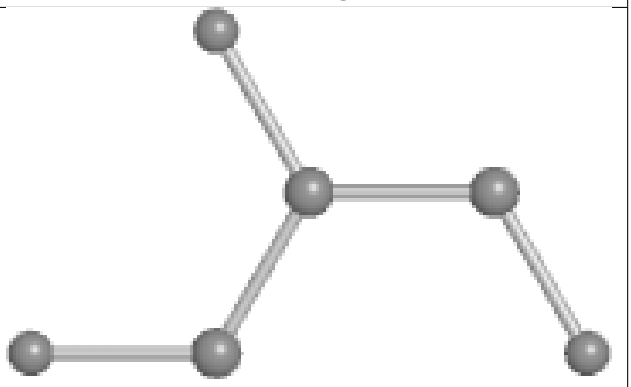
Bond lengths



Bond angles

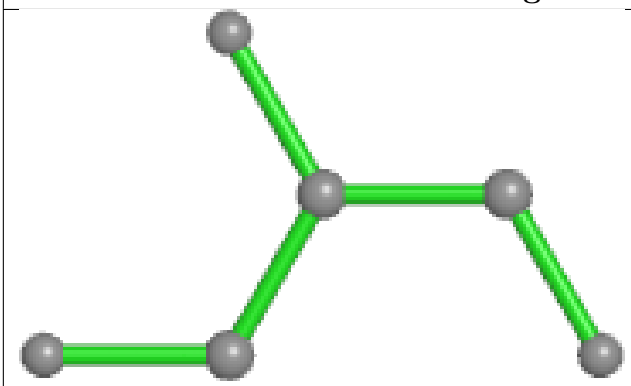


Torsions



Rings

Ligand GOL C 502



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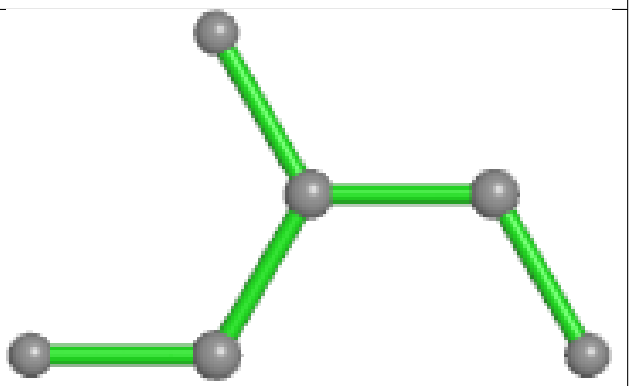
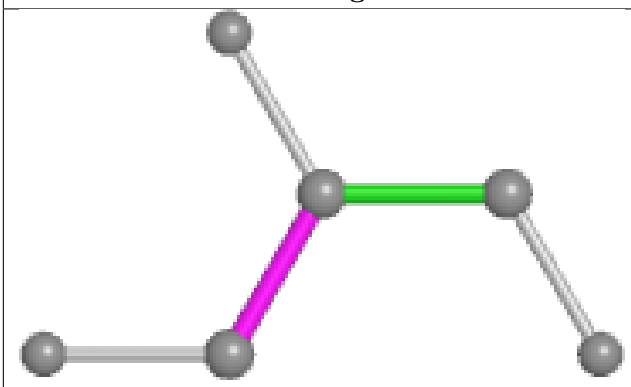
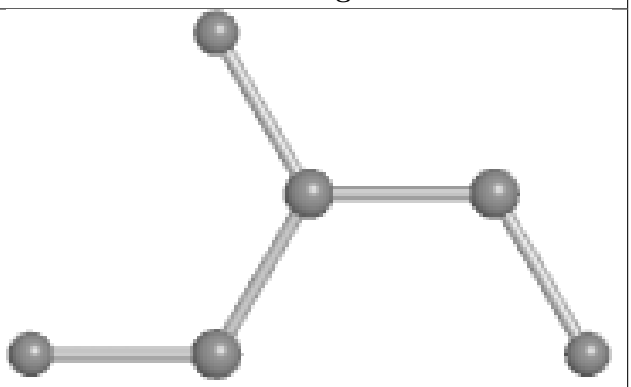


Bond angles

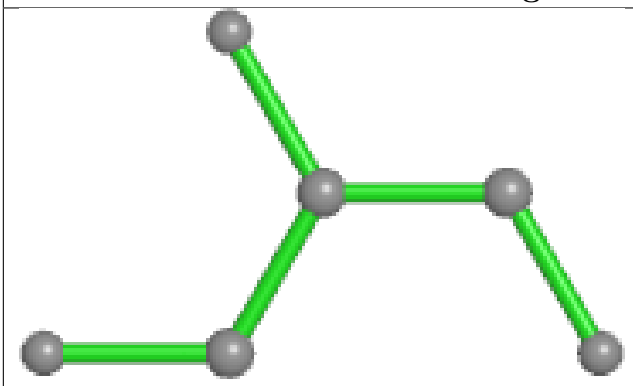


Torsions

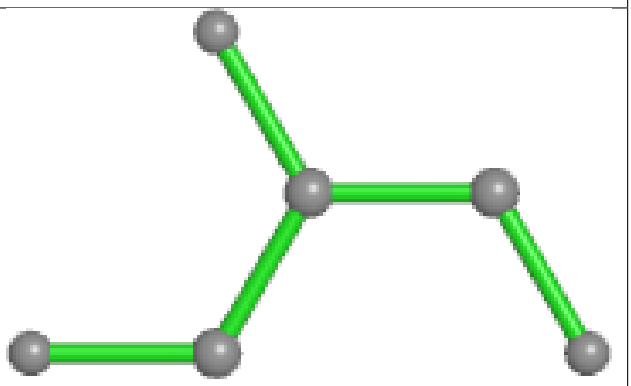


Rings

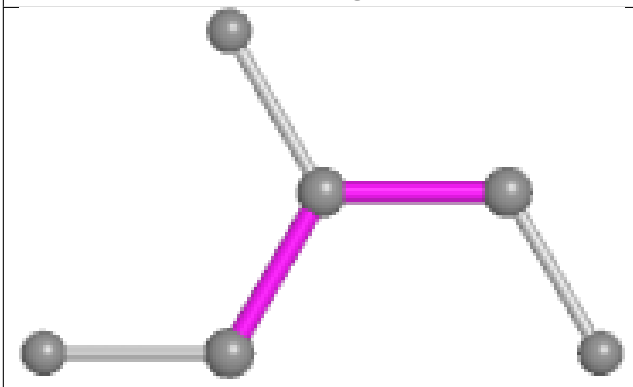
Ligand GOL A 503



Bond lengths



Bond angles



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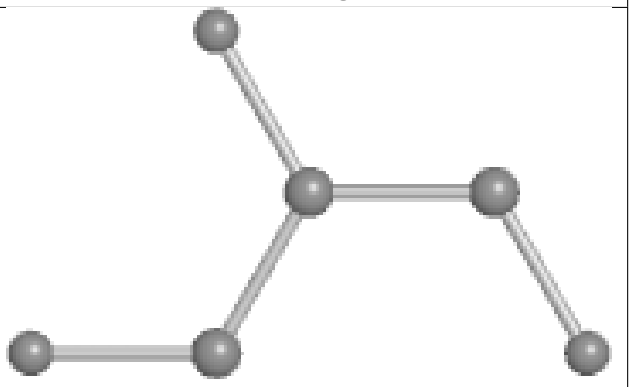
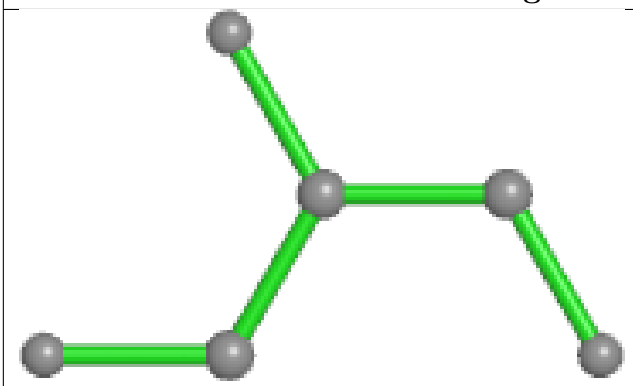
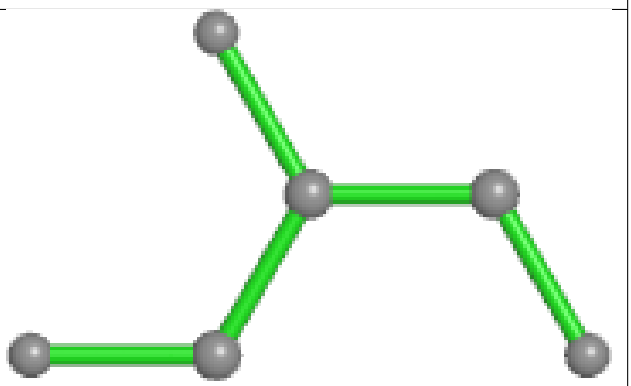


Rings

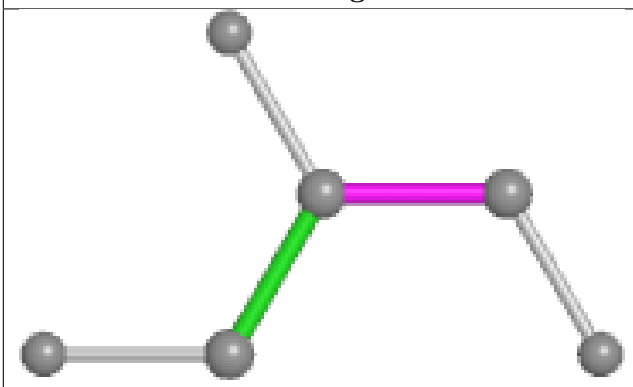
Ligand GOL C 503



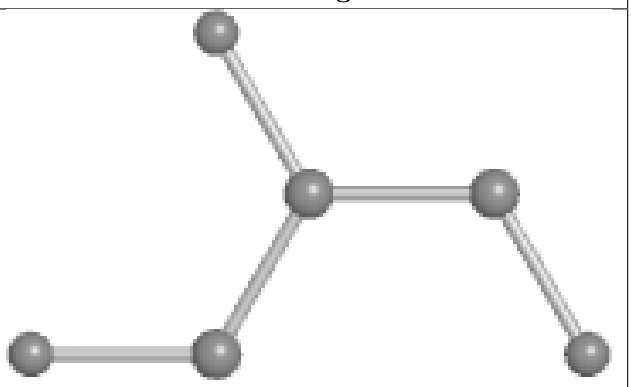
Bond lengths



Bond angles

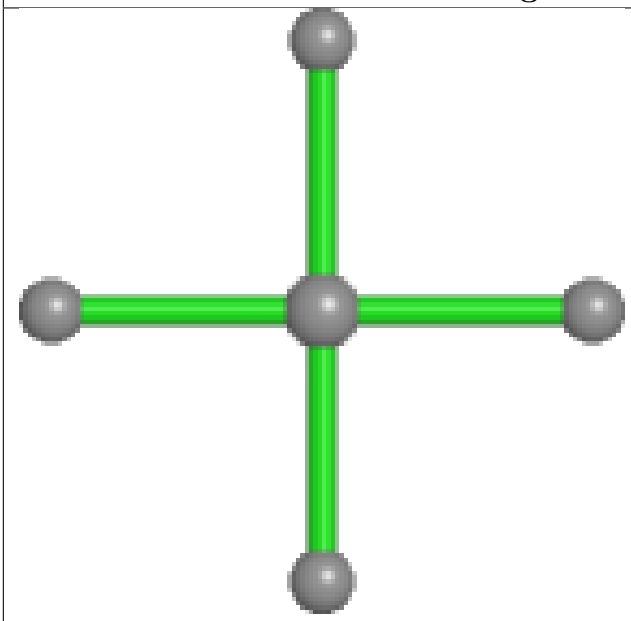


Torsions

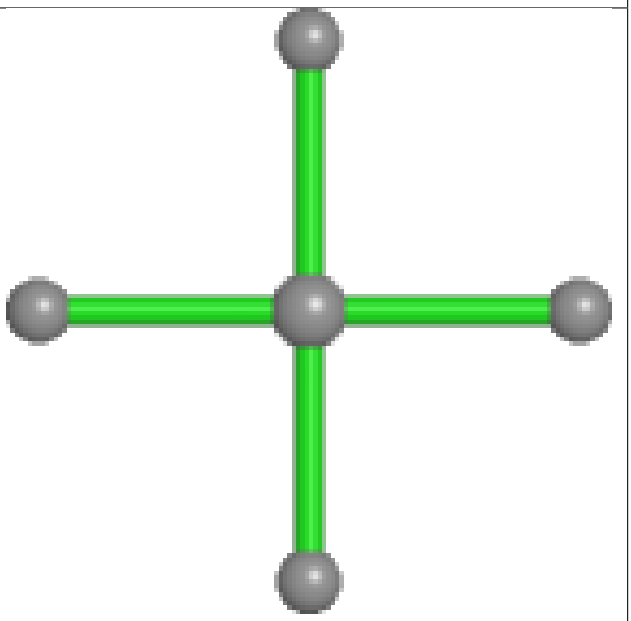


Rings

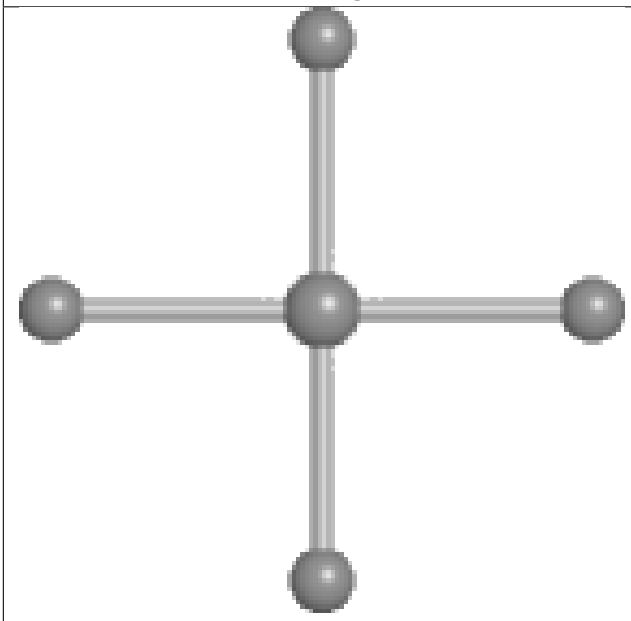
Ligand SO4 B 1215



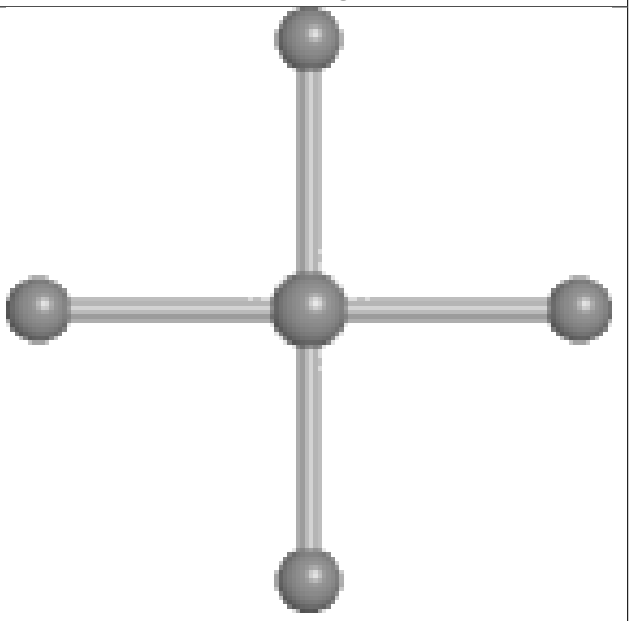
Bond lengths



Bond angles

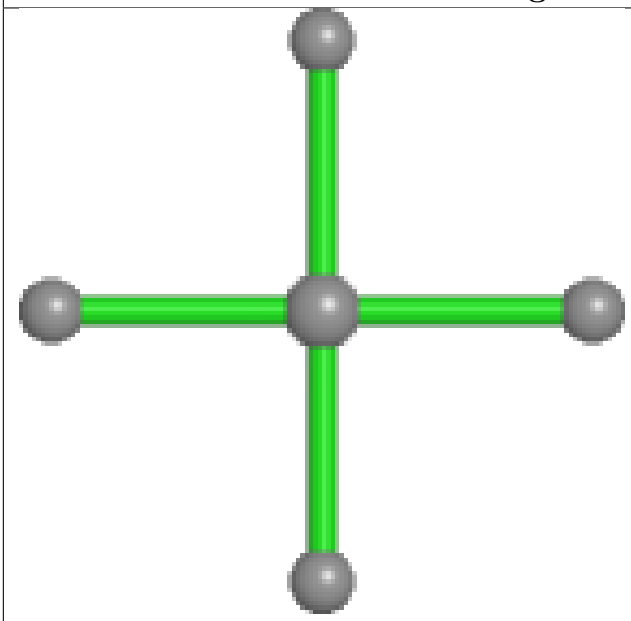


Torsions

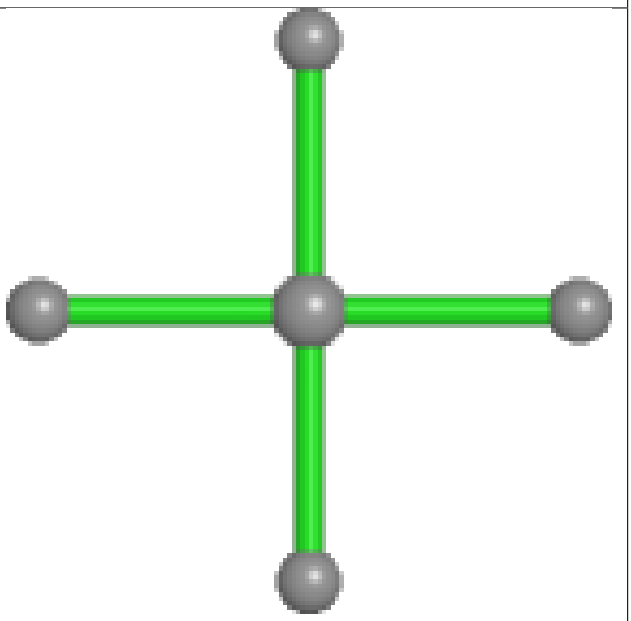


Rings

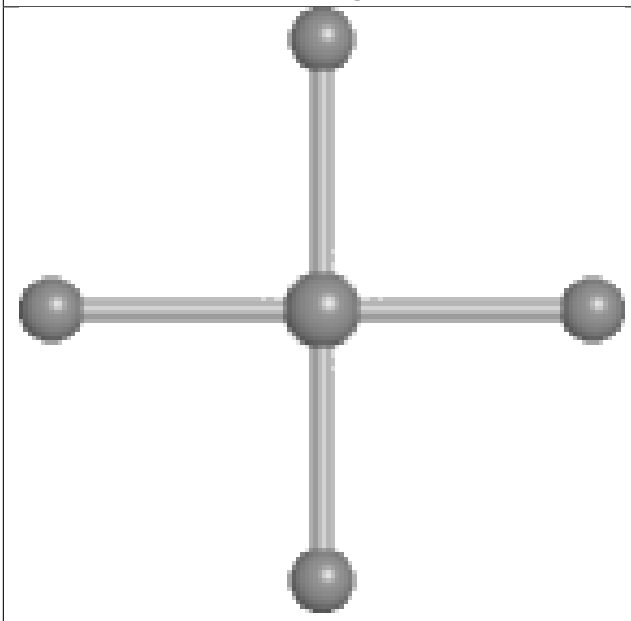
Ligand SO4 A 508



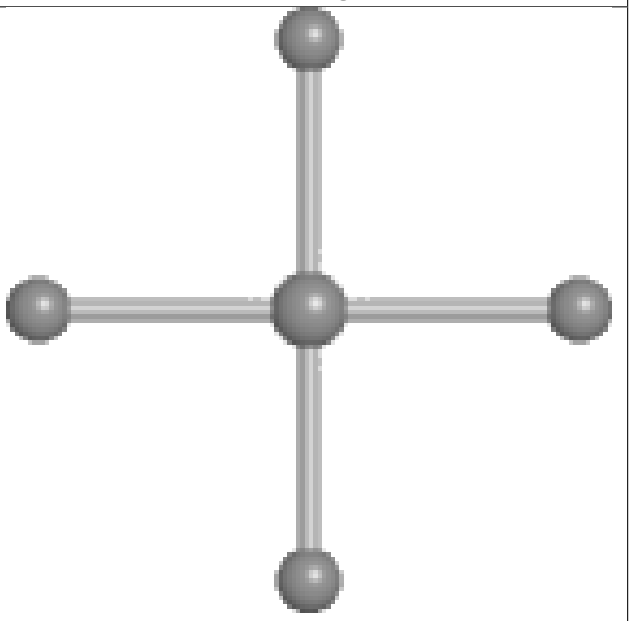
Bond lengths



Bond angles

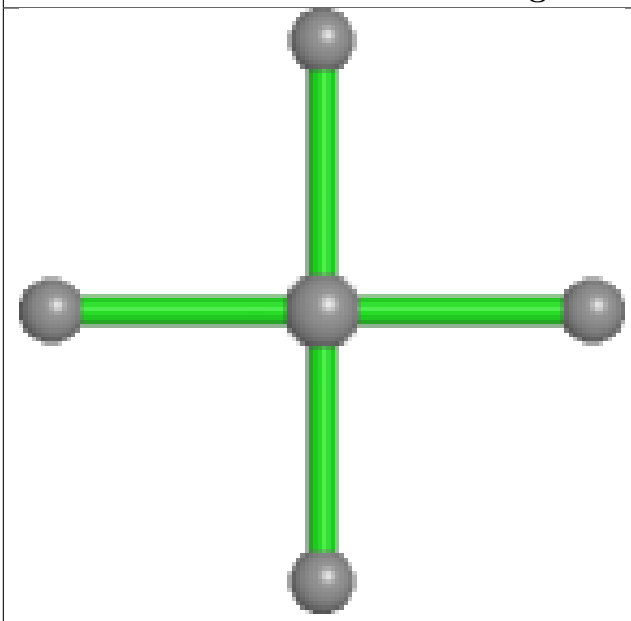


Torsions

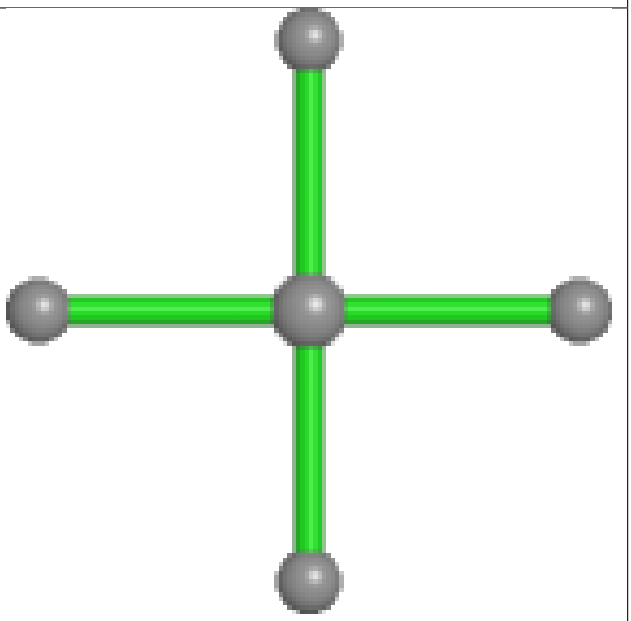


Rings

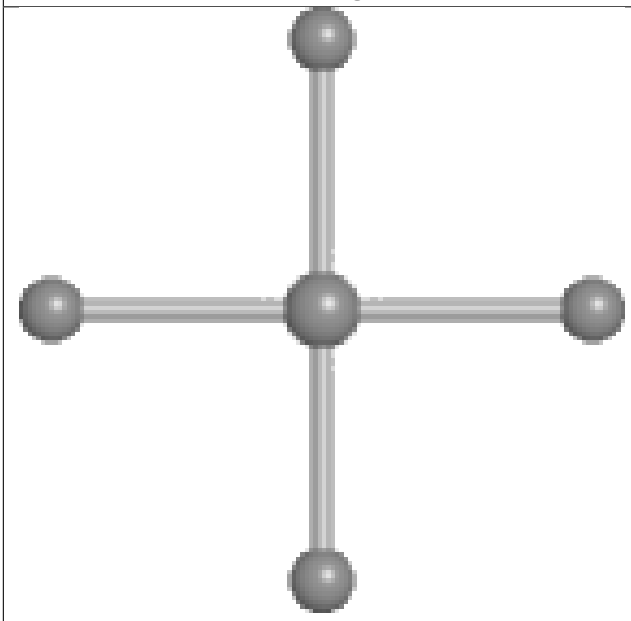
Ligand SO4 C 513



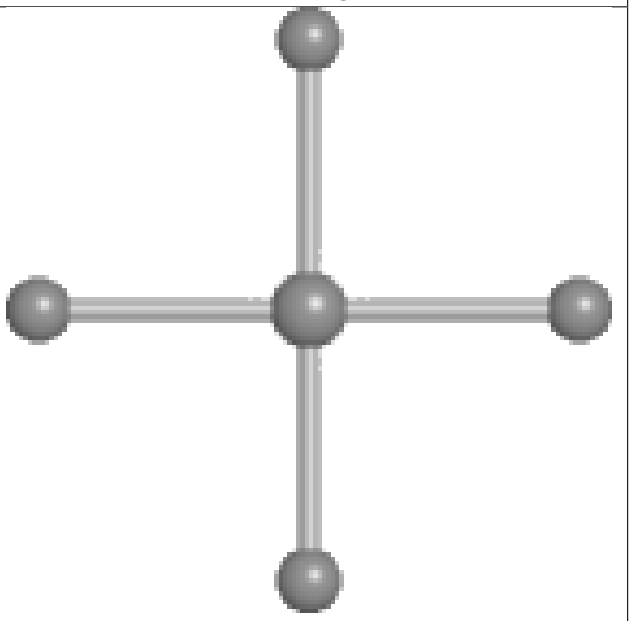
Bond lengths



Bond angles

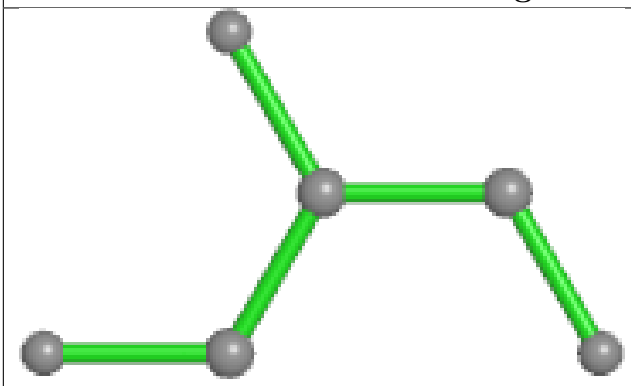


Torsions

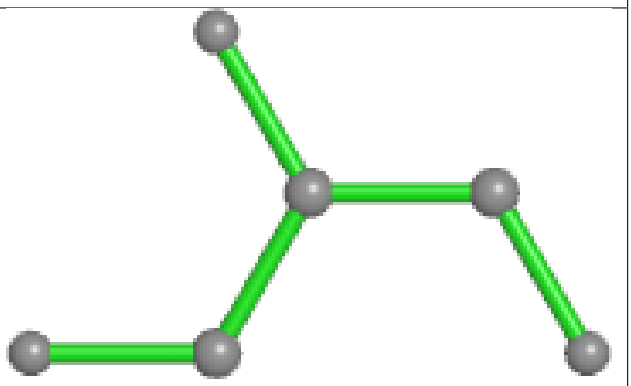


Rings

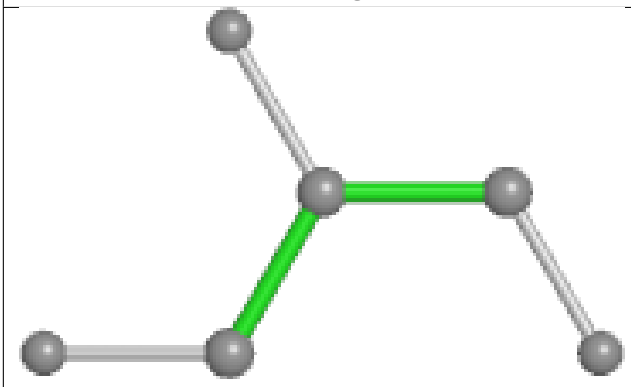
Ligand GOL B 1211



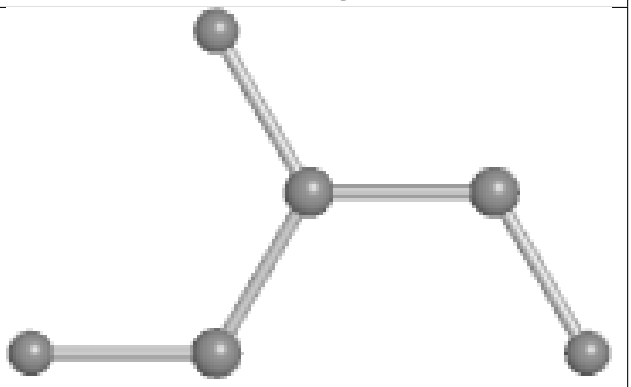
Bond lengths



Bond angles

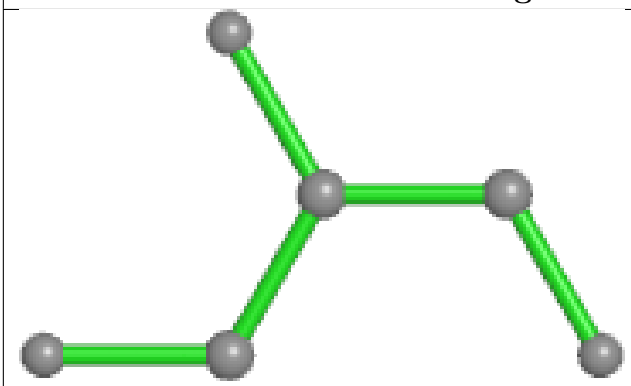


Torsions

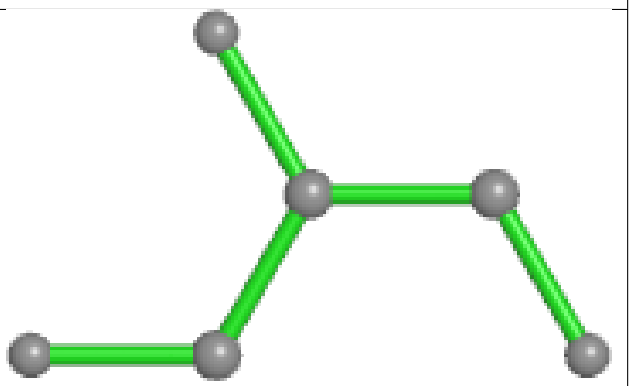


Rings

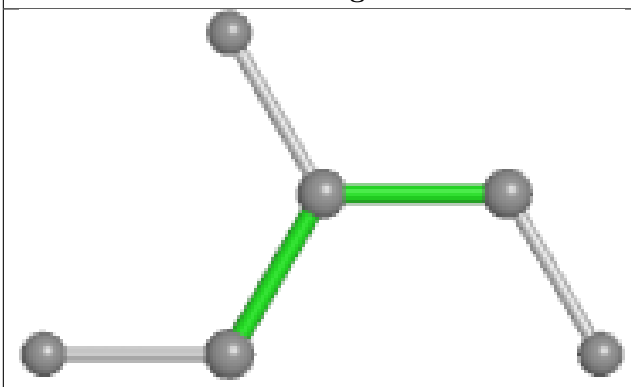
Ligand GOL B 1209



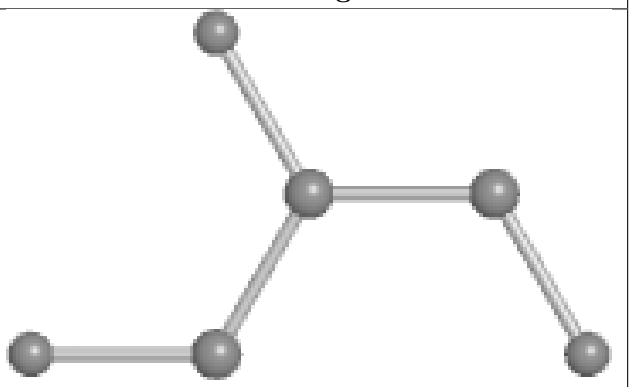
Bond lengths



Bond angles

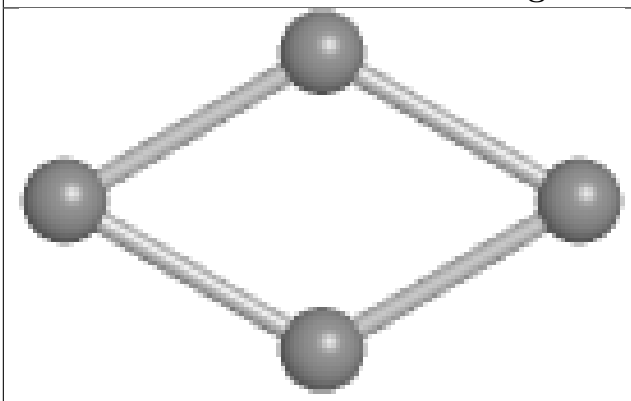


Torsions

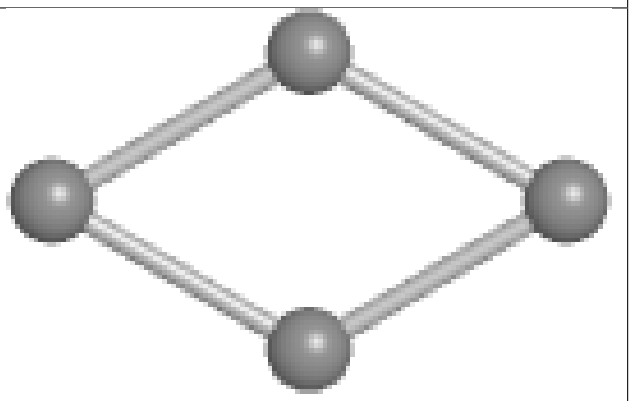


Rings

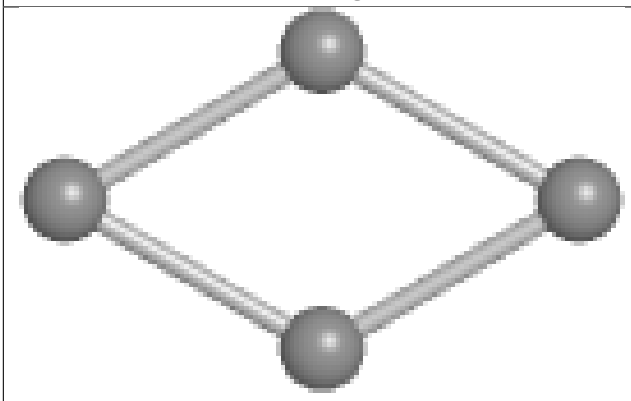
Ligand FES A 501



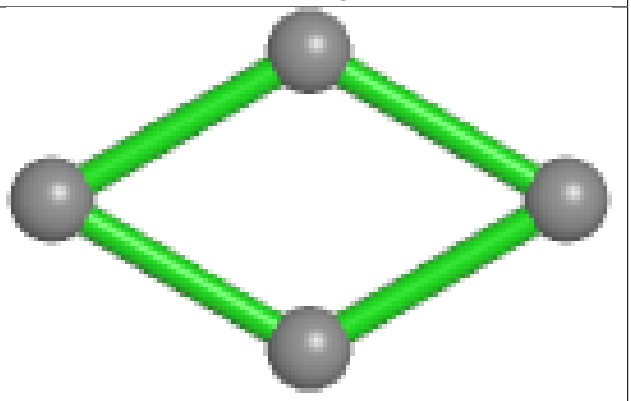
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	323/334 (96%)	0.44	23 (7%) 16 12	26, 40, 78, 118	0
1	B	327/334 (97%)	0.64	39 (11%) 4 3	26, 35, 63, 82	0
1	C	319/334 (95%)	0.36	19 (5%) 21 17	30, 43, 76, 105	0
All	All	969/1002 (96%)	0.48	81 (8%) 11 8	26, 40, 71, 118	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	ALA	9.3
1	A	205	ILE	6.7
1	C	297	PRO	6.2
1	A	6	LEU	6.1
1	C	200	PHE	6.0
1	C	202	THR	5.9
1	B	44	GLN	5.8
1	A	178	TYR	5.5
1	C	201	GLN	5.4
1	A	210	GLU	5.3
1	B	228[A]	CYS	5.3
1	B	6	LEU	5.0
1	B	229	VAL	5.0
1	B	1	MET	5.0
1	A	209	ILE	4.8
1	B	296	ALA	4.8
1	A	200	PHE	4.7
1	A	201	GLN	4.7
1	C	44	GLN	4.6
1	C	190	LYS	4.5
1	B	217	TRP	4.4
1	B	227	TYR	4.4
1	B	304	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	3	THR	4.2
1	C	1	MET	4.0
1	A	212	ASP	4.0
1	B	240	LEU	3.9
1	B	220	LEU	3.9
1	C	4	ALA	3.8
1	B	45	ASN	3.7
1	C	212	ASP	3.7
1	C	43	GLU	3.7
1	C	45	ASN	3.6
1	B	218	PHE	3.6
1	B	42	GLN	3.6
1	B	178	TYR	3.4
1	C	124	VAL	3.4
1	B	131	PRO	3.4
1	B	334	CYS	3.4
1	B	238	VAL	3.4
1	A	211	ASP	3.4
1	A	190	LYS	3.3
1	B	129[A]	SER	3.3
1	B	130	PHE	3.2
1	C	42	GLN	3.1
1	A	213	SER	3.1
1	A	233	PRO	3.0
1	A	202	THR	3.0
1	A	304	GLY	2.9
1	A	296	ALA	2.9
1	C	137	ASN	2.8
1	B	194	THR	2.8
1	B	237	ILE	2.8
1	A	206	VAL	2.8
1	B	2	THR	2.7
1	B	291	ARG	2.7
1	B	241[A]	MET	2.7
1	B	225[A]	CYS	2.6
1	C	70[A]	ASN	2.6
1	C	22	LYS	2.6
1	A	225[A]	CYS	2.6
1	C	233	PRO	2.6
1	B	230[A]	SER	2.6
1	B	256	LEU	2.5
1	A	127	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	127	ILE	2.4
1	C	198	TYR	2.4
1	C	304	GLY	2.4
1	B	193[A]	LEU	2.4
1	A	198	TYR	2.4
1	B	43	GLU	2.4
1	B	23	PRO	2.3
1	B	330	THR	2.3
1	A	234	GLU	2.2
1	B	22	LYS	2.2
1	A	113	TYR	2.2
1	B	160	ILE	2.1
1	B	70	ASN	2.1
1	A	228[A]	CYS	2.1
1	B	219	ARG	2.1
1	B	69	ASN	2.1

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	1211	6/6	0.54	0.21	69,79,81,84	0
6	SO4	C	513	5/5	0.57	0.36	115,118,130,139	0
3	GOL	B	1205	6/6	0.71	0.34	69,76,78,85	0
3	GOL	B	1208	6/6	0.72	0.30	48,59,60,61	0
7	CL	A	509	1/1	0.72	0.20	83,83,83,83	0
3	GOL	C	510	6/6	0.73	0.18	73,74,76,78	0
4	D82	B	1212	20/20	0.74	0.34	36,44,52,54	20

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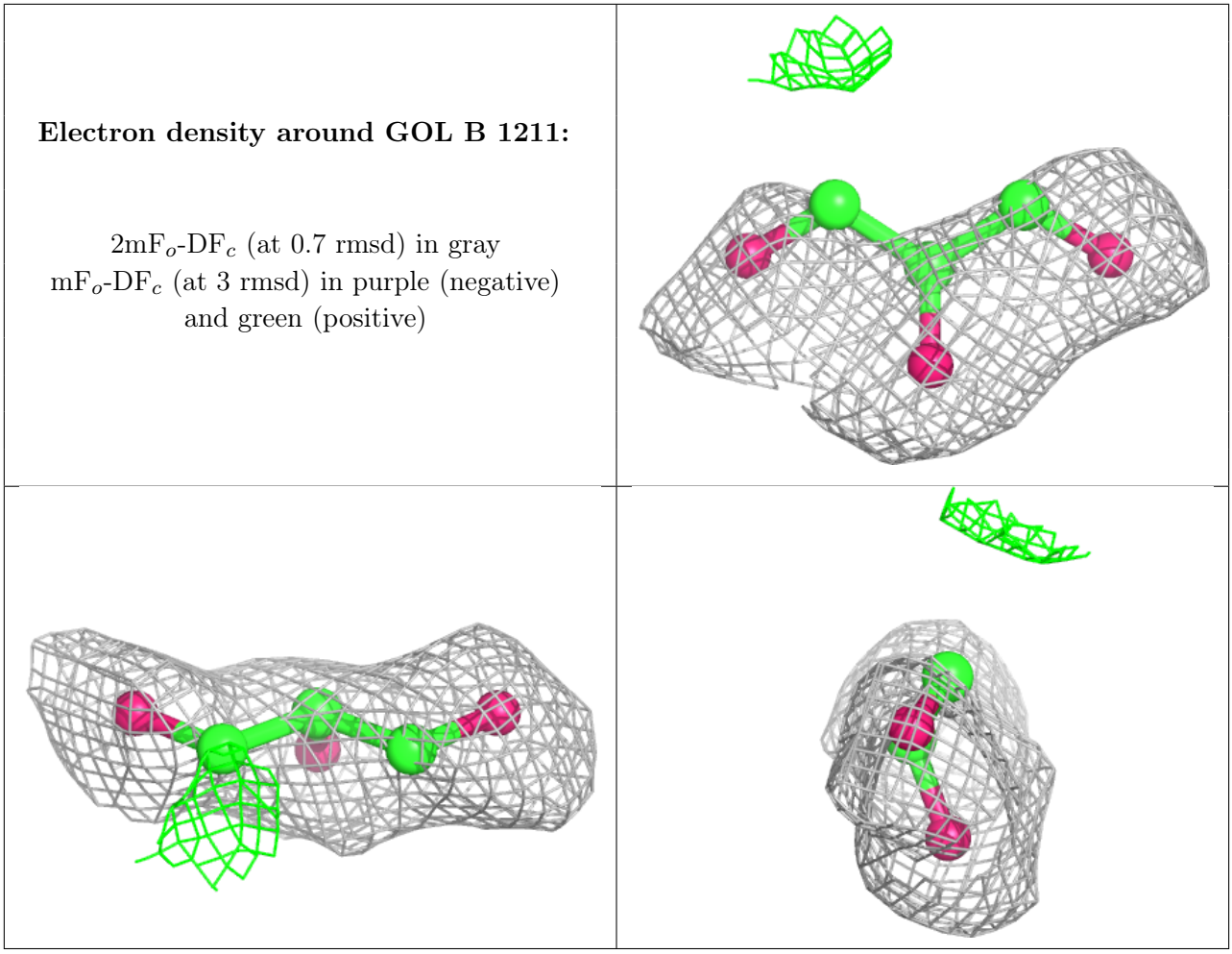
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	1210	6/6	0.78	0.26	37,45,56,60	0
3	GOL	C	505	6/6	0.80	0.23	66,70,72,83	0
3	GOL	C	509	6/6	0.80	0.32	73,82,83,85	0
3	GOL	B	1209	6/6	0.81	0.32	70,73,78,80	0
3	GOL	C	508	6/6	0.82	0.14	41,57,63,70	0
3	GOL	A	505	6/6	0.82	0.18	44,61,64,65	0
3	GOL	C	507	6/6	0.82	0.34	52,66,72,72	0
3	GOL	B	1201	6/6	0.83	0.30	60,65,72,77	0
4	D82	C	506	20/20	0.83	0.17	42,53,60,61	20
3	GOL	B	1207	6/6	0.85	0.18	40,62,72,72	0
3	GOL	C	504	6/6	0.86	0.31	59,67,74,82	0
3	GOL	B	1206	6/6	0.86	0.34	60,65,68,74	0
4	D82	A	506	20/20	0.87	0.14	37,55,59,59	20
7	CL	A	510	1/1	0.87	0.17	70,70,70,70	0
3	GOL	C	502	6/6	0.88	0.27	67,71,72,78	0
3	GOL	C	503	6/6	0.89	0.21	54,55,70,75	0
6	SO4	B	1216	5/5	0.91	0.29	82,88,114,122	0
3	GOL	A	503	6/6	0.91	0.26	48,72,76,82	0
3	GOL	B	1203	6/6	0.91	0.34	42,61,64,82	0
3	GOL	B	1204	6/6	0.91	0.24	52,56,69,77	0
3	GOL	A	502	6/6	0.93	0.12	60,66,71,74	0
3	GOL	A	504	6/6	0.93	0.23	57,65,68,71	0
6	SO4	C	512	5/5	0.94	0.21	69,76,101,104	0
6	SO4	A	508	5/5	0.94	0.10	67,70,77,87	0
6	SO4	B	1215	5/5	0.95	0.19	49,77,97,97	0
6	SO4	B	1214	5/5	0.97	0.10	55,59,85,90	0
2	FES	C	501	4/4	0.99	0.09	32,33,33,35	0
2	FES	B	1202	4/4	0.99	0.13	29,29,30,32	0
2	FES	A	501	4/4	1.00	0.11	26,26,26,27	0
5	FE	A	507	1/1	1.00	0.12	33,33,33,33	0
5	FE	B	1213	1/1	1.00	0.17	27,27,27,27	0
5	FE	C	511	1/1	1.00	0.14	29,29,29,29	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.

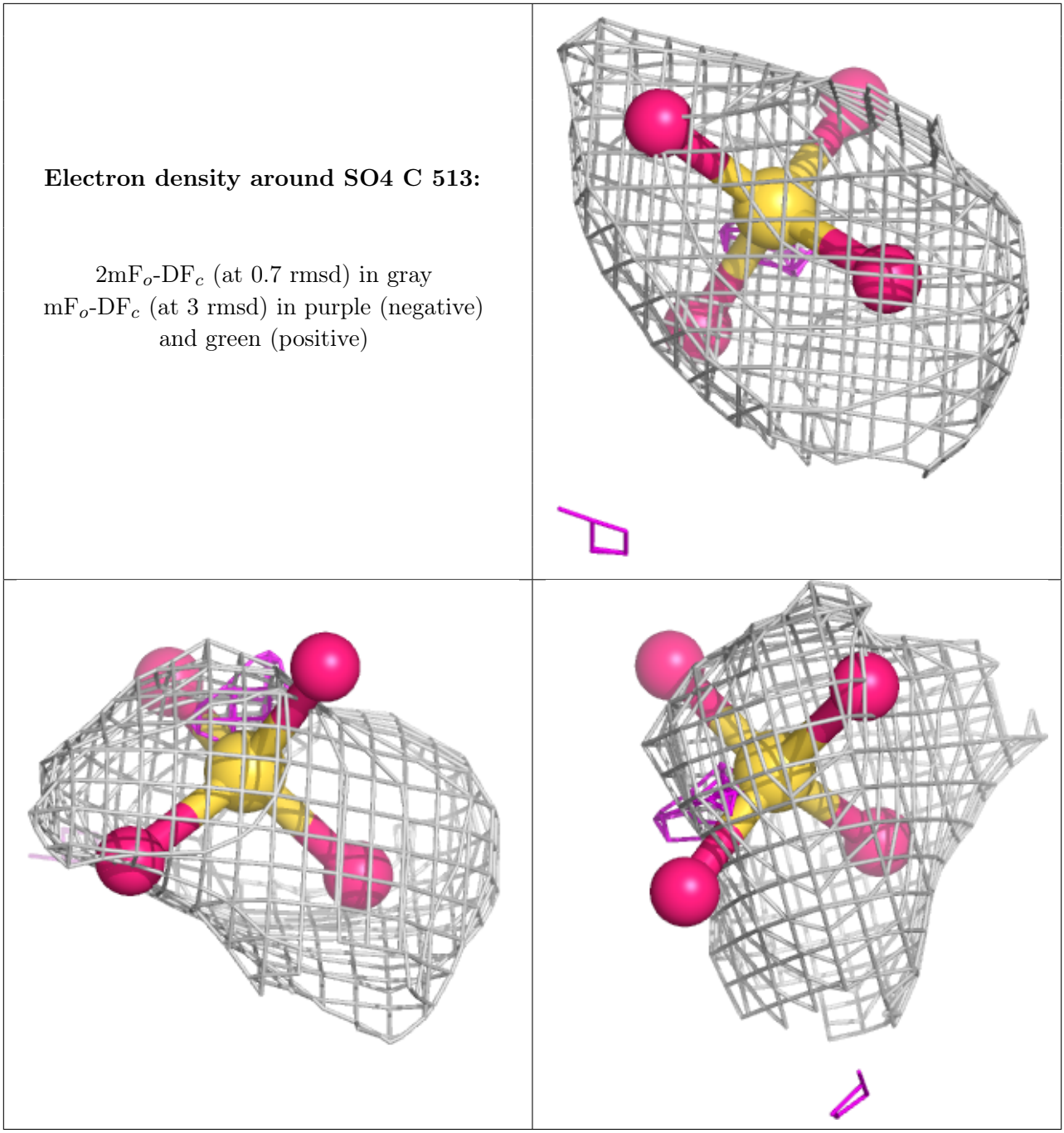
Electron density around GOL B 1211:

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



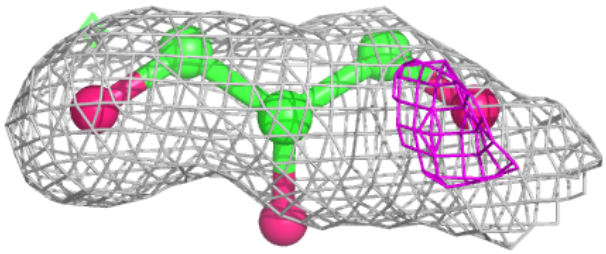
Electron density around SO4 C 513:

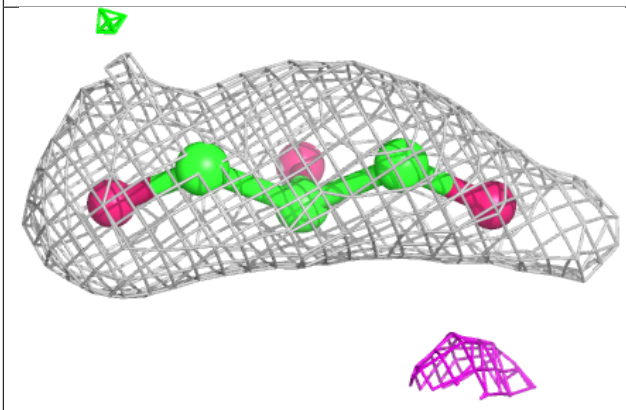
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

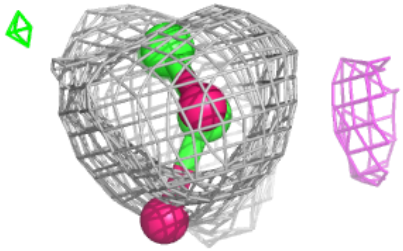


Electron density around GOL B 1205:

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

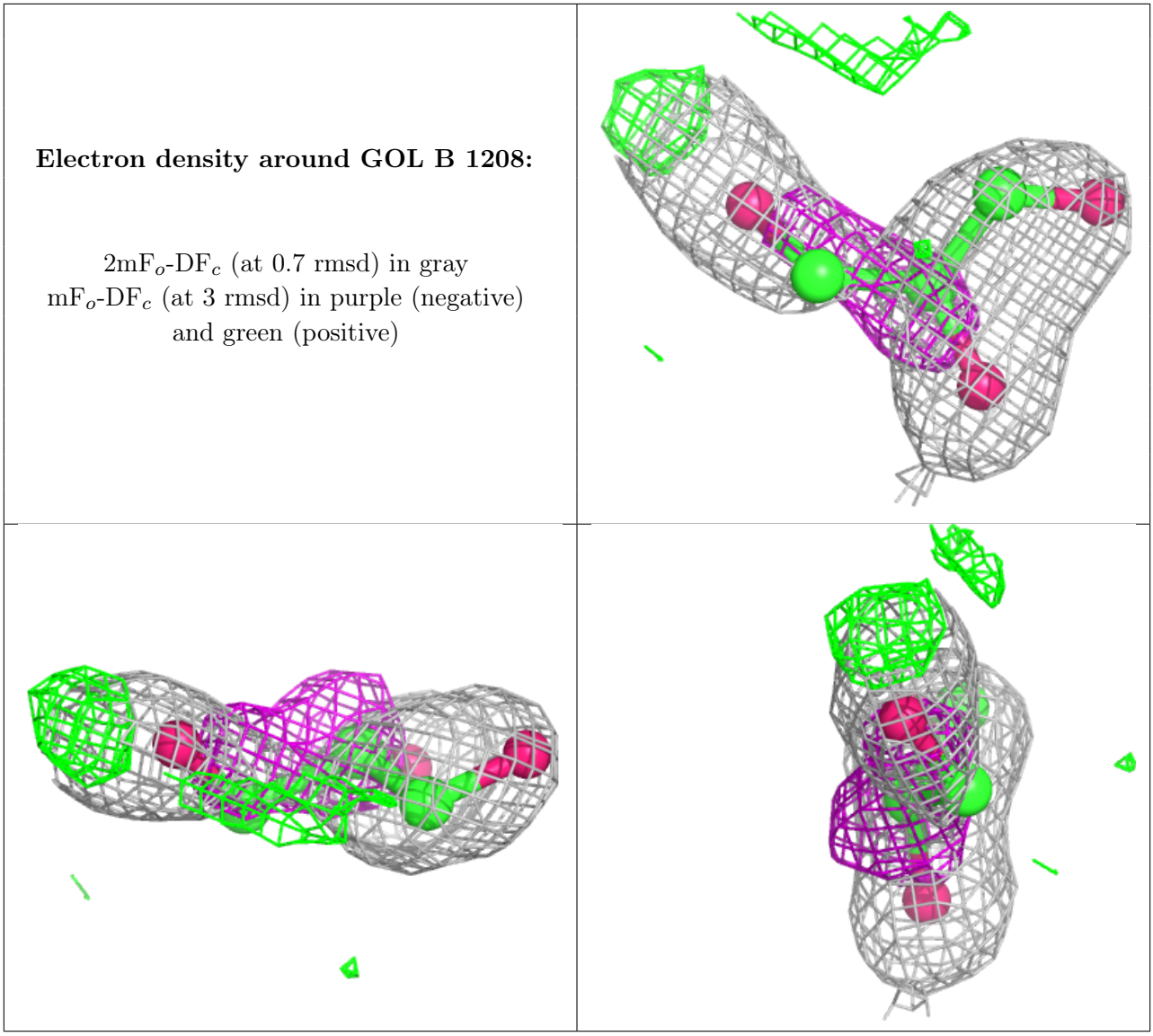






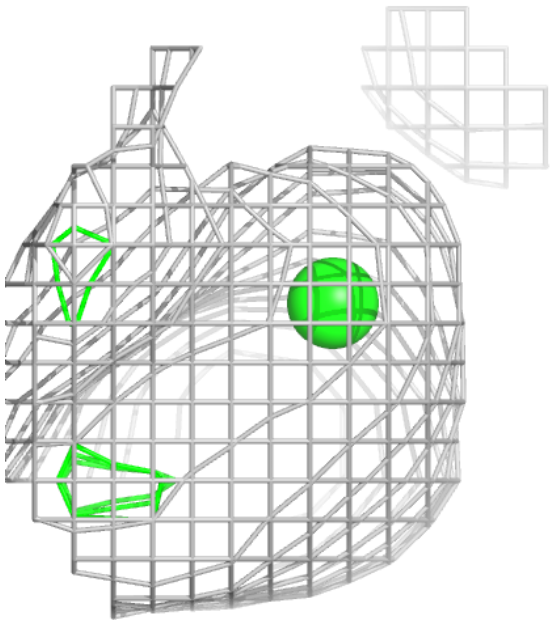
Electron density around GOL B 1208:

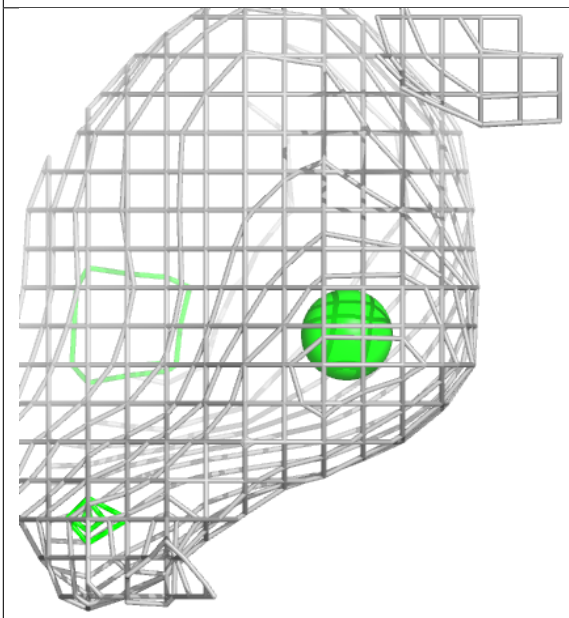
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

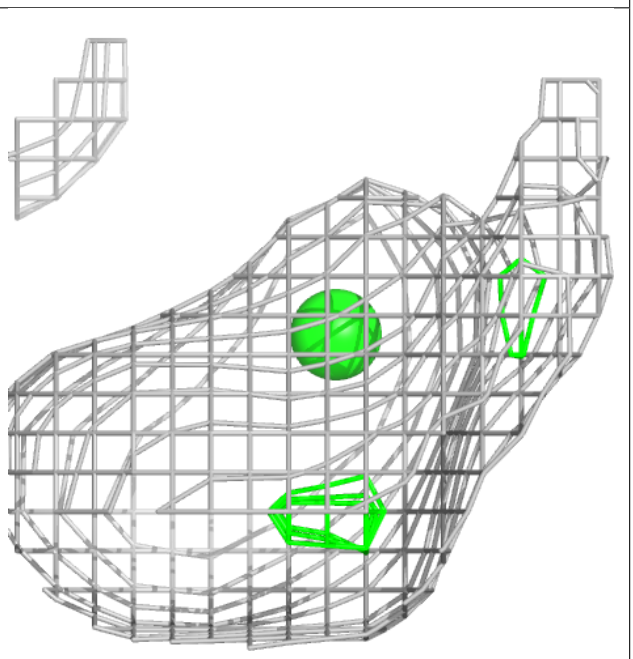


Electron density around CL A 509:

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

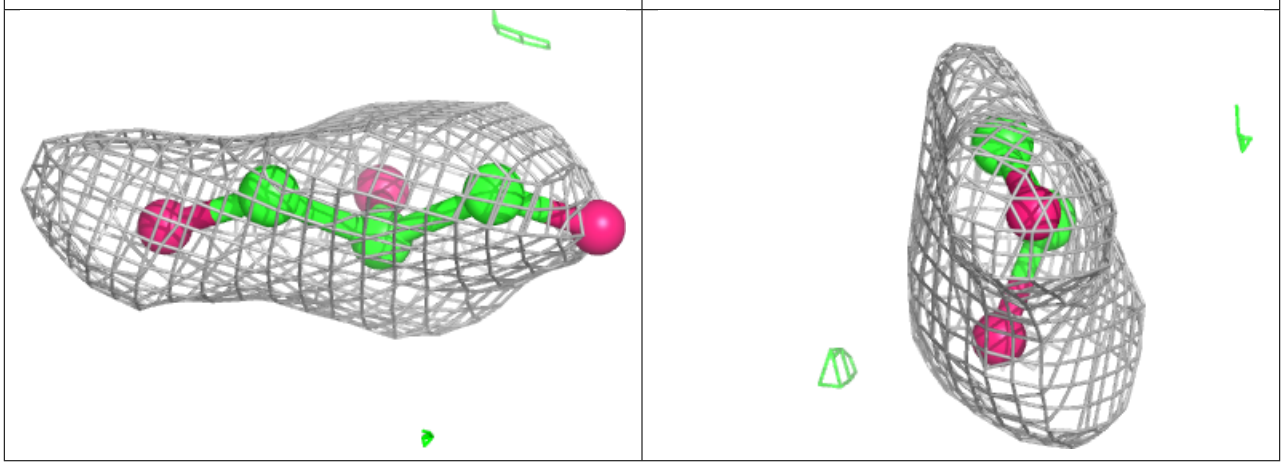






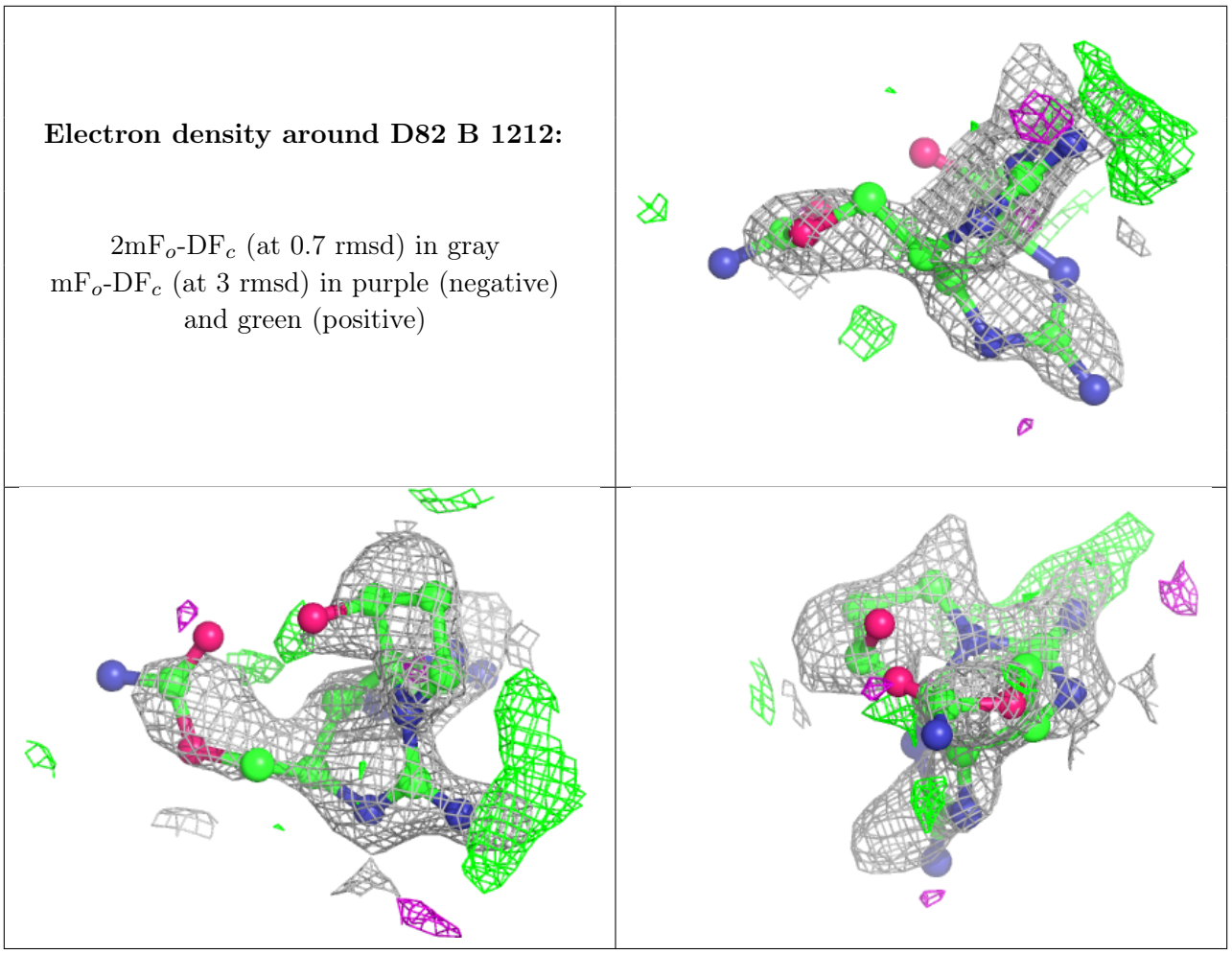
Electron density around GOL C 510:

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



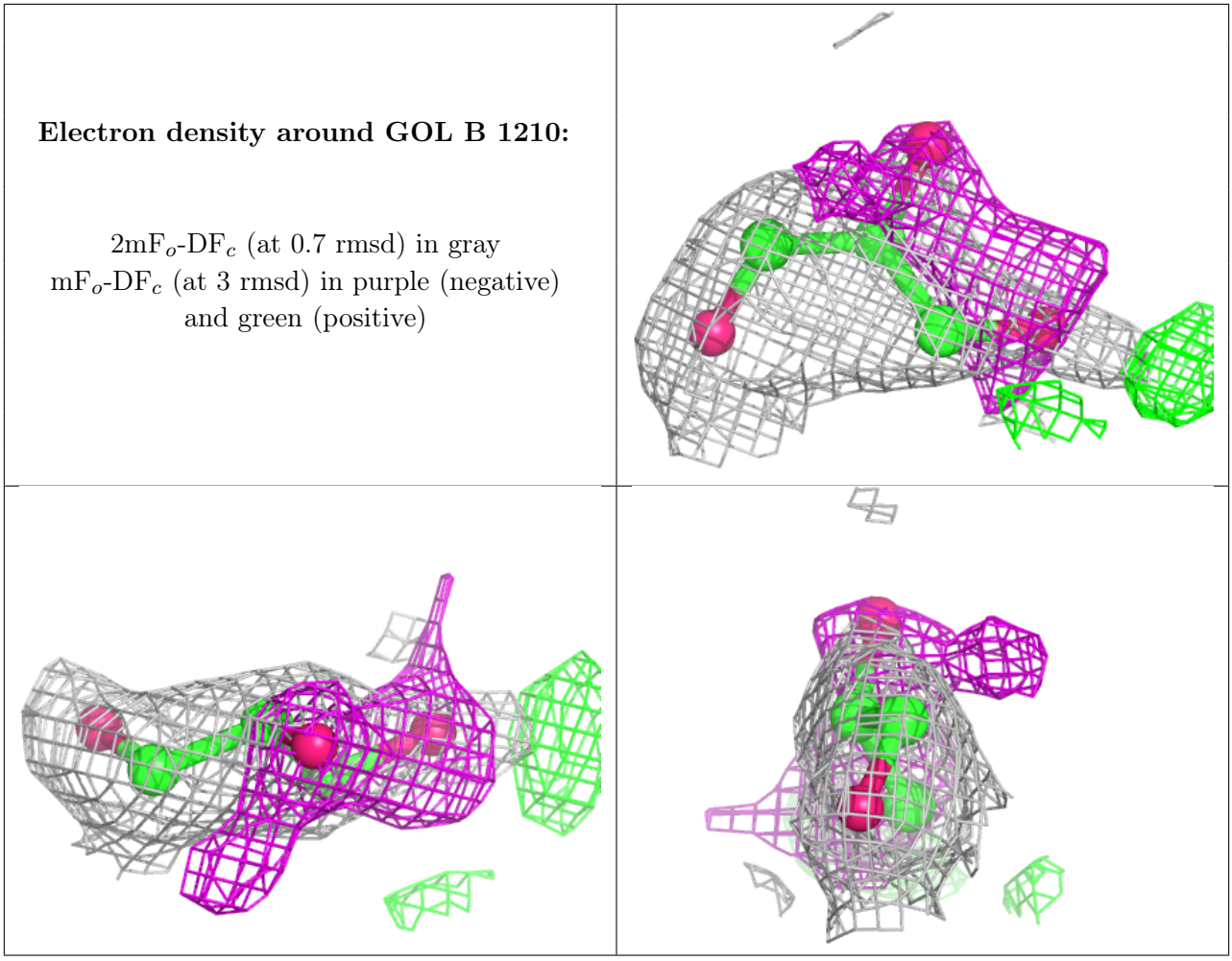
Electron density around D82 B 1212:

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



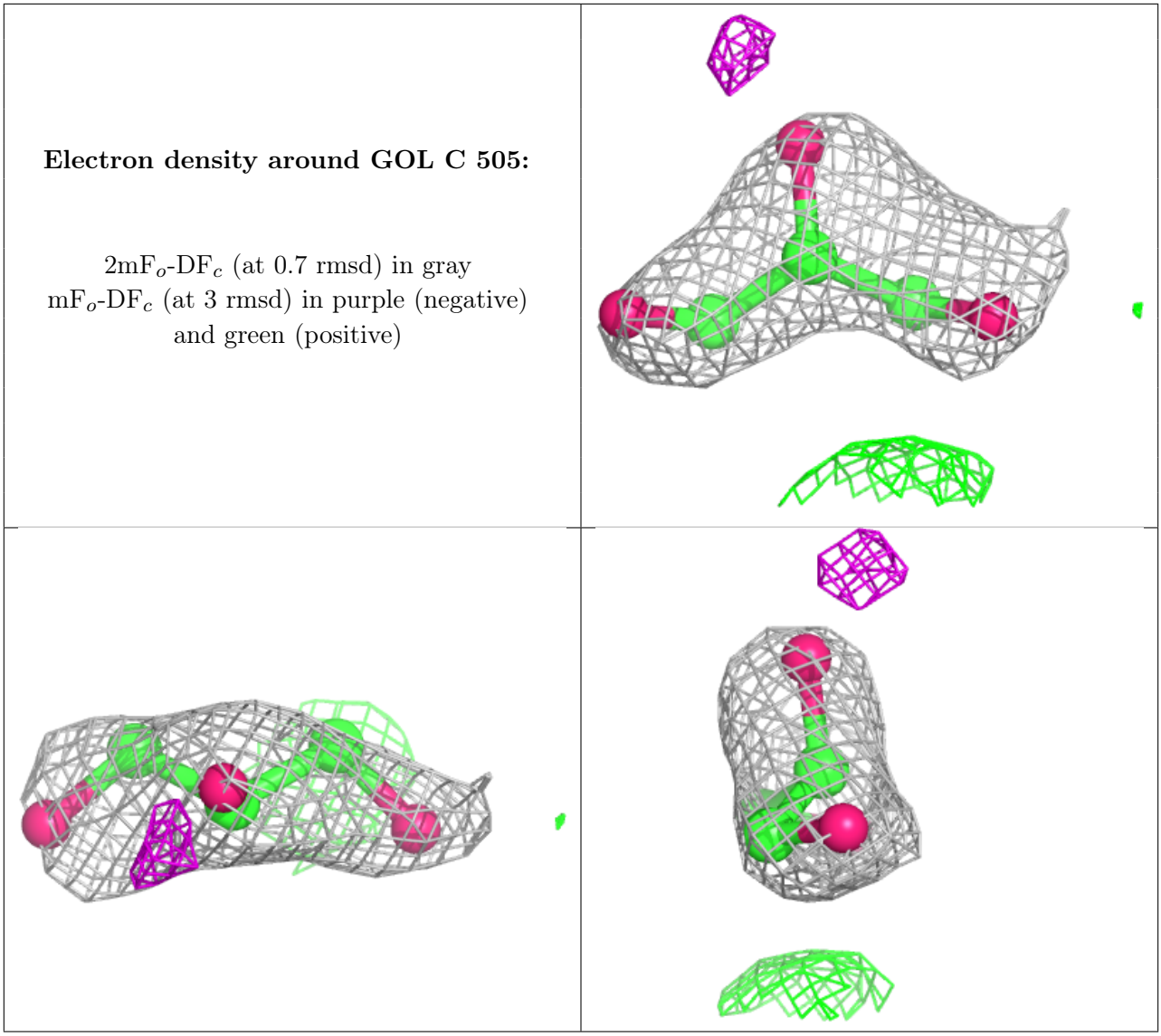
Electron density around GOL B 1210:

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



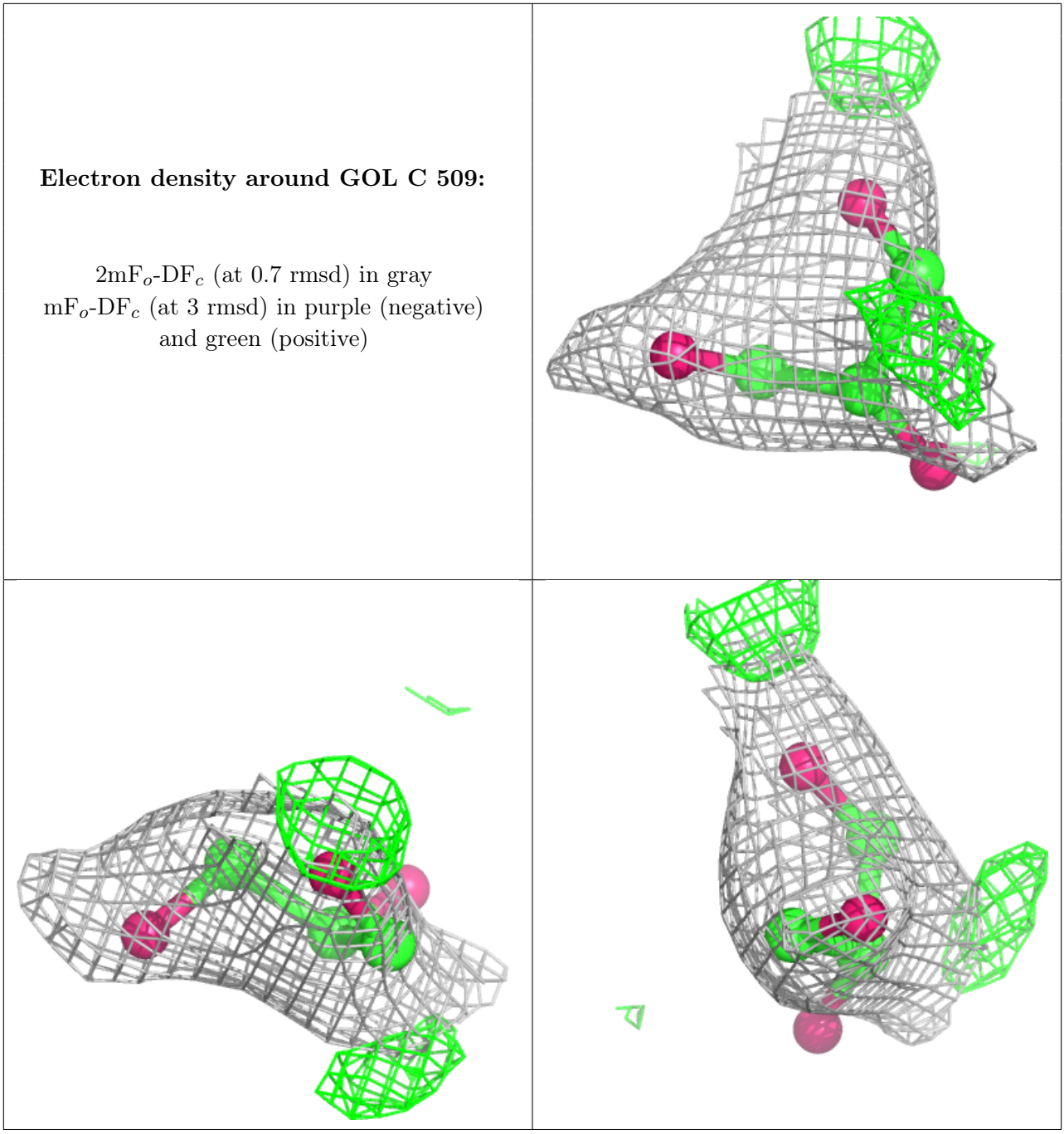
Electron density around GOL C 505:

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



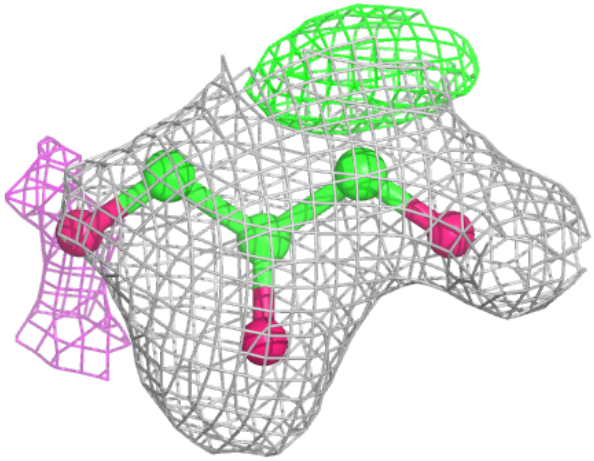
Electron density around GOL C 509:

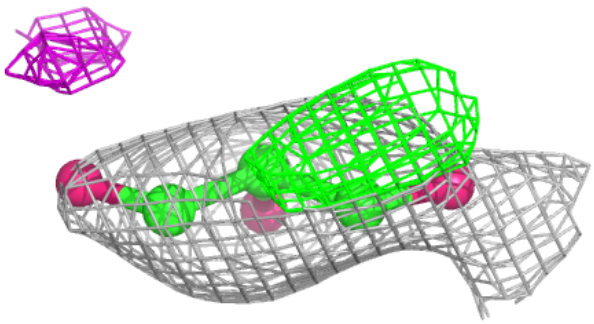
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

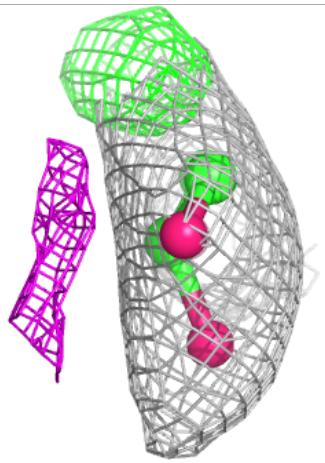


Electron density around GOL B 1209:

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

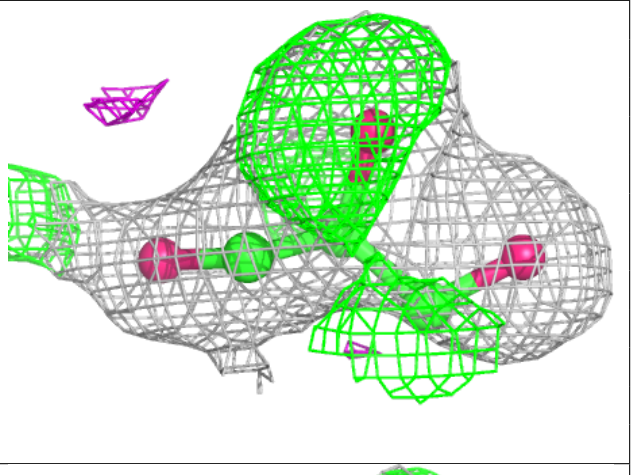


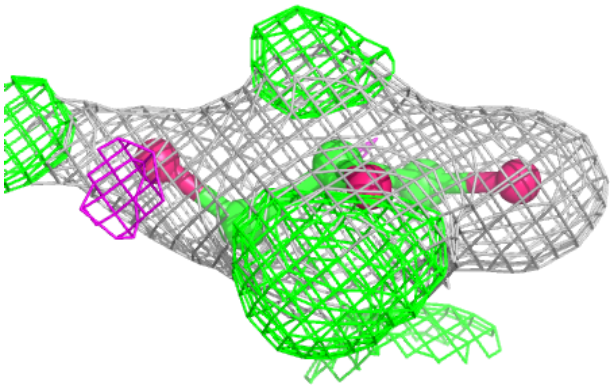


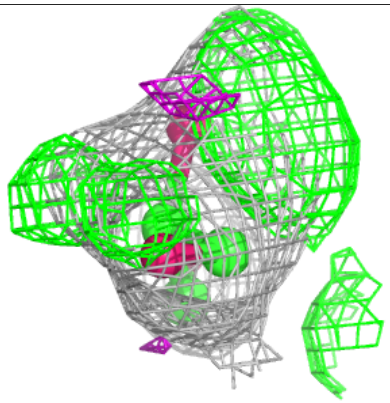


Electron density around GOL C 508:

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

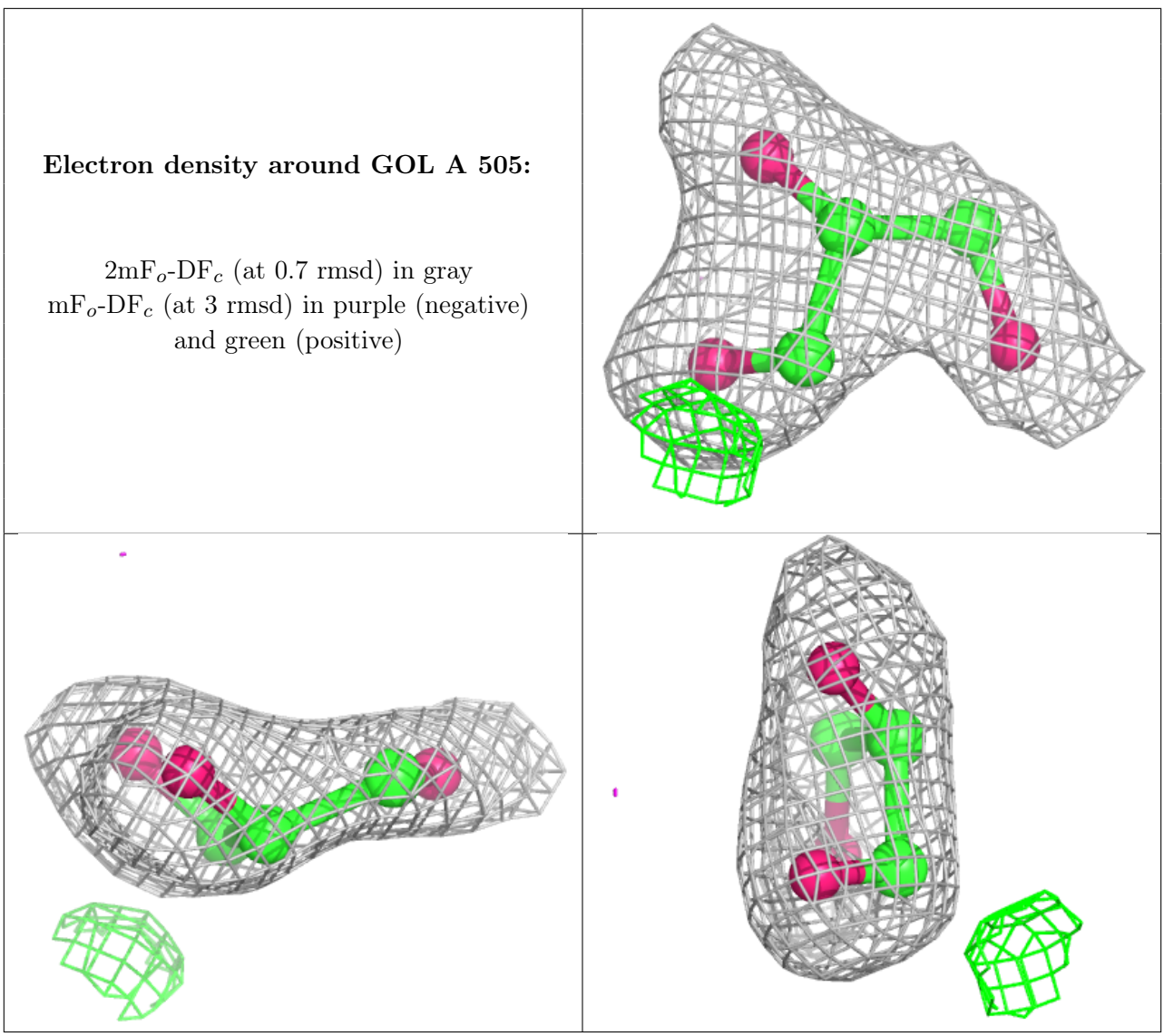






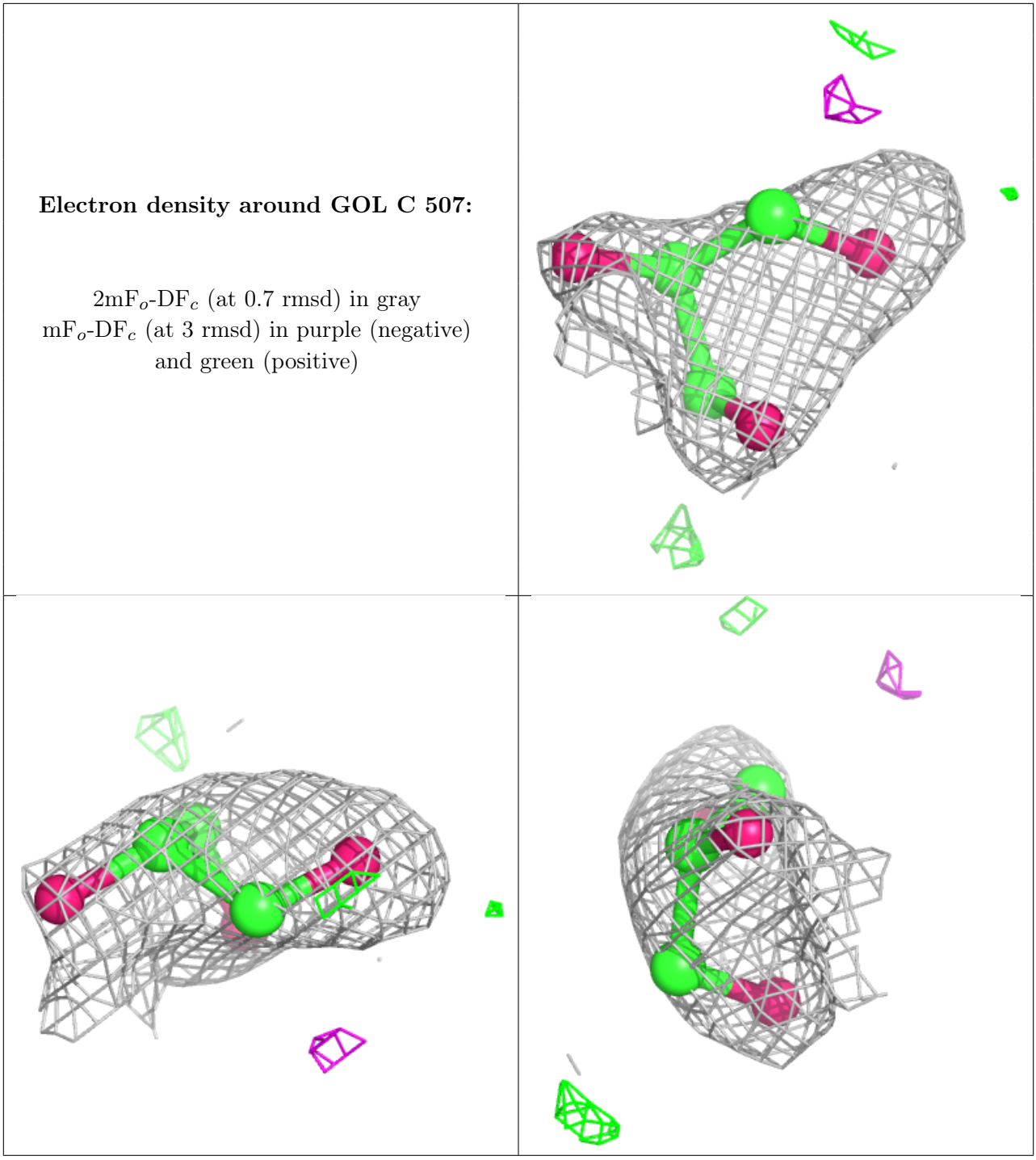
Electron density around GOL A 505:

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



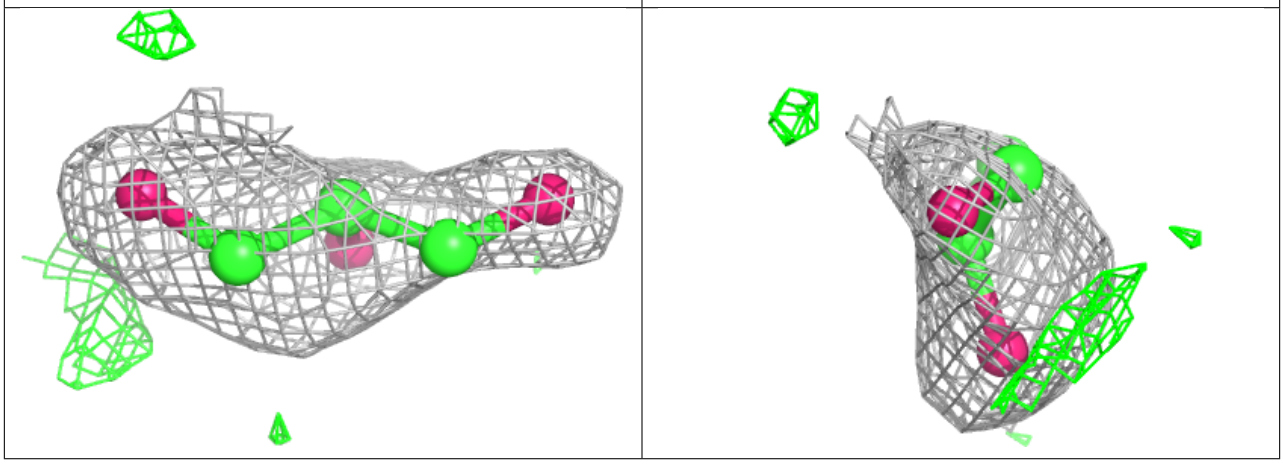
Electron density around GOL C 507:

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



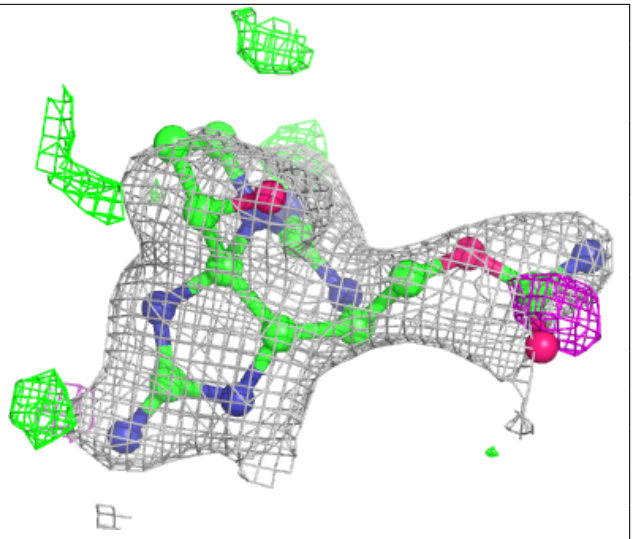
Electron density around GOL B 1201:

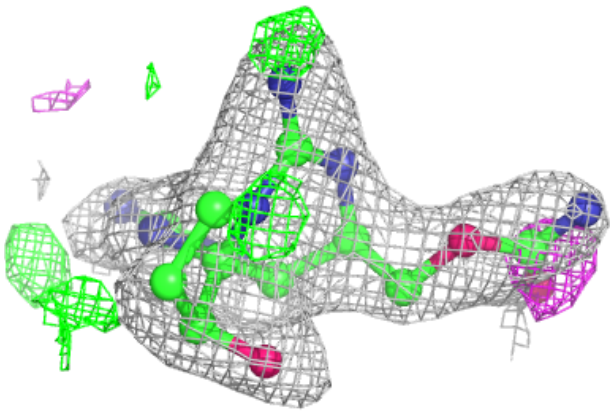
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

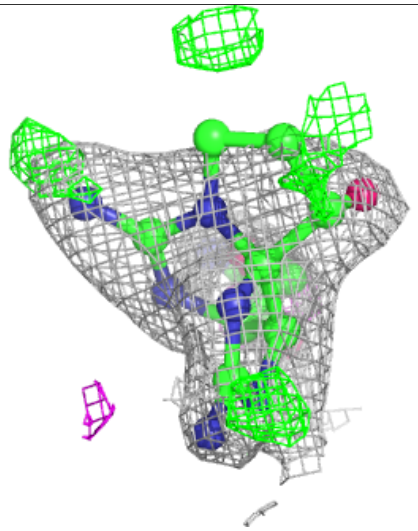


Electron density around D82 C 506:

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

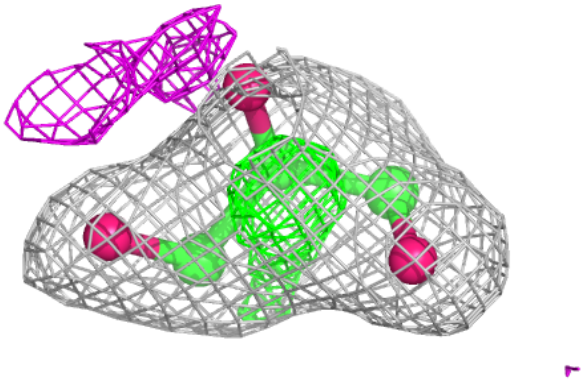


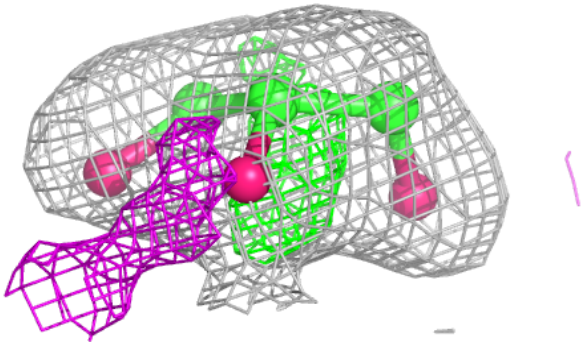


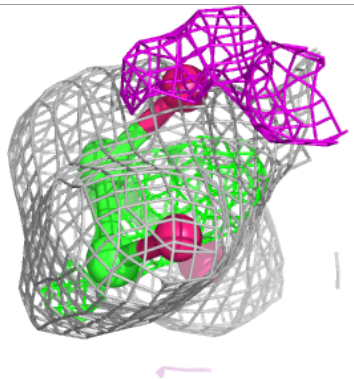


Electron density around GOL B 1207:

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

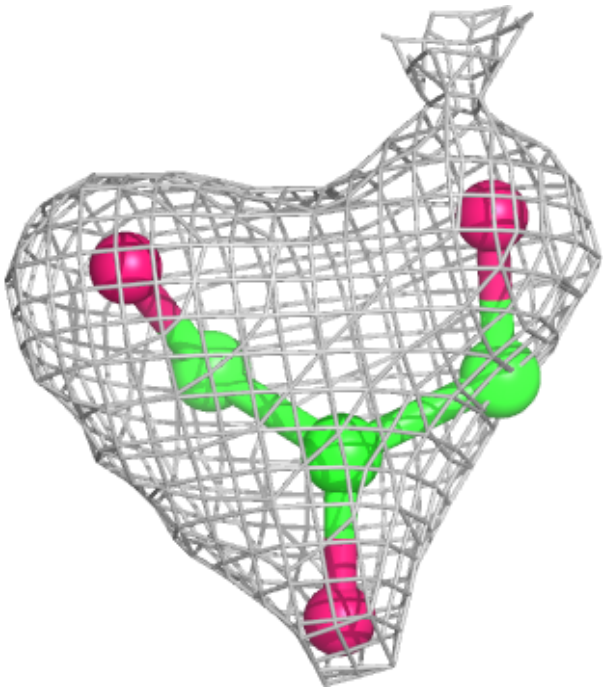


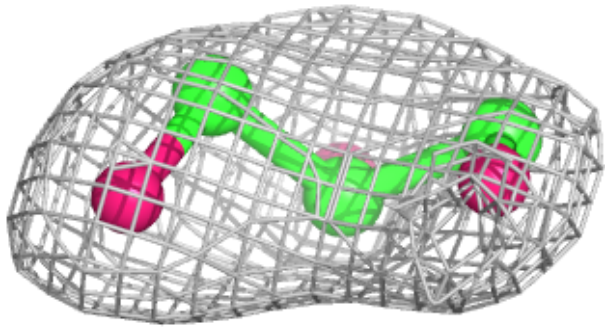


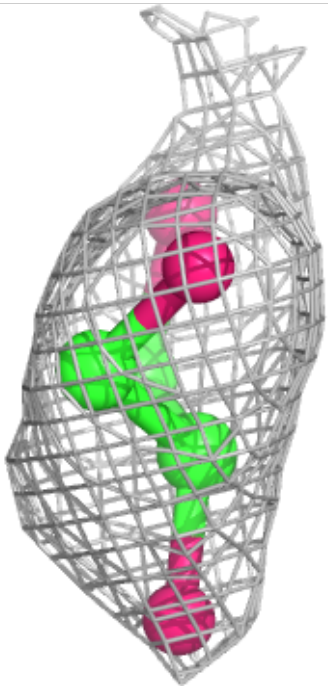


Electron density around GOL C 504:

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

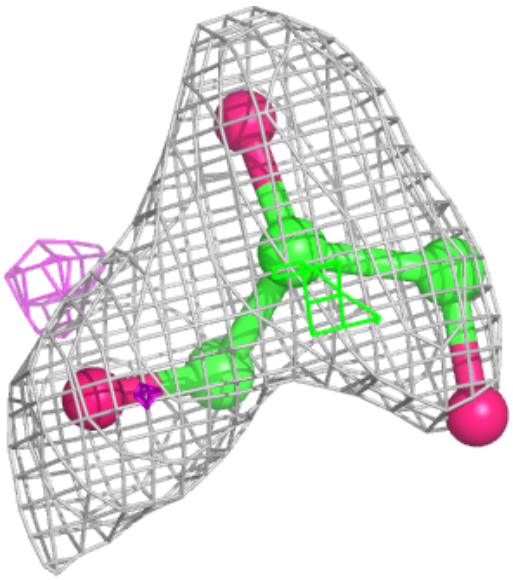


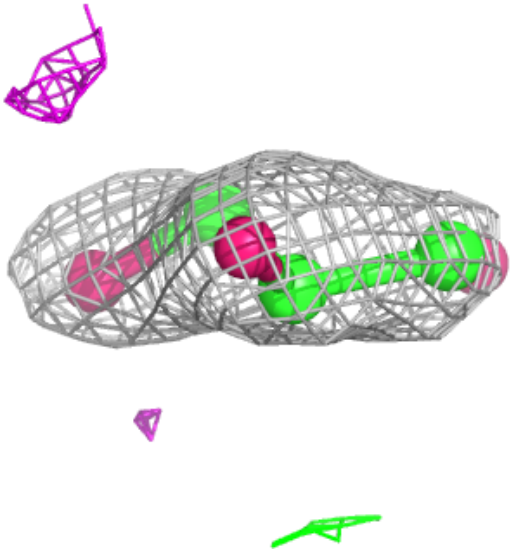


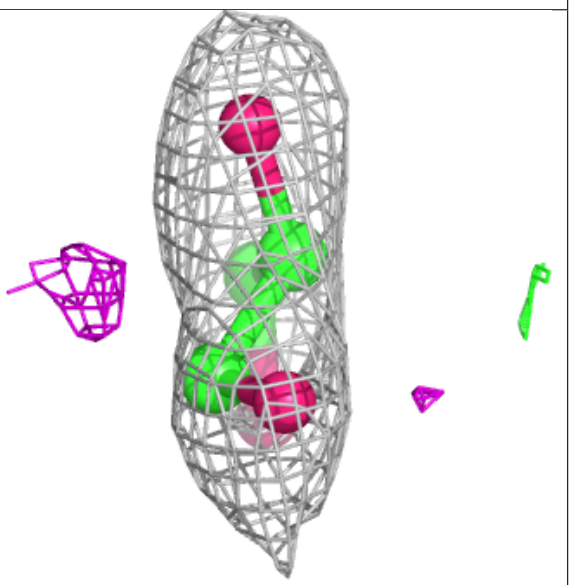


Electron density around GOL B 1206:

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

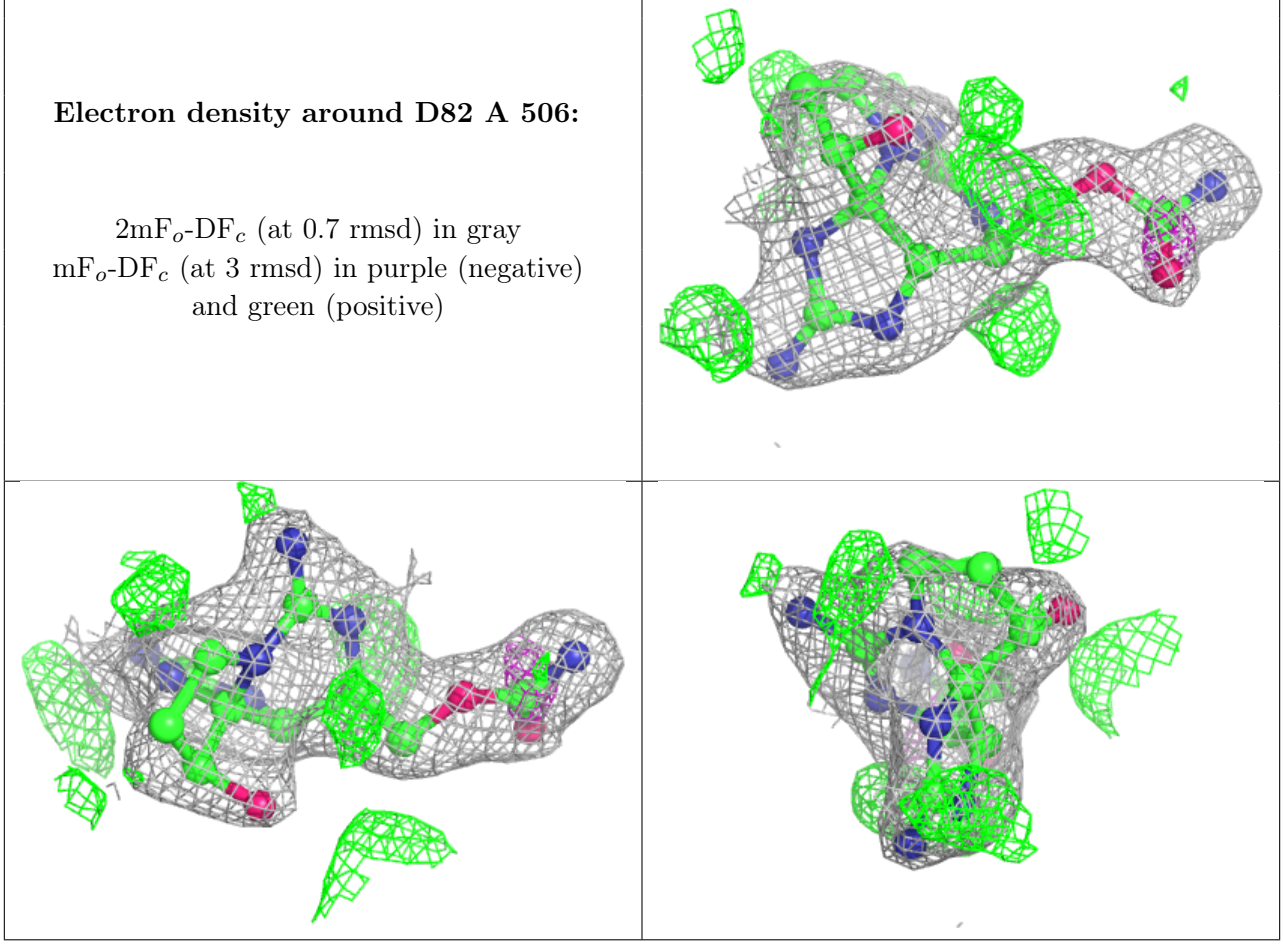






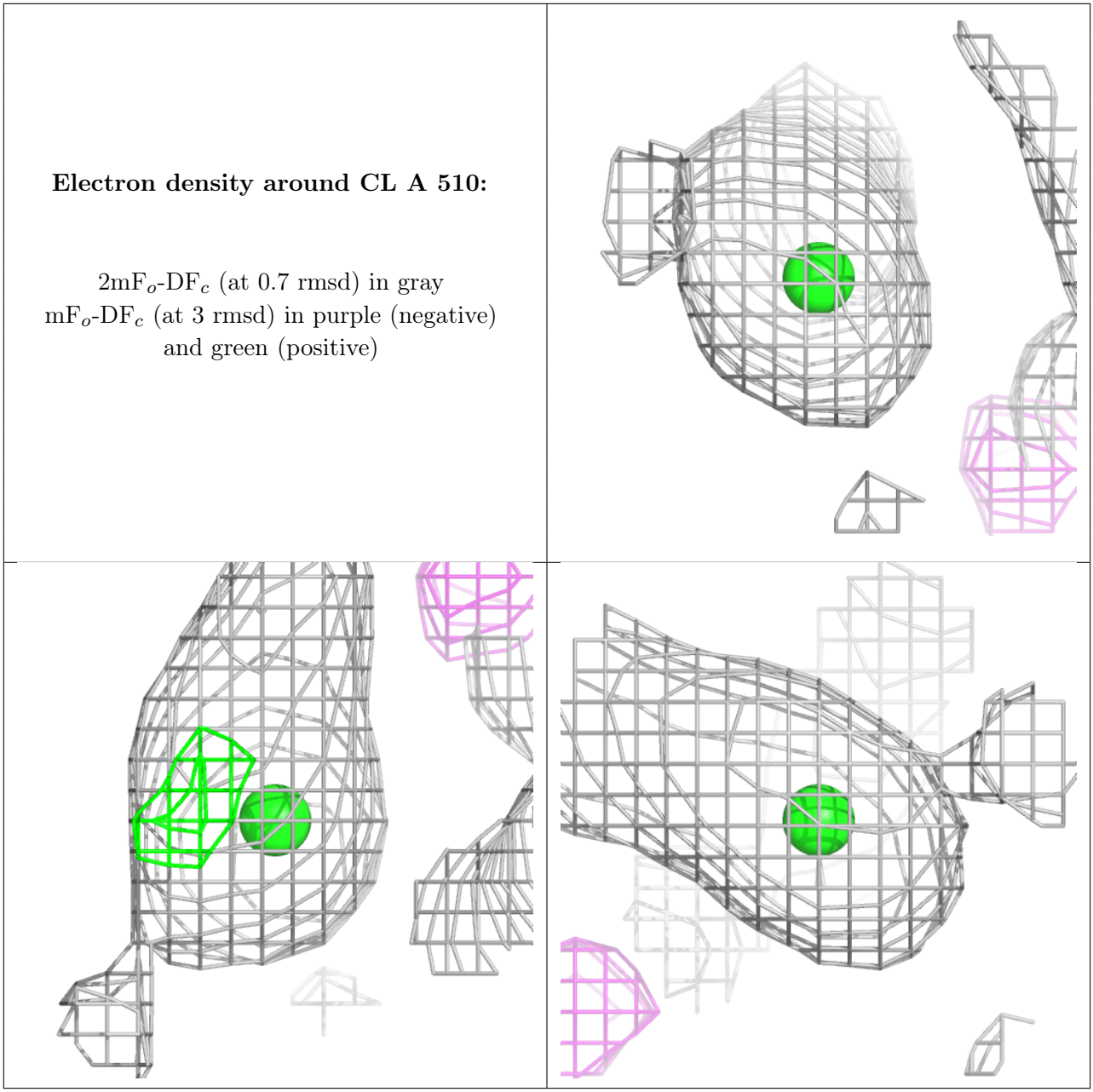
Electron density around D82 A 506:

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



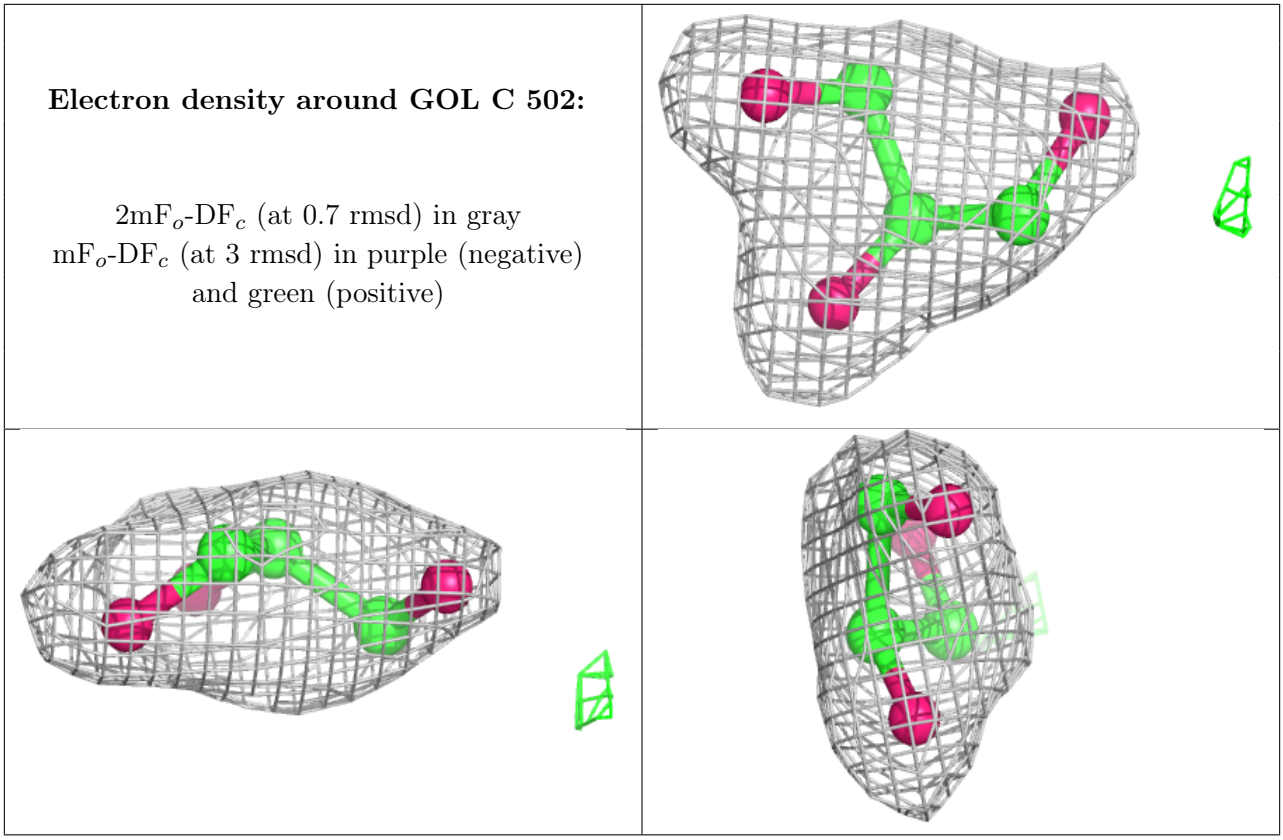
Electron density around CL A 510:

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



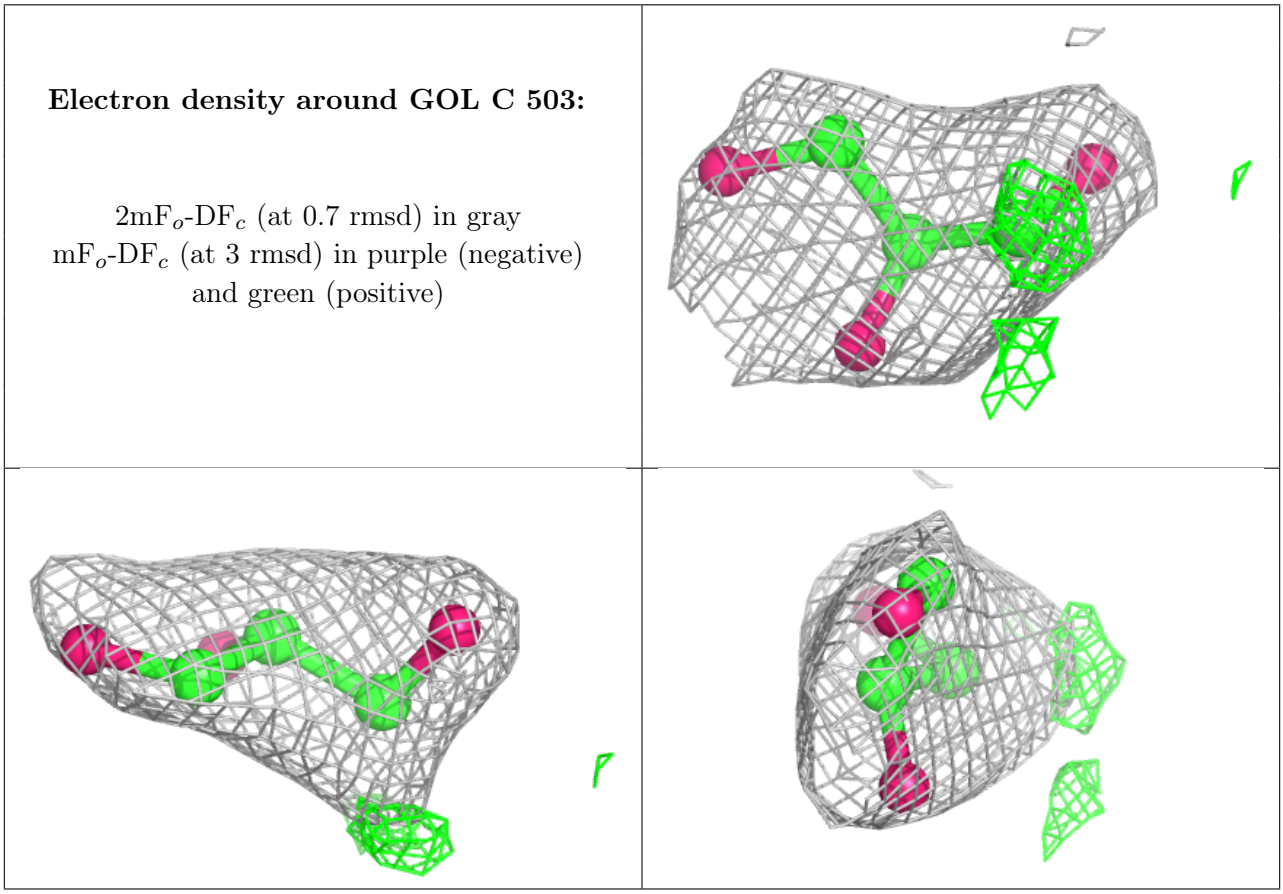
Electron density around GOL C 502:

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



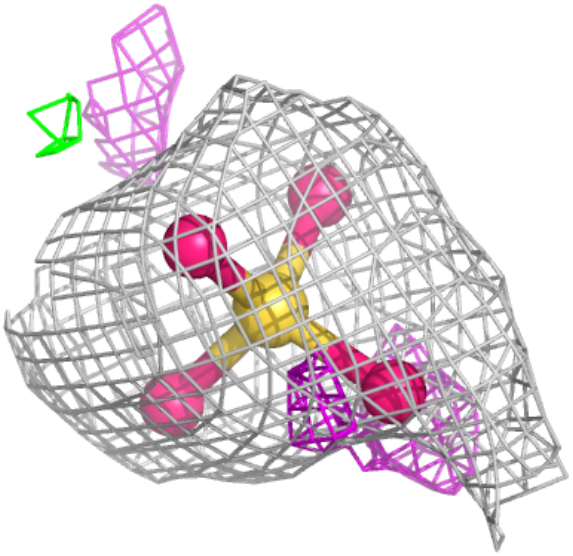
Electron density around GOL C 503:

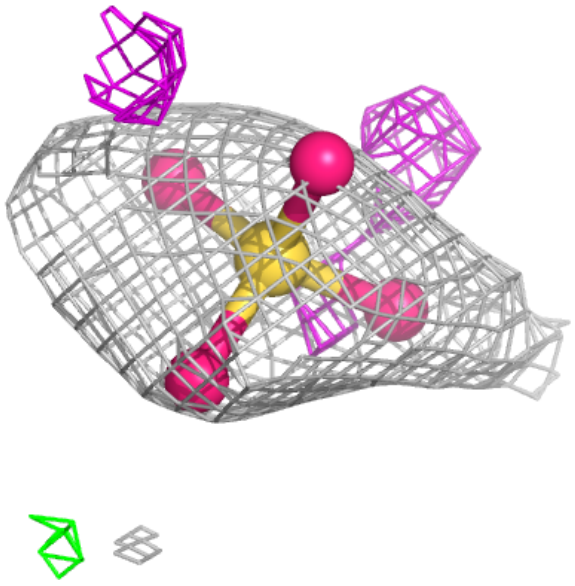
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

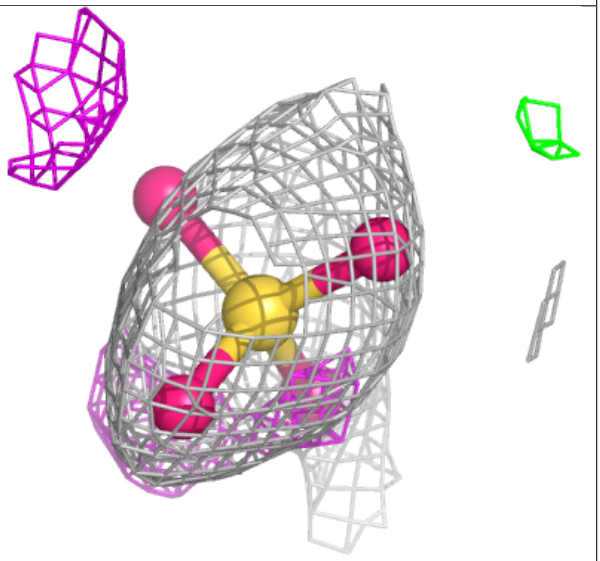


Electron density around SO4 B 1216:

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

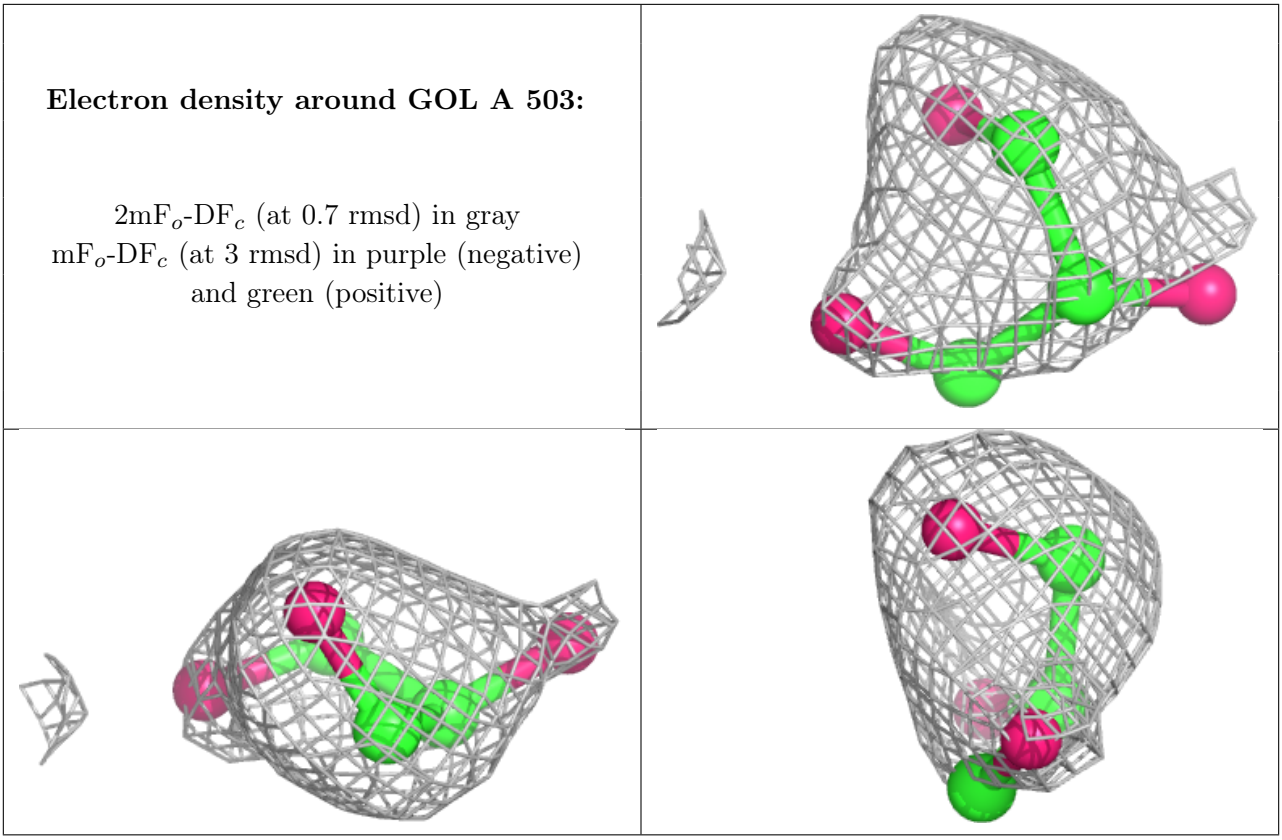






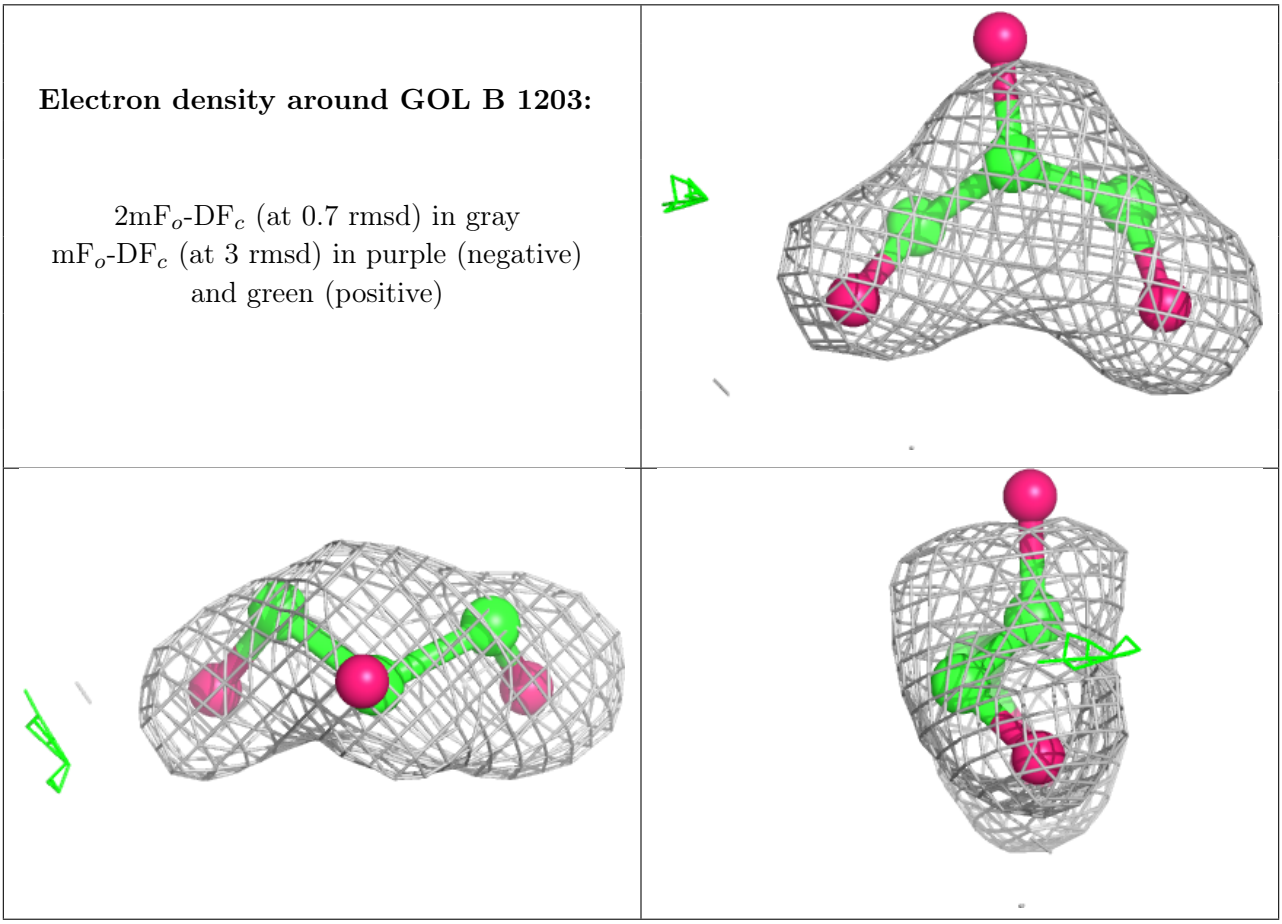
Electron density around GOL A 503:

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



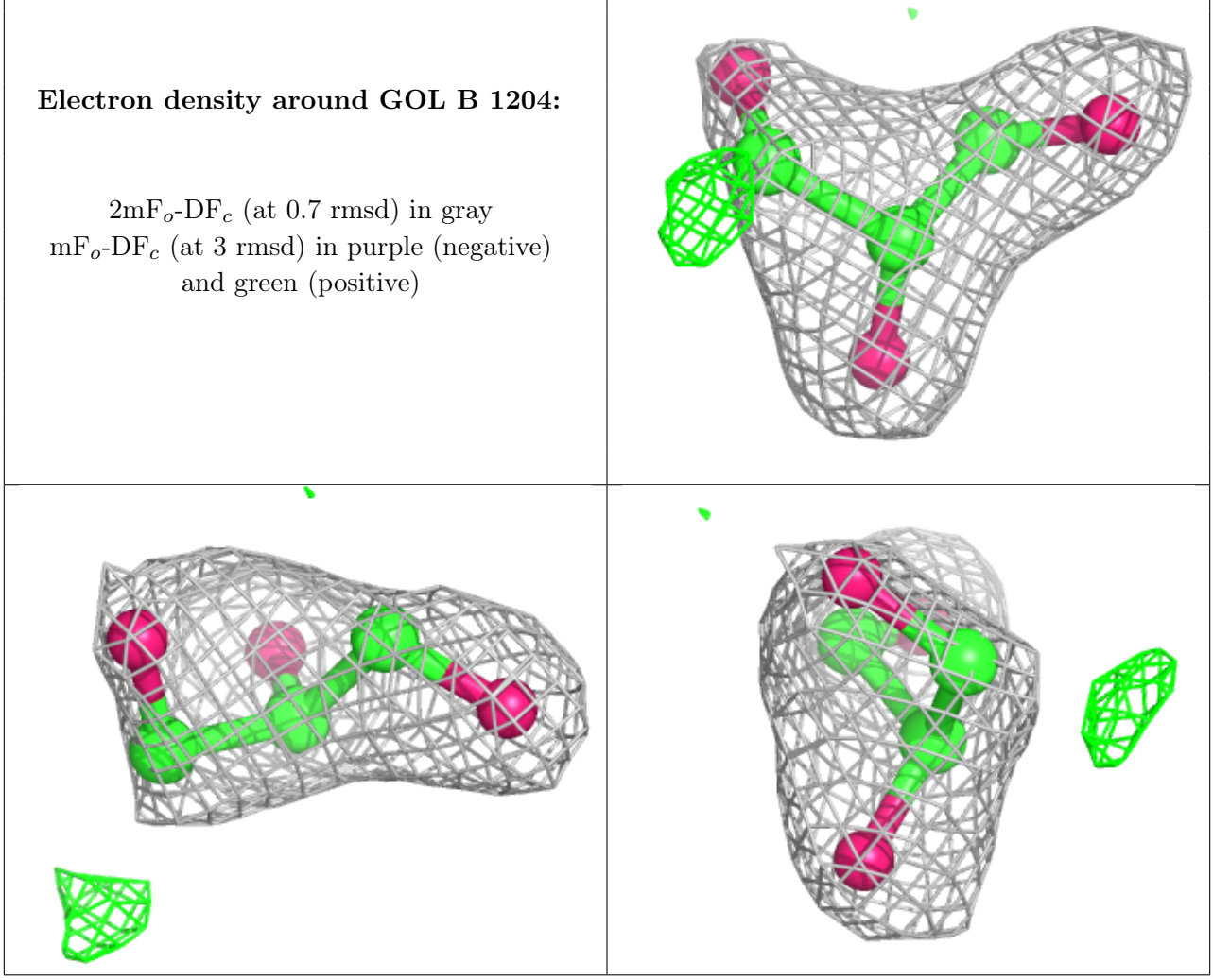
Electron density around GOL B 1203:

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



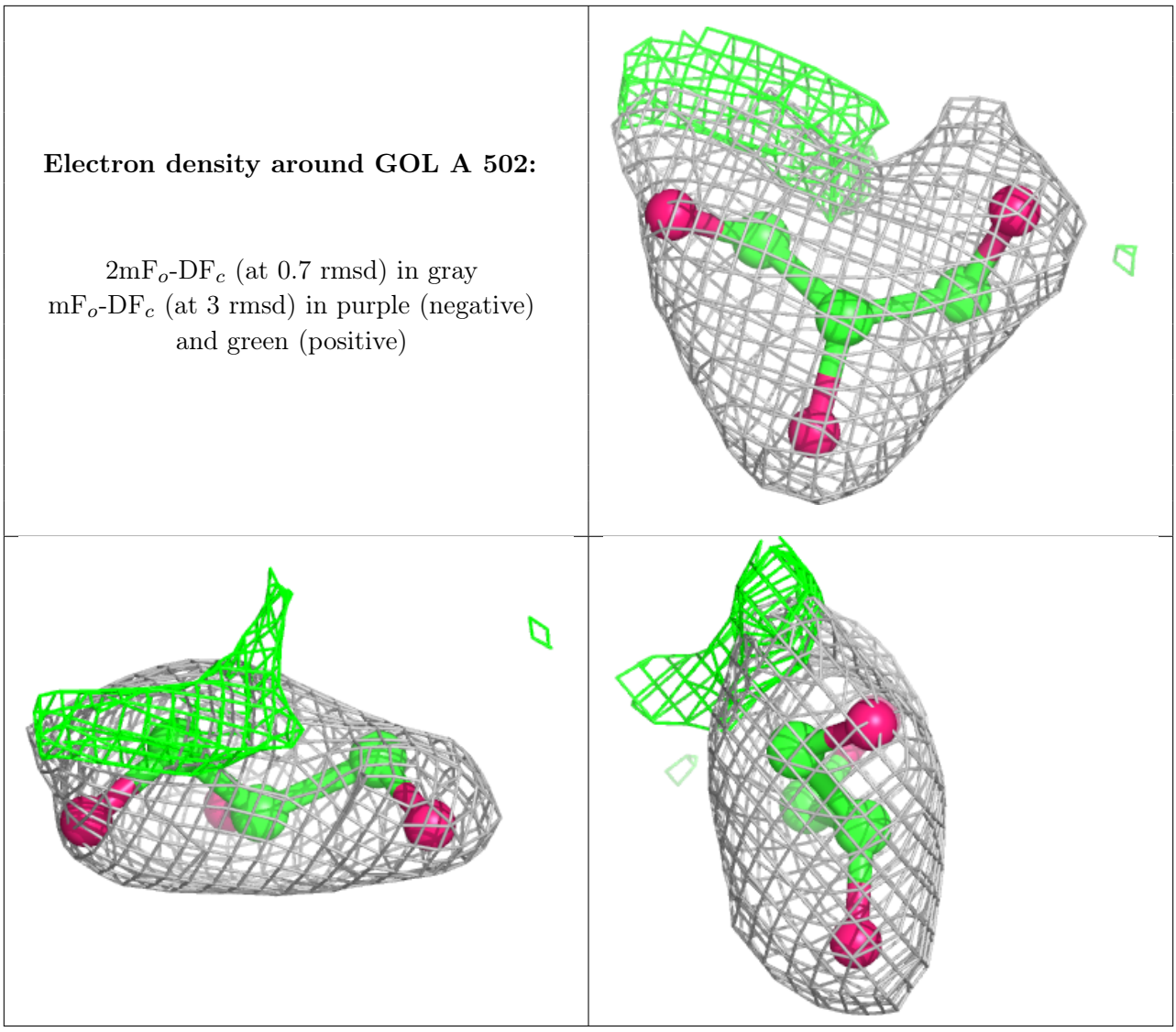
Electron density around GOL B 1204:

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



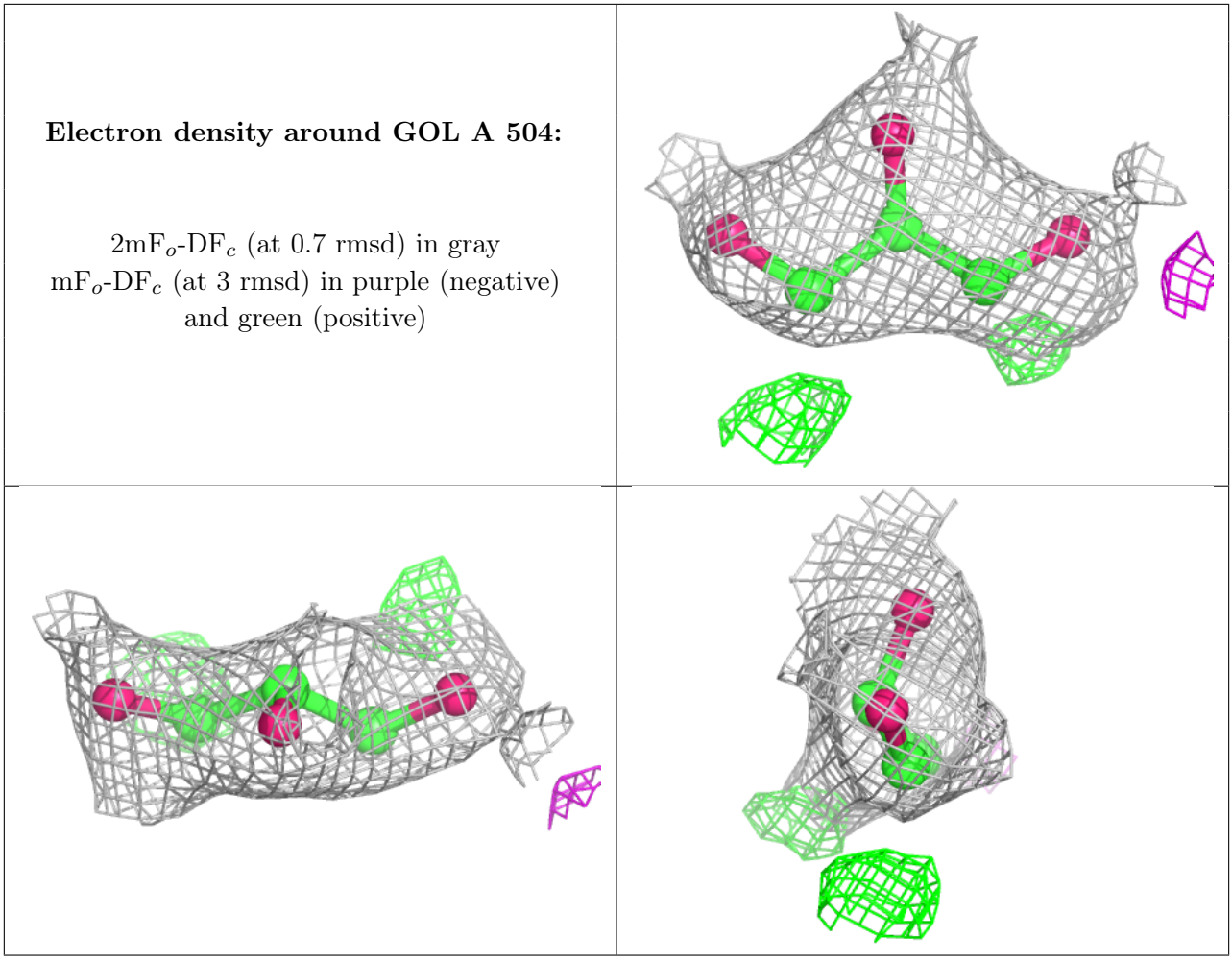
Electron density around GOL A 502:

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



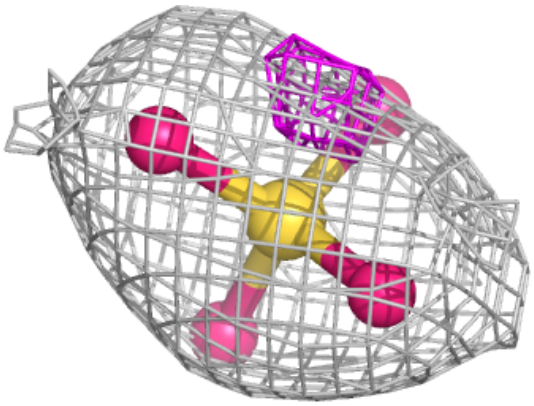
Electron density around GOL A 504:

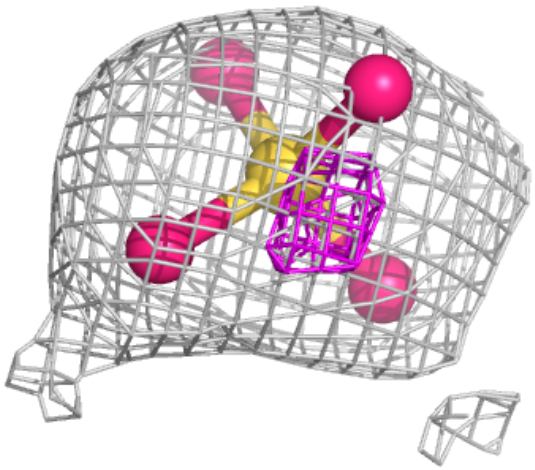
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

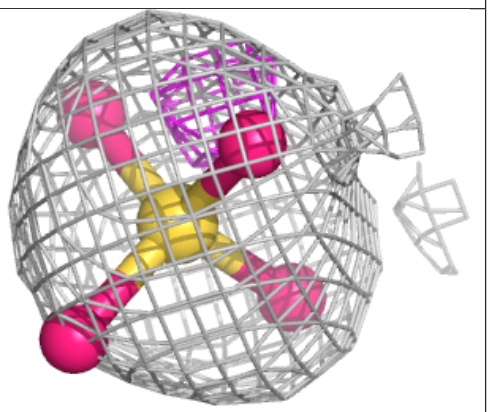


Electron density around SO4 C 512:

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

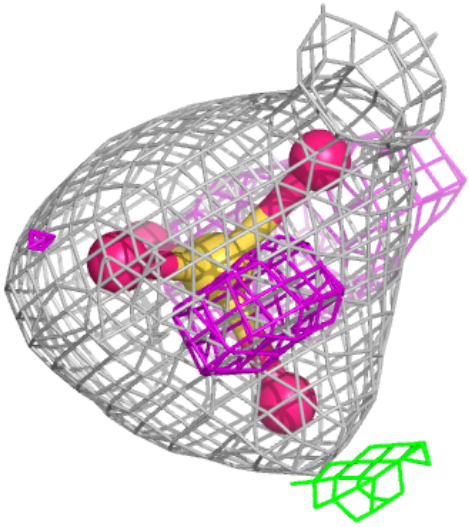


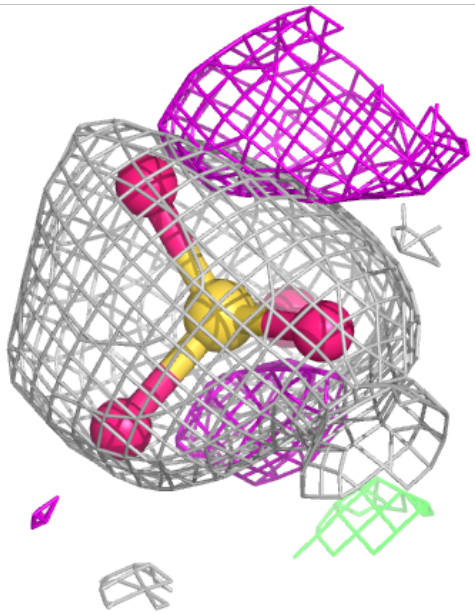


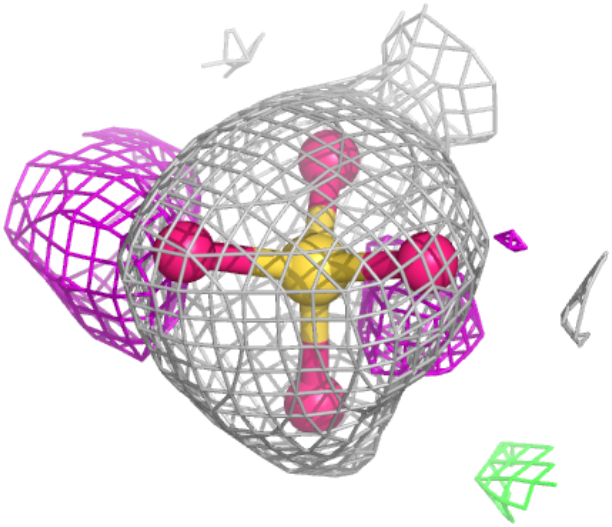


Electron density around SO4 A 508:

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

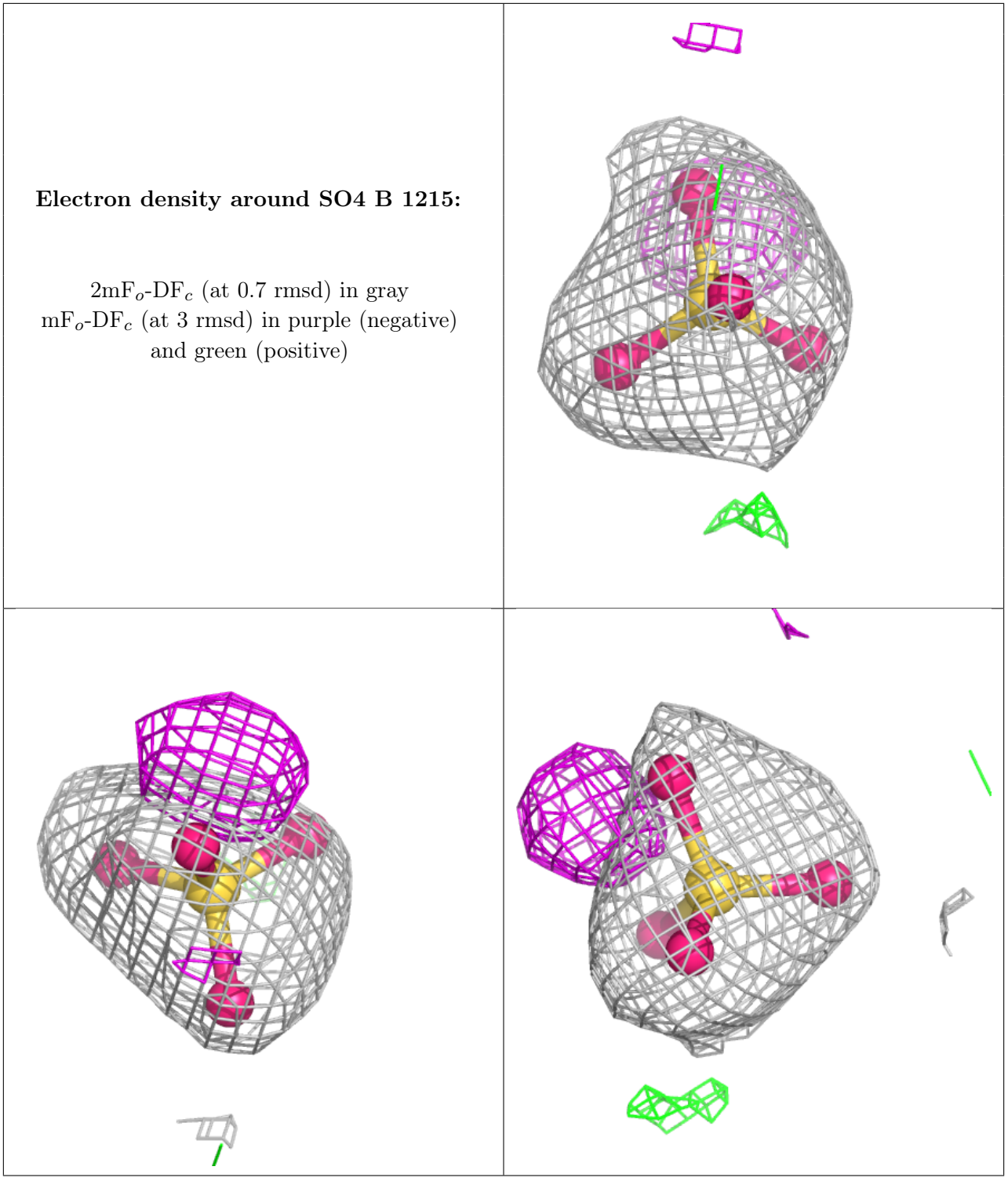






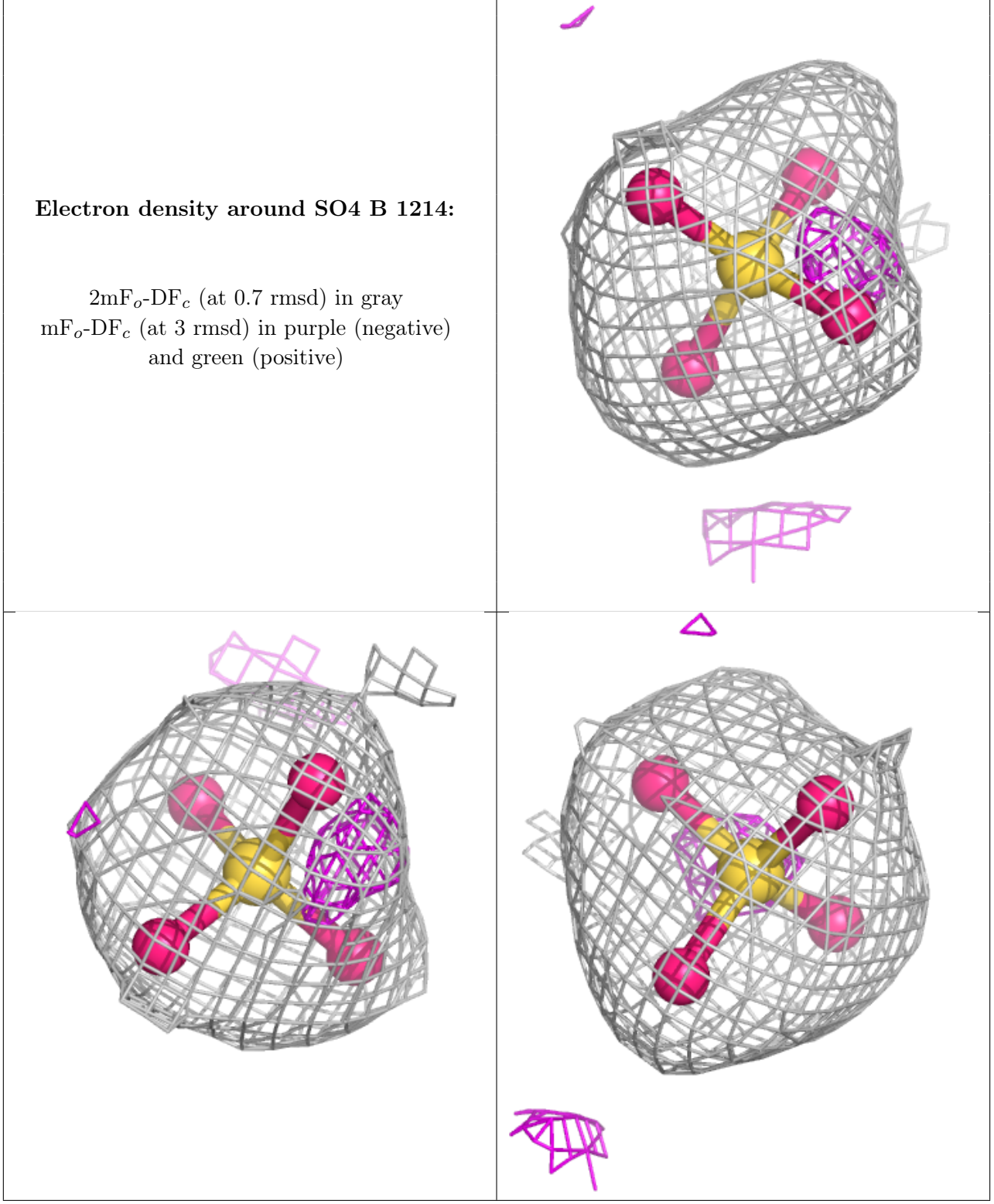
Electron density around SO4 B 1215:

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



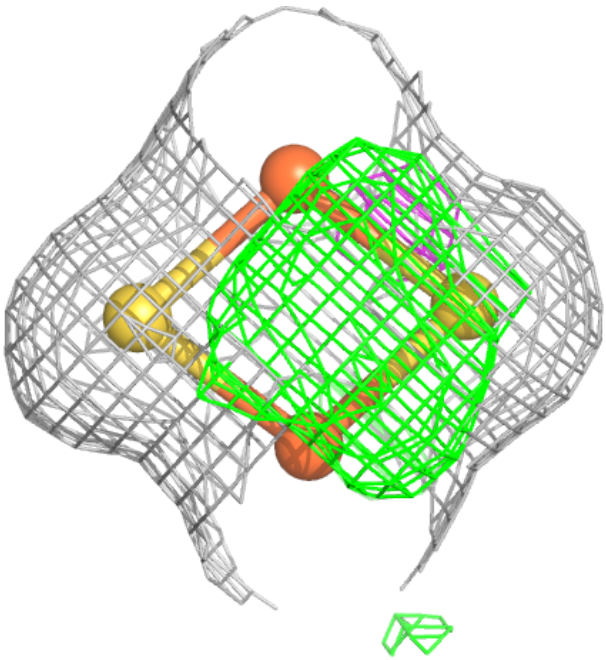
Electron density around SO4 B 1214:

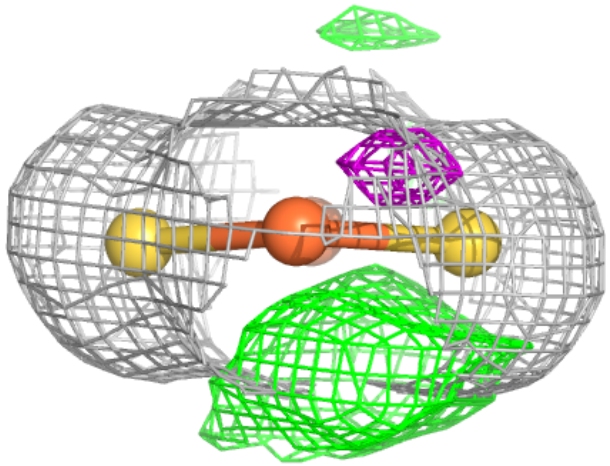
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

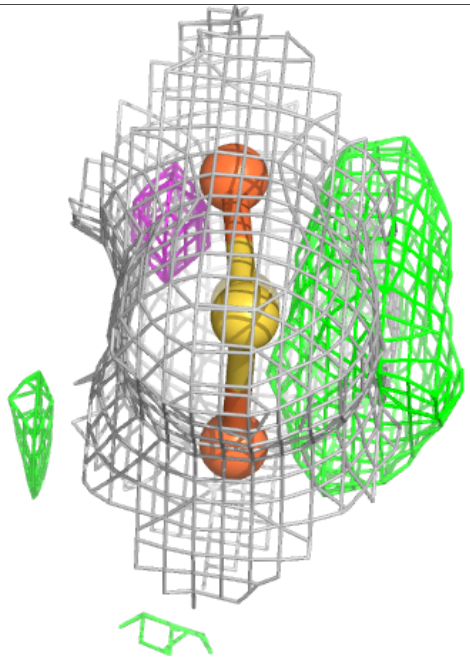


Electron density around FES C 501:

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

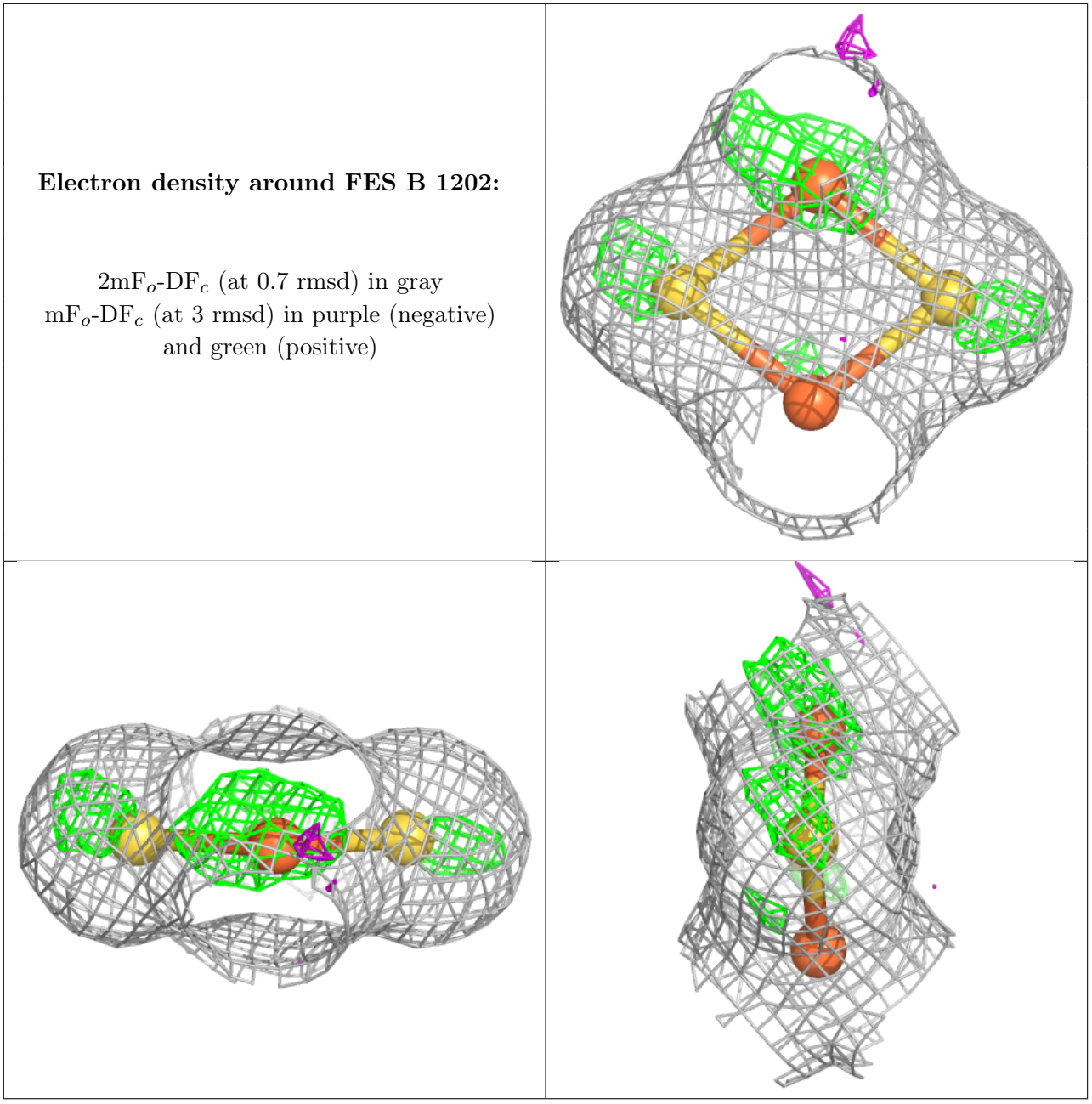






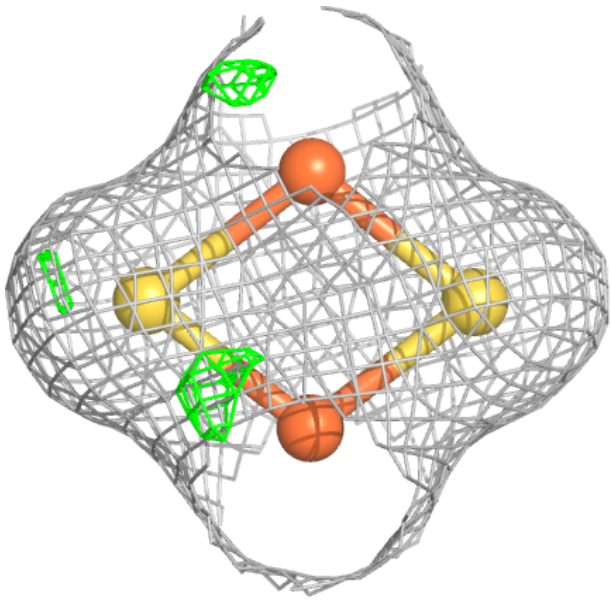
Electron density around FES B 1202:

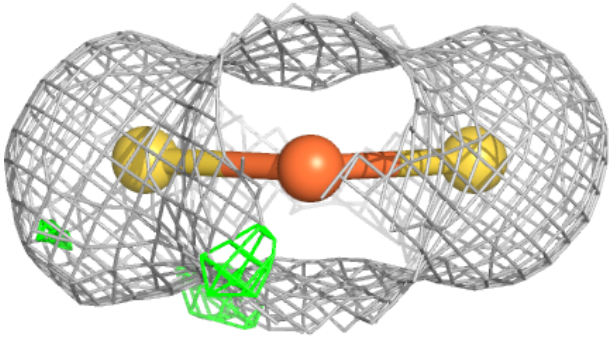
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

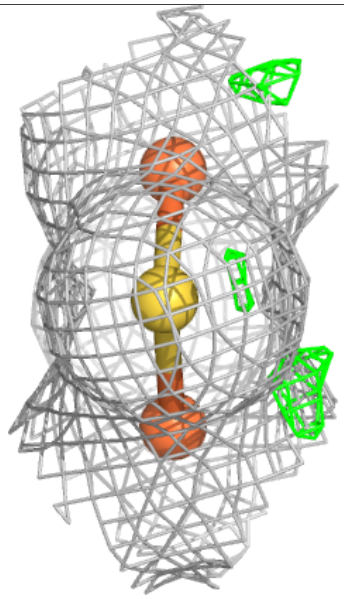


Electron density around FES A 501:

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

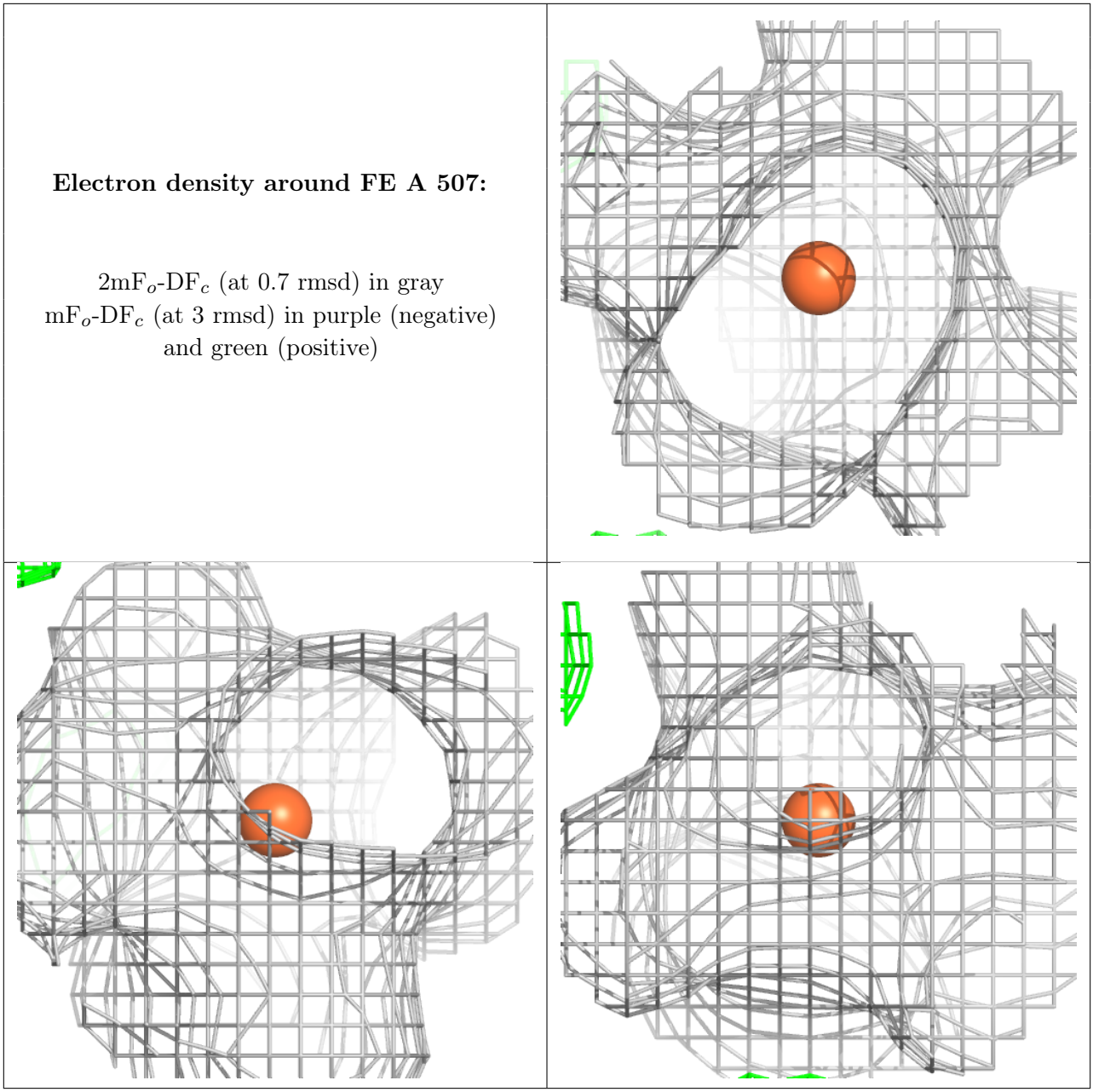






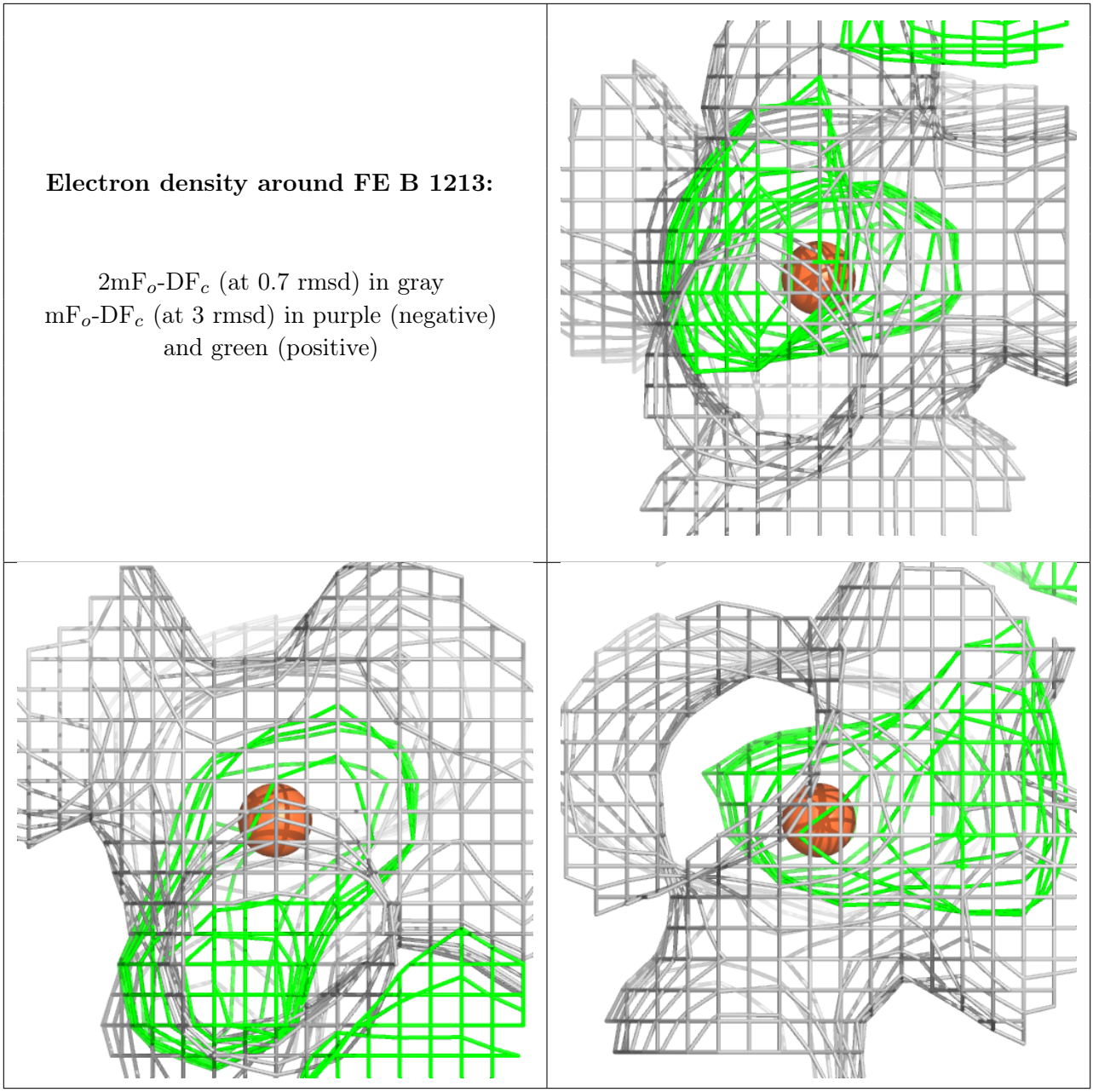
Electron density around FE A 507:

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



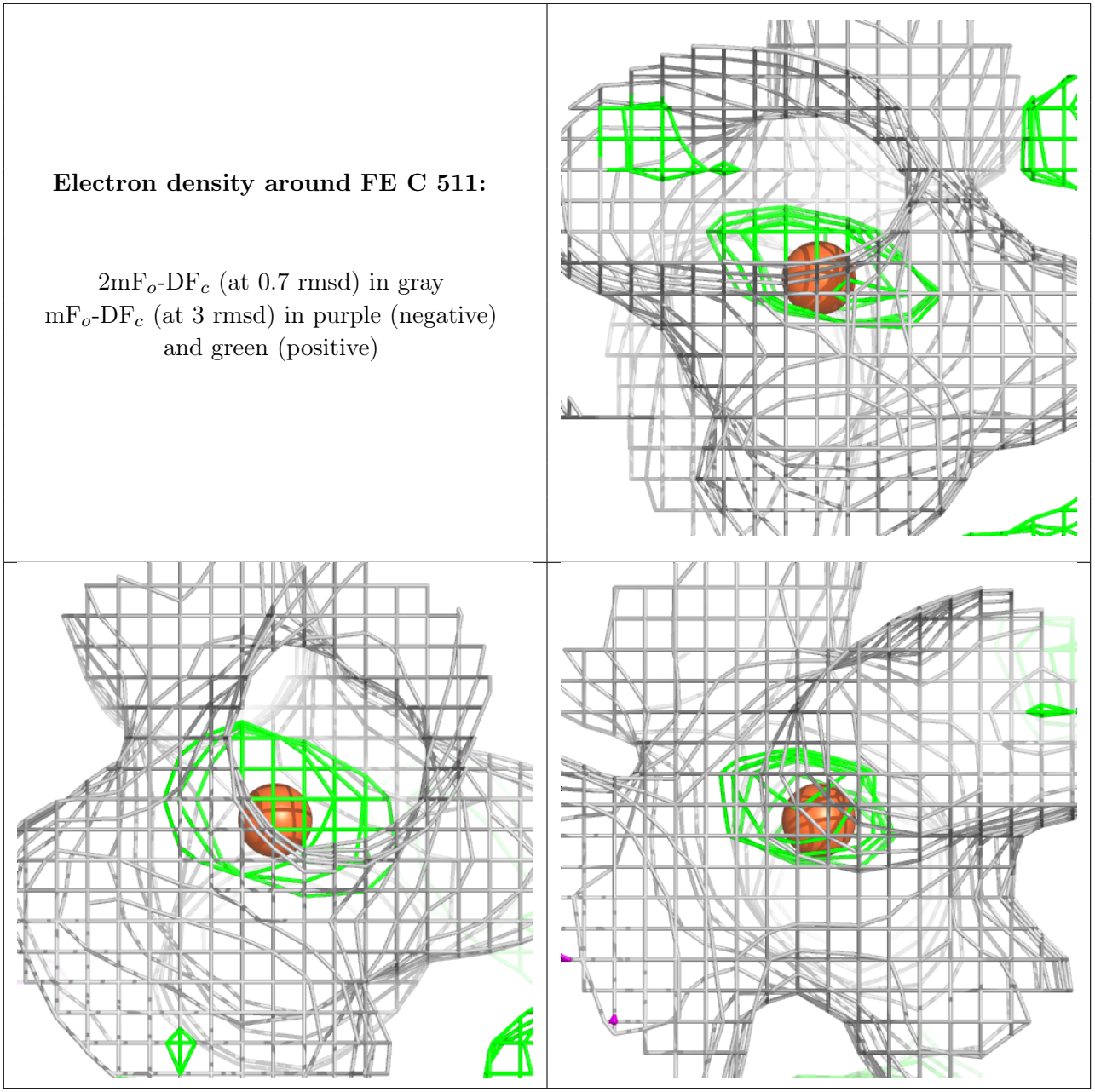
Electron density around FE B 1213:

$2mF_o$-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 511:

$2mF_o$-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.