Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2022 – 01:33 pm BST

PDB ID	:	6TXN
Title	:	Crystal structure of thermotoga maritima Ferritin in apo form
Authors	:	Wilk, P.; Grudnik, P.; Kumar, M.; Heddle, J.; Chakraborti, S.
Deposited on	:	2020-01-14
Resolution	:	2.01 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 (i) 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 (i)) were used in the production of this report:

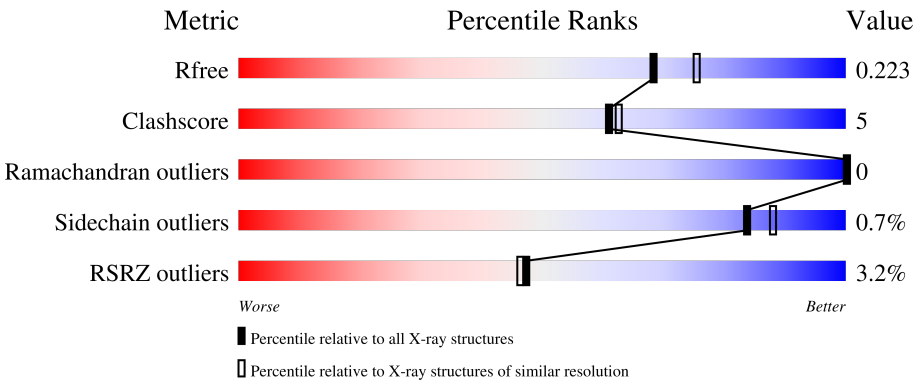
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	164	.% 90% 9% •
1	B	164	2% 87% 12% •
1	C	164	3% 88% 11% •
1	D	164	2% 90% 10%
1	E	164	.% 94% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	164	8% 89% 11%
1	G	164	2% 92% 7%
1	H	164	6% 88% 12%

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	SO4	C	203	-	-	-	X
3	SO4	C	204	-	-	-	X

2 Entry composition (i)

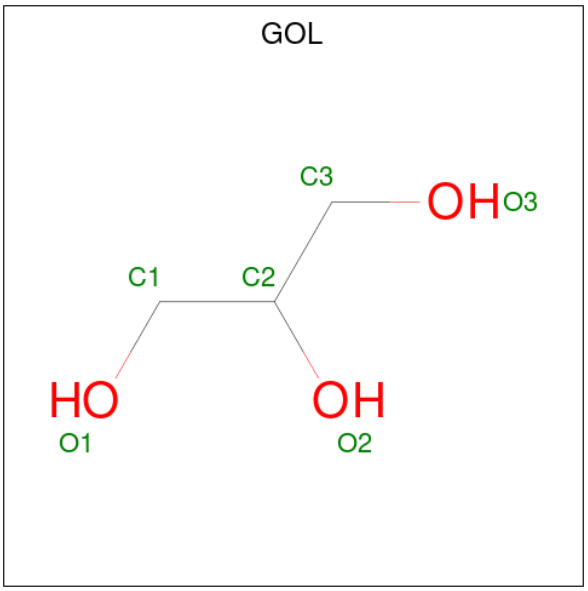
There are 6 unique types of molecules in this entry. The entry contains 22696 atoms, of which 10836 are hydrogens and 0 are deuteriums.

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 Ferritin.

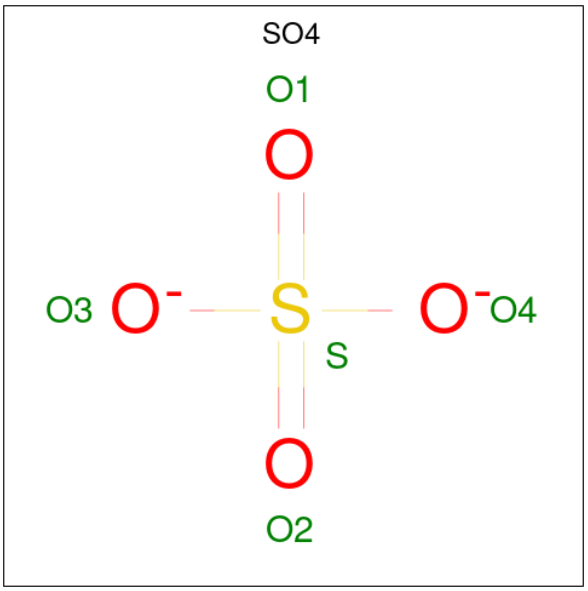
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	164	2702	879	1329	224	264	6	0	1	0
1	B	164	2728	887	1341	226	268	6	0	4	0
1	C	164	2693	878	1320	223	266	6	0	1	0
1	D	164	2724	886	1343	225	264	6	0	3	0
1	E	164	2712	881	1334	226	265	6	0	2	0
1	F	164	2663	868	1304	222	263	6	0	1	0
1	G	164	2668	871	1305	222	264	6	0	0	0
1	H	164	2757	893	1362	231	265	6	0	4	0

- 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 9	C 3	H 3	O 3	0	0
2	B	1	Total 9	C 3	H 3	O 3	0	0
2	B	1	Total 9	C 3	H 3	O 3	0	0
2	C	1	Total 9	C 3	H 3	O 3	0	0
2	C	1	Total 9	C 3	H 3	O 3	0	0
2	D	1	Total 9	C 3	H 3	O 3	0	0
2	D	1	Total 9	C 3	H 3	O 3	0	0
2	E	1	Total 9	C 3	H 3	O 3	0	0
2	G	1	Total 9	C 3	H 3	O 3	0	0
2	H	1	Total 9	C 3	H 3	O 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).

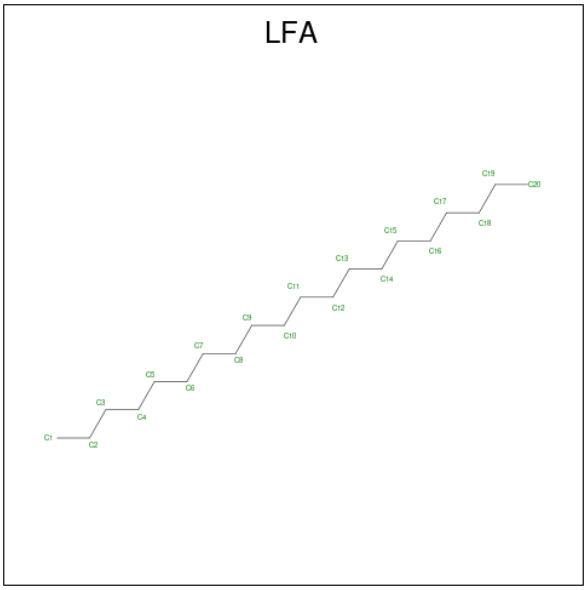


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	H		
5	B	1	62	20	42	0	0
5	D	1	62	20	42	0	0
5	E	1	62	20	42	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	H		
5	G	1	62	20	42	0	0

- Molecule 6 is water.

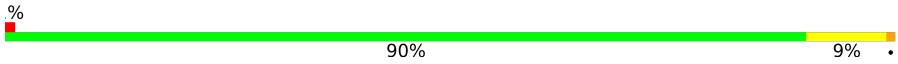
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	115	115	115	0	0
6	B	105	105	105	0	0
6	C	76	76	76	0	0
6	D	81	81	81	0	0
6	E	91	91	91	0	0
6	F	66	66	66	0	0
6	G	63	63	63	0	0
6	H	46	46	46	0	0

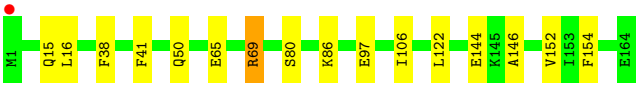
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ferritin

Chain A:



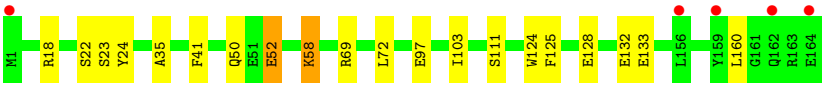


• Molecule 1: Ferritin

Chain B:

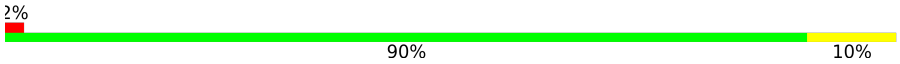
• Molecule 1: Ferritin

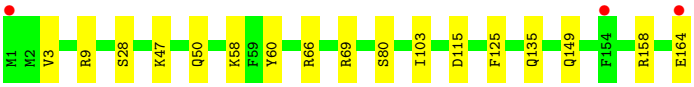
Chain C:



• Molecule 1: Ferritin

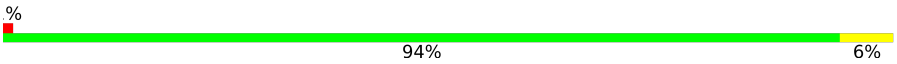
Chain D:

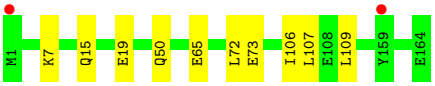




• Molecule 1: Ferritin

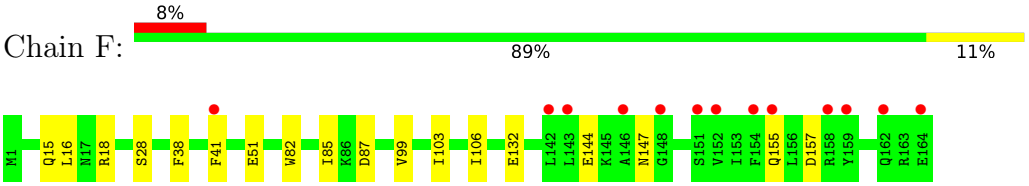
Chain E:





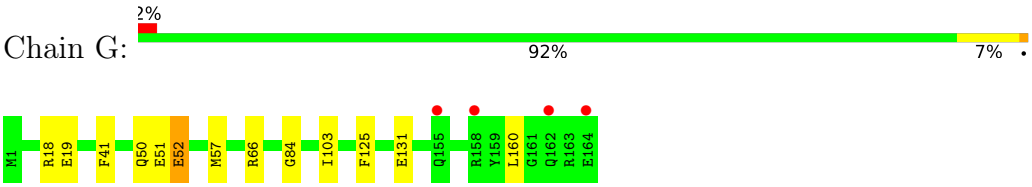
• Molecule 1: Ferritin

Chain F:



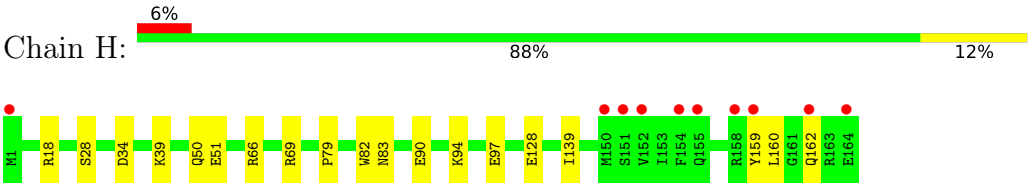
• Molecule 1: Ferritin

Chain G:



• Molecule 1: Ferritin

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	176.02Å 176.02Å 356.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.28 – 2.01 48.28 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.28-2.01) 93.2 (48.28-2.01)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.73 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.193 , 0.221 0.195 , 0.223	Depositor DCC
R_{free} test set	2000 reflections (1.43%)	wwPDB-VP
Wilson B-factor (Å^2)	40.9	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22696	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, LFA, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.79	1/1405 (0.1%)	0.82	2/1887 (0.1%)
1	B	0.78	0/1438	0.81	4/1933 (0.2%)
1	C	0.73	0/1405	0.77	3/1888 (0.2%)
1	D	0.72	0/1419	0.76	6/1905 (0.3%)
1	E	0.72	0/1413	0.73	0/1898
1	F	0.77	0/1390	0.79	2/1869 (0.1%)
1	G	0.73	2/1392 (0.1%)	0.66	0/1872
1	H	0.60	0/1436	0.64	0/1927
All	All	0.73	3/11298 (0.0%)	0.75	17/15179 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	52	GLU	CD-OE1	-9.11	1.15	1.25
1	G	51	GLU	CD-OE2	-6.56	1.18	1.25
1	A	65	GLU	CD-OE1	-5.72	1.19	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	69	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	C	69	ARG	NE-CZ-NH2	-9.91	115.35	120.30
1	C	69	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	A	69	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	C	18	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	B	45	MET	CB-CG-SD	6.80	132.81	112.40
1	B	69	ARG	NE-CZ-NH1	-6.39	117.11	120.30
1	D	58[A]	LYS	CA-C-O	6.39	133.52	120.10
1	D	58[B]	LYS	CA-C-O	6.39	133.52	120.10
1	B	9	ARG	NE-CZ-NH1	5.84	123.22	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	9	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	D	58[A]	LYS	O-C-N	-5.43	114.00	122.70
1	D	58[B]	LYS	O-C-N	-5.43	114.00	122.70
1	D	60	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	F	155[A]	GLN	O-C-N	-5.09	114.55	122.70
1	F	155[B]	GLN	O-C-N	-5.09	114.55	122.70
1	D	60	TYR	CB-CG-CD1	5.05	124.03	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1373	1329	1332	11	0
1	B	1387	1341	1334	14	2
1	C	1373	1320	1325	13	0
1	D	1381	1343	1347	15	0
1	E	1378	1334	1337	9	0
1	F	1359	1304	1308	12	0
1	G	1363	1305	1308	12	0
1	H	1395	1362	1366	16	0
2	A	6	3	8	0	0
2	B	12	6	15	0	0
2	C	12	6	16	2	0
2	D	12	6	16	1	0
2	E	6	3	7	0	0
2	G	6	3	8	1	0
2	H	6	3	8	0	0
3	A	5	0	0	0	0
3	B	15	0	0	2	0
3	C	10	0	0	2	0
3	D	5	0	0	1	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
3	H	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	B	20	42	42	0	0
5	D	20	42	42	1	0
5	E	20	42	42	0	0
5	G	20	42	42	4	0
6	A	115	0	0	4	0
6	B	105	0	0	7	0
6	C	76	0	0	2	0
6	D	81	0	0	6	0
6	E	91	0	0	3	0
6	F	66	0	0	3	0
6	G	63	0	0	2	0
6	H	46	0	0	8	0
All	All	11860	10836	10903	100	2

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 5.

All (100) 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)
3:B:201:SO4:O1	6:B:301:HOH:O	1.53	1.27
1:C:50:GLN:NE2	6:C:301:HOH:O	1.91	1.01
1:H:18[B]:ARG:NH2	6:H:303:HOH:O	2.03	0.91
1:F:18:ARG:NH2	6:F:301:HOH:O	2.04	0.91
1:H:97:GLU:OE1	6:H:302:HOH:O	1.94	0.85
3:C:204:SO4:O3	6:C:302:HOH:O	1.95	0.84
1:D:66[B]:ARG:NH2	1:D:115:ASP:OD1	2.10	0.84
2:D:202:GOL:O3	6:D:302:HOH:O	1.97	0.82
1:D:135:GLN:OE1	6:D:301:HOH:O	1.97	0.81
1:B:80:SER:OG	6:B:302:HOH:O	1.99	0.79
1:E:19:GLU:OE2	6:E:301:HOH:O	2.02	0.77
1:G:18:ARG:NH2	6:G:301:HOH:O	2.18	0.76
1:D:69:ARG:NH2	6:D:303:HOH:O	2.02	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:GLU:OE2	6:E:302:HOH:O	2.06	0.74
1:D:69:ARG:NE	6:D:303:HOH:O	2.16	0.74
1:F:87:ASP:OD2	6:F:303:HOH:O	2.06	0.73
1:B:76:GLU:OE2	6:B:303:HOH:O	2.06	0.72
1:H:51:GLU:OE2	6:H:304:HOH:O	2.08	0.70
1:C:111:SER:OG	3:C:203:SO4:O2	2.10	0.67
1:D:50:GLN:NE2	6:D:305:HOH:O	2.28	0.67
1:H:128:GLU:OE2	6:H:304:HOH:O	2.11	0.66
1:D:3:VAL:HG23	1:D:66[B]:ARG:HH11	1.60	0.66
1:A:50:GLN:OE1	6:A:301:HOH:O	2.14	0.65
1:A:80:SER:OG	6:A:302:HOH:O	2.15	0.63
1:H:83:ASN:OD1	6:H:305:HOH:O	2.16	0.62
1:E:65:GLU:OE1	1:G:131:GLU:OE1	2.19	0.61
1:A:97:GLU:OE1	6:A:303:HOH:O	2.16	0.61
1:C:22:SER:HB2	1:C:52:GLU:HG3	1.82	0.61
1:G:52:GLU:HA	1:G:52:GLU:OE1	2.00	0.59
1:C:41:PHE:CE1	1:C:160:LEU:HD12	2.38	0.59
1:C:41:PHE:CD1	1:C:160:LEU:HD12	2.38	0.59
1:G:84:GLY:HA3	2:G:201:GOL:H32	1.84	0.58
1:B:80:SER:CB	6:B:302:HOH:O	2.51	0.57
1:G:103:ILE:HD13	1:G:125:PHE:HB3	1.87	0.57
1:F:82:TRP:NE1	6:F:302:HOH:O	2.05	0.56
5:G:202:LFA:H22	1:H:50:GLN:HG3	1.87	0.56
1:D:103:ILE:HD13	1:D:125:PHE:HB3	1.88	0.56
1:D:3:VAL:HG23	1:D:66[B]:ARG:HD2	1.86	0.56
1:G:41:PHE:CE1	1:G:160:LEU:HD12	2.43	0.54
1:A:69:ARG:HG3	1:B:35:ALA:HB2	1.90	0.52
1:E:15:GLN:HB2	1:E:106:ILE:HD11	1.91	0.52
1:G:41:PHE:CD1	1:G:160:LEU:HD12	2.44	0.52
1:D:158:ARG:O	6:D:304:HOH:O	2.19	0.51
1:E:107:LEU:O	1:E:107:LEU:HD23	2.11	0.51
1:F:51:GLU:OE2	1:F:132:GLU:OE1	2.28	0.51
1:A:146:ALA:HB2	1:A:152:VAL:HG11	1.94	0.50
1:B:131[B]:GLU:HG2	6:B:322:HOH:O	2.10	0.50
1:G:19:GLU:OE2	6:G:302:HOH:O	2.19	0.50
1:F:99:VAL:O	1:F:103:ILE:HG12	2.11	0.50
1:A:15:GLN:HB2	1:A:106:ILE:HD11	1.94	0.49
1:A:86:LYS:HE3	1:A:144:GLU:OE2	2.13	0.49
1:C:23:SER:HB2	1:C:52:GLU:HB3	1.94	0.48
1:E:7:LYS:HE2	1:E:109:LEU:HD11	1.96	0.48
1:G:57:MET:HG3	5:G:202:LFA:H32	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ILE:HD13	1:C:125:PHE:HB3	1.97	0.47
1:H:139:ILE:HG12	1:H:160:LEU:HD11	1.96	0.47
1:F:16:LEU:C	1:F:16:LEU:HD23	2.35	0.47
1:H:69[B]:ARG:NH2	6:H:308:HOH:O	2.38	0.46
1:D:50:GLN:OE1	5:D:203:LFA:H21	2.16	0.46
1:F:144:GLU:O	1:F:144:GLU:HG3	2.16	0.46
1:G:50:GLN:HG3	5:G:202:LFA:H181	1.97	0.46
1:D:47:LYS:HE3	1:D:164:GLU:OXT	2.16	0.46
1:A:80:SER:CB	6:A:302:HOH:O	2.63	0.45
1:H:90:GLU:O	1:H:94:LYS:HG2	2.17	0.45
1:B:40:GLY:HA3	1:B:157:ASP:O	2.17	0.45
1:B:107:LEU:O	1:B:107:LEU:HD23	2.16	0.45
1:B:80:SER:HB3	6:B:302:HOH:O	2.17	0.45
1:B:26:TYR:CD1	1:B:45:MET:HE1	2.52	0.44
1:F:15:GLN:HB2	1:F:106:ILE:HD11	1.99	0.44
1:G:66:ARG:HA	1:G:66:ARG:HD2	1.83	0.44
1:H:159:TYR:HA	1:H:162:GLN:OE1	2.17	0.44
1:C:72:LEU:HD12	1:D:28:SER:HB2	2.00	0.44
1:H:66:ARG:HA	1:H:66:ARG:HD2	1.82	0.44
1:C:58:LYS:HE3	1:C:124:TRP:CE3	2.52	0.44
1:H:159:TYR:HD1	1:H:162:GLN:OE1	2.01	0.44
1:C:97:GLU:HB3	2:C:202:GOL:H32	1.99	0.44
1:A:106:ILE:HG22	1:A:122:LEU:HD11	2.00	0.43
1:F:41:PHE:HE1	1:F:157:ASP:HB2	1.84	0.43
1:H:69[B]:ARG:HD3	6:H:301:HOH:O	2.19	0.43
1:B:80:SER:HB3	6:B:329:HOH:O	2.18	0.43
1:F:38:PHE:CD2	1:F:85:ILE:HD11	2.54	0.43
1:A:38:PHE:HB3	1:A:41:PHE:HD2	1.84	0.42
1:E:50:GLN:NE2	6:E:306:HOH:O	2.52	0.42
1:E:72:LEU:HD12	1:F:28:SER:HB2	2.02	0.42
1:H:34:ASP:OD1	1:H:39:LYS:HE2	2.20	0.42
1:D:80:SER:OG	3:D:204:SO4:O4	2.34	0.42
1:C:35:ALA:HB2	1:D:69:ARG:HG3	2.00	0.42
1:E:107:LEU:HD23	1:E:107:LEU:C	2.39	0.42
1:F:38:PHE:CE2	1:F:85:ILE:HD11	2.55	0.42
1:B:142:LEU:HB3	1:B:156:LEU:HD11	2.02	0.41
1:B:15:GLN:HB2	1:B:106:ILE:HD11	2.03	0.41
1:A:16:LEU:C	1:A:16:LEU:HD23	2.41	0.41
1:B:66:ARG:HA	1:B:66:ARG:HD2	1.88	0.41
1:G:50:GLN:CG	5:G:202:LFA:H181	2.50	0.41
1:H:79:PRO:HG2	1:H:82:TRP:CZ2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:GLU:OE2	2:C:202:GOL:H11	2.21	0.41
1:B:128:GLU:O	1:B:132:GLU:HG2	2.21	0.41
1:C:128:GLU:O	1:C:132:GLU:HG2	2.21	0.41
1:H:69[B]:ARG:NH1	6:H:301:HOH:O	2.04	0.41
3:B:203:SO4:O1	1:D:149:GLN:NE2	2.55	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:GLU:OE1	1:B:114:LYS:NZ[2_665]	2.01	0.19
1:B:108:GLU:OE1	1:B:114:LYS:HZ2[2_665]	1.45	0.15

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	163/164 (99%)	163 (100%)	0	0	100	100
1	B	166/164 (101%)	165 (99%)	1 (1%)	0	100	100
1	C	163/164 (99%)	163 (100%)	0	0	100	100
1	D	165/164 (101%)	163 (99%)	2 (1%)	0	100	100
1	E	164/164 (100%)	163 (99%)	1 (1%)	0	100	100
1	F	163/164 (99%)	161 (99%)	2 (1%)	0	100	100
1	G	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	H	166/164 (101%)	164 (99%)	2 (1%)	0	100	100
All	All	1312/1312 (100%)	1301 (99%)	11 (1%)	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	145/144 (101%)	144 (99%)	1 (1%)	84	88
1	B	148/144 (103%)	147 (99%)	1 (1%)	84	88
1	C	145/144 (101%)	142 (98%)	3 (2%)	53	57
1	D	146/144 (101%)	145 (99%)	1 (1%)	84	88
1	E	146/144 (101%)	146 (100%)	0	100	100
1	F	142/144 (99%)	141 (99%)	1 (1%)	84	88
1	G	143/144 (99%)	143 (100%)	0	100	100
1	H	148/144 (103%)	147 (99%)	1 (1%)	84	88
All	All	1163/1152 (101%)	1155 (99%)	8 (1%)	84	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	PHE
1	B	7	LYS
1	C	24	TYR
1	C	52	GLU
1	C	58	LYS
1	D	9	ARG
1	F	147	ASN
1	H	28	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	81	ASN
1	F	147	ASN
1	G	55	HIS

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 34 ligands modelled in this entry, 8 are monoatomic - leaving 26 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	202	-	5,5,5	1.15	1 (20%)	5,5,5	1.26	1 (20%)
5	LFA	G	202	-	19,19,19	0.36	0	18,18,18	0.45	0
2	GOL	A	201	-	5,5,5	1.14	0	5,5,5	0.82	0
2	GOL	E	202	-	5,5,5	1.19	1 (20%)	5,5,5	0.87	0
5	LFA	B	205	-	19,19,19	0.25	0	18,18,18	0.41	0
3	SO4	H	201	-	4,4,4	0.11	0	6,6,6	0.18	0
3	SO4	D	204	-	4,4,4	0.14	0	6,6,6	0.18	0
2	GOL	B	202	-	5,5,5	1.45	1 (20%)	5,5,5	1.06	0
3	SO4	F	202	-	4,4,4	0.17	0	6,6,6	0.05	0
3	SO4	B	201	-	4,4,4	0.15	0	6,6,6	0.05	0
2	GOL	G	201	-	5,5,5	1.31	0	5,5,5	1.04	0
3	SO4	A	202	-	4,4,4	0.24	0	6,6,6	0.27	0
5	LFA	D	203	-	19,19,19	0.24	0	18,18,18	0.50	0
2	GOL	H	202	-	5,5,5	0.69	0	5,5,5	1.03	0
2	GOL	D	201	-	5,5,5	0.83	0	5,5,5	1.05	0
3	SO4	C	204	-	4,4,4	0.14	0	6,6,6	0.23	0
2	GOL	C	201	-	5,5,5	0.79	0	5,5,5	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	B	206	-	4,4,4	0.19	0	6,6,6	0.16	0
3	SO4	B	203	-	4,4,4	0.14	0	6,6,6	0.05	0
2	GOL	B	204	-	5,5,5	0.74	0	5,5,5	0.88	0
5	LFA	E	203	-	19,19,19	0.19	0	18,18,18	0.27	0
3	SO4	E	201	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	F	201	-	4,4,4	0.14	0	6,6,6	0.04	0
2	GOL	D	202	-	5,5,5	0.73	0	5,5,5	1.28	0
3	SO4	E	204	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	C	203	-	4,4,4	0.68	0	6,6,6	0.13	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	B	204	-	-	4/4/4/4	-
2	GOL	B	202	-	-	4/4/4/4	-
2	GOL	C	202	-	-	2/4/4/4	-
5	LFA	G	202	-	-	8/17/17/17	-
2	GOL	G	201	-	-	3/4/4/4	-
5	LFA	E	203	-	-	7/17/17/17	-
5	LFA	D	203	-	-	5/17/17/17	-
2	GOL	H	202	-	-	2/4/4/4	-
2	GOL	D	201	-	-	0/4/4/4	-
2	GOL	A	201	-	-	2/4/4/4	-
2	GOL	E	202	-	-	2/4/4/4	-
5	LFA	B	205	-	-	3/17/17/17	-
2	GOL	C	201	-	-	4/4/4/4	-
2	GOL	D	202	-	-	4/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	202	GOL	O2-C2	-2.43	1.36	1.43
2	E	202	GOL	O2-C2	-2.22	1.36	1.43
2	C	202	GOL	C1-C2	2.20	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	202	GOL	C3-C2-C1	-2.04	103.77	111.70

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	204	GOL	O1-C1-C2-C3
2	C	202	GOL	O1-C1-C2-C3
2	D	202	GOL	O1-C1-C2-O2
2	D	202	GOL	O1-C1-C2-C3
2	D	202	GOL	C1-C2-C3-O3
2	D	202	GOL	O2-C2-C3-O3
2	G	201	GOL	C1-C2-C3-O3
5	D	203	LFA	C2-C3-C4-C5
5	E	203	LFA	C11-C12-C13-C14
5	D	203	LFA	C11-C12-C13-C14
5	G	202	LFA	C10-C11-C12-C13
2	A	201	GOL	O1-C1-C2-C3
2	B	202	GOL	O1-C1-C2-C3
2	B	204	GOL	C1-C2-C3-O3
2	C	201	GOL	O1-C1-C2-C3
2	C	201	GOL	C1-C2-C3-O3
2	E	202	GOL	O1-C1-C2-C3
2	G	201	GOL	O1-C1-C2-C3
5	G	202	LFA	C9-C10-C11-C12
5	G	202	LFA	C4-C5-C6-C7
2	A	201	GOL	O1-C1-C2-O2
2	B	204	GOL	O1-C1-C2-O2
2	B	204	GOL	O2-C2-C3-O3
2	C	202	GOL	O1-C1-C2-O2
5	E	203	LFA	C9-C10-C11-C12
5	G	202	LFA	C3-C4-C5-C6
5	B	205	LFA	C9-C10-C11-C12
5	E	203	LFA	C13-C14-C15-C16
2	G	201	GOL	O2-C2-C3-O3
5	G	202	LFA	C6-C7-C8-C9
5	B	205	LFA	C11-C12-C13-C14
5	E	203	LFA	C1-C2-C3-C4
5	B	205	LFA	C11-C10-C9-C8
5	E	203	LFA	C12-C13-C14-C15
5	D	203	LFA	C1-C2-C3-C4
2	C	201	GOL	O1-C1-C2-O2
2	C	201	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	202	GOL	O1-C1-C2-O2
2	H	202	GOL	O1-C1-C2-O2
5	G	202	LFA	C2-C3-C4-C5
5	G	202	LFA	C17-C18-C19-C20
5	E	203	LFA	C7-C8-C9-C10
5	E	203	LFA	C10-C11-C12-C13
2	B	202	GOL	C1-C2-C3-O3
5	D	203	LFA	C3-C4-C5-C6
5	G	202	LFA	C7-C8-C9-C10
5	D	203	LFA	C15-C16-C17-C18
2	B	202	GOL	O1-C1-C2-O2
2	B	202	GOL	O2-C2-C3-O3
2	H	202	GOL	O1-C1-C2-C3

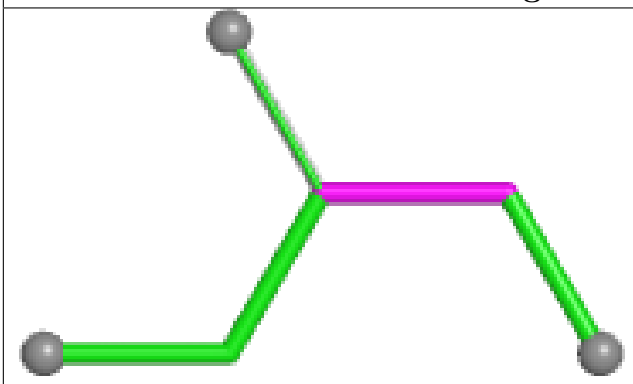
There are no ring outliers.

10 monomers are involved in 14 short contacts:

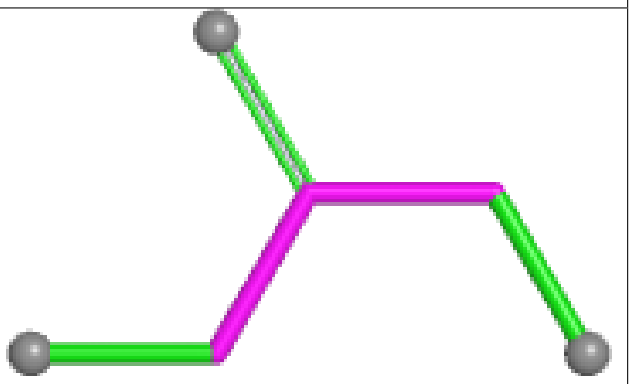
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	202	GOL	2	0
5	G	202	LFA	4	0
3	D	204	SO4	1	0
3	B	201	SO4	1	0
2	G	201	GOL	1	0
5	D	203	LFA	1	0
3	C	204	SO4	1	0
3	B	203	SO4	1	0
2	D	202	GOL	1	0
3	C	203	SO4	1	0

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

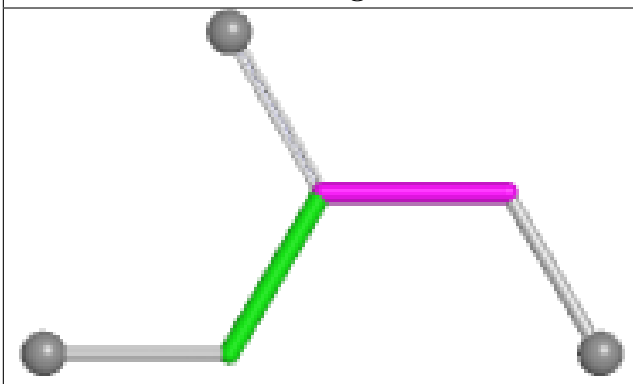
Ligand GOL C 202



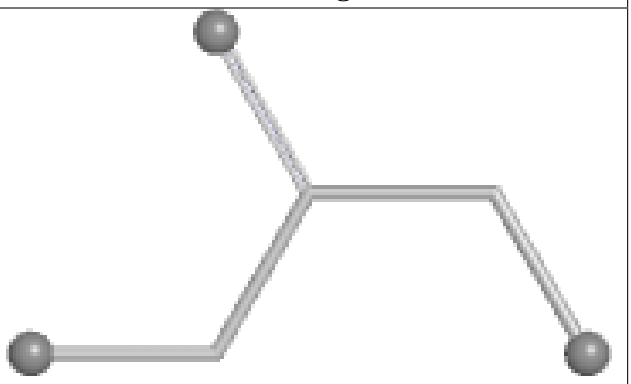
Bond lengths



Bond angles

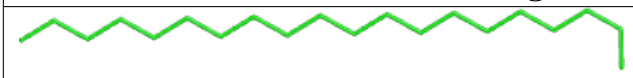


Torsions

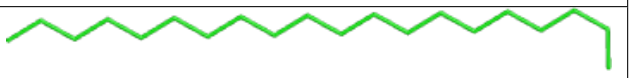


Rings

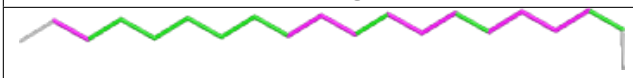
Ligand LFA G 202



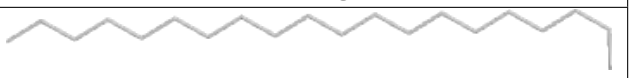
Bond lengths



Bond angles

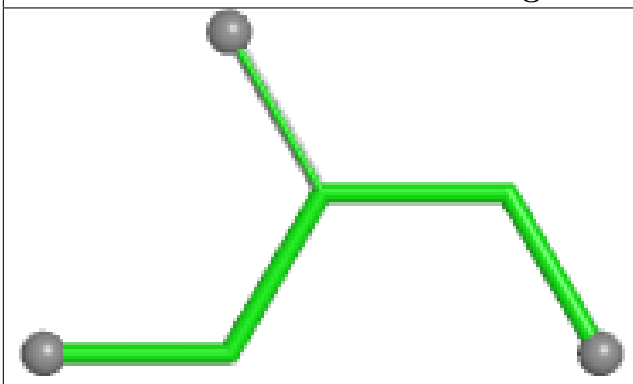


Torsions

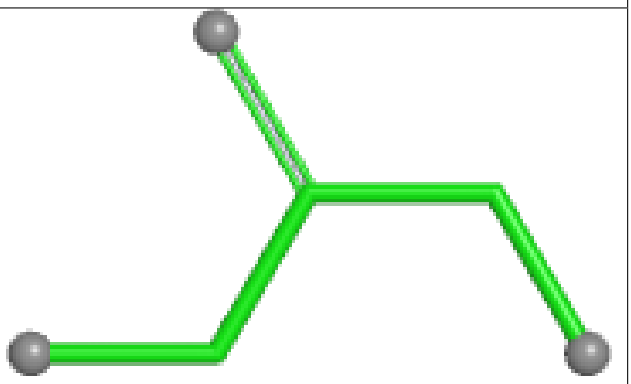


Rings

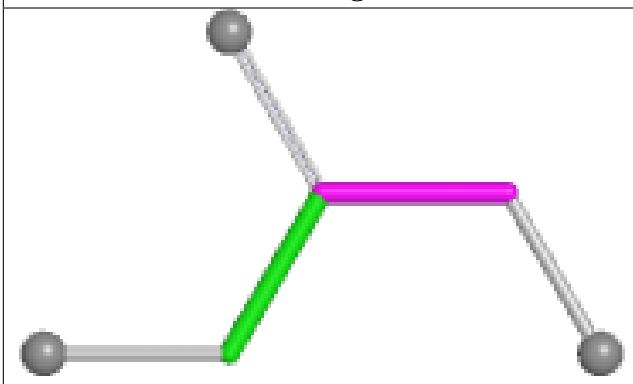
Ligand GOL A 201



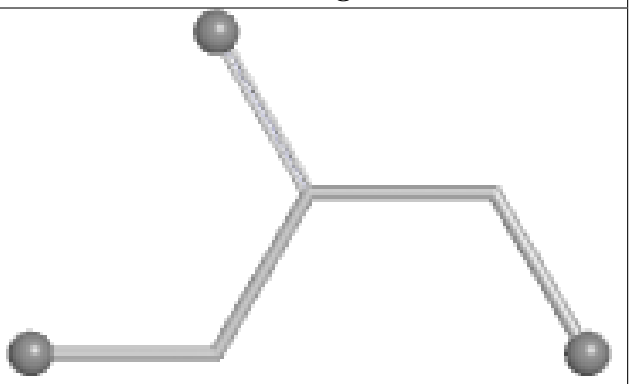
Bond lengths



Bond angles

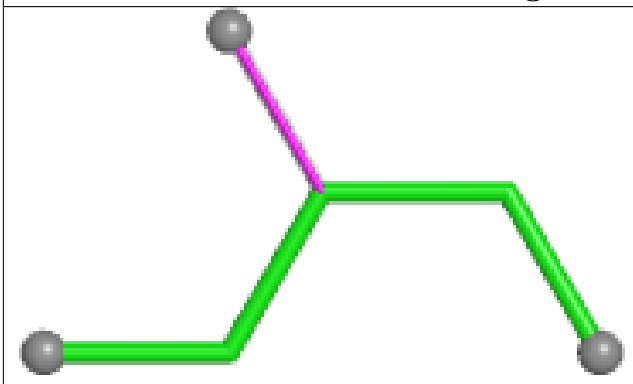


Torsions

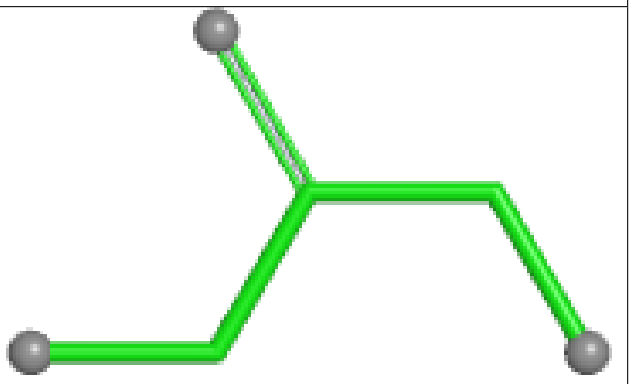


Rings

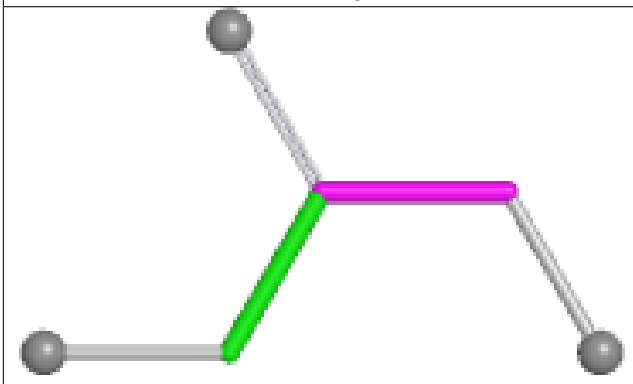
Ligand GOL E 202



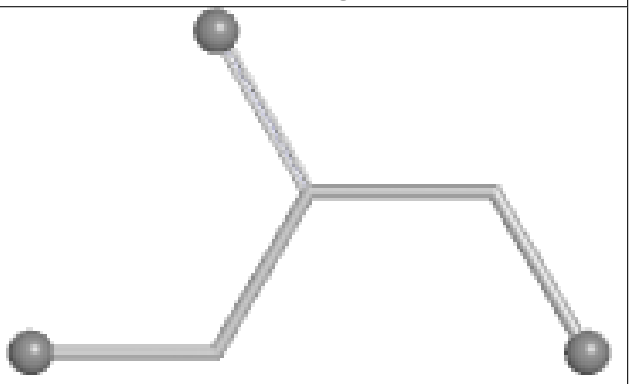
Bond lengths



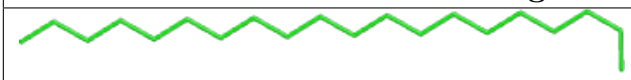
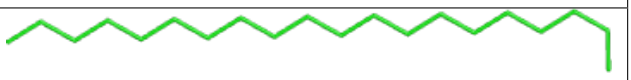
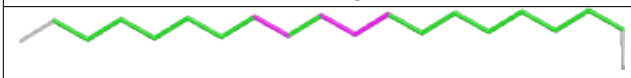
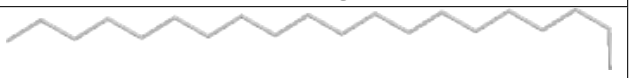
Bond angles

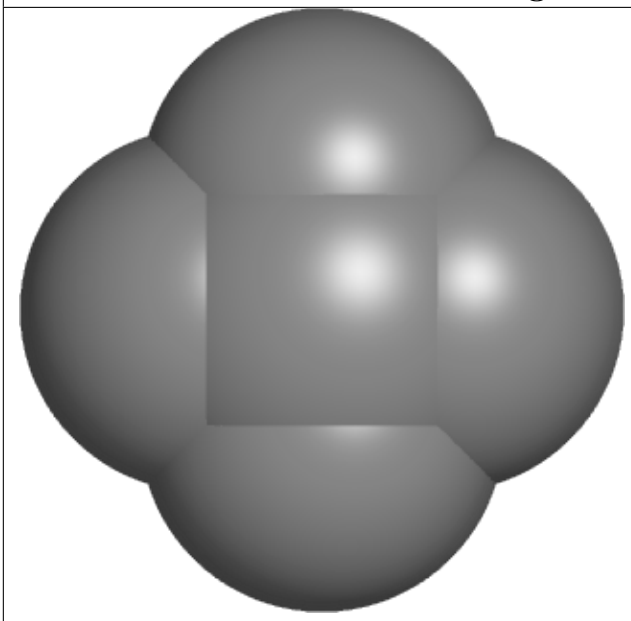
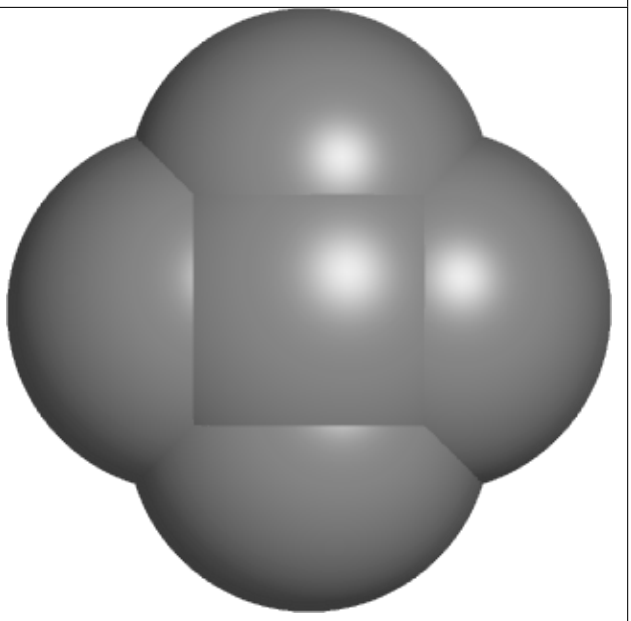
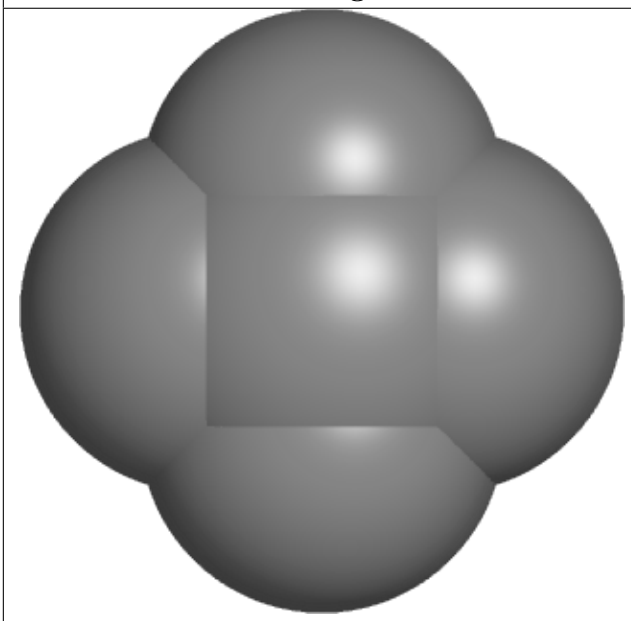
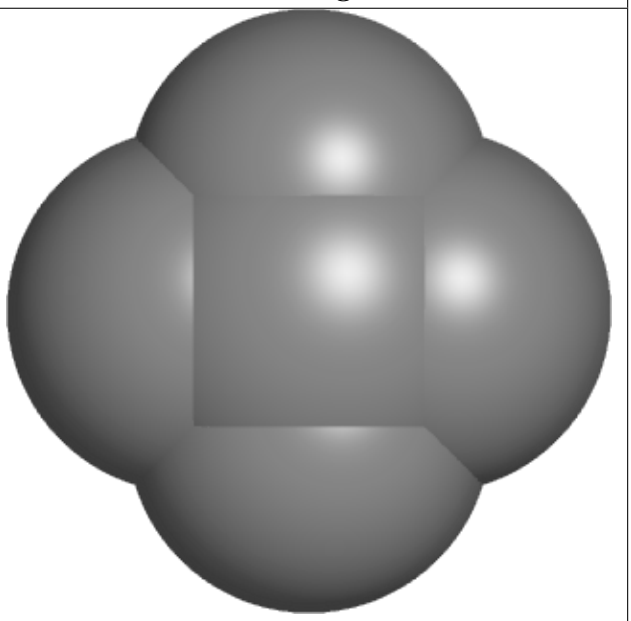


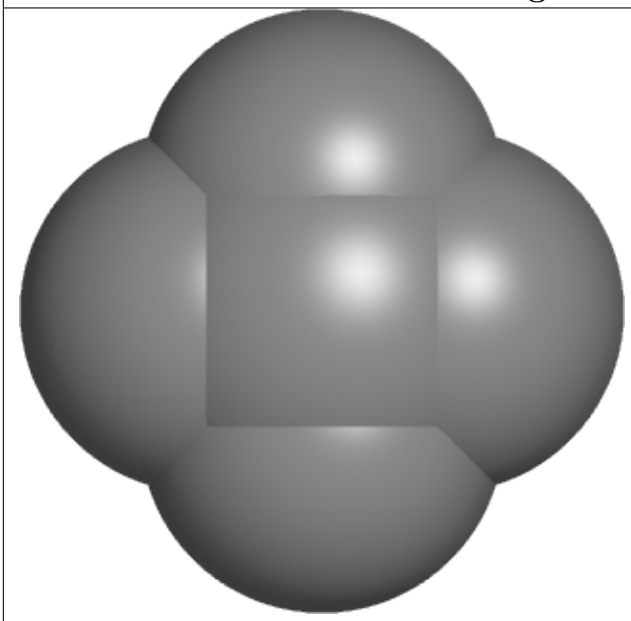
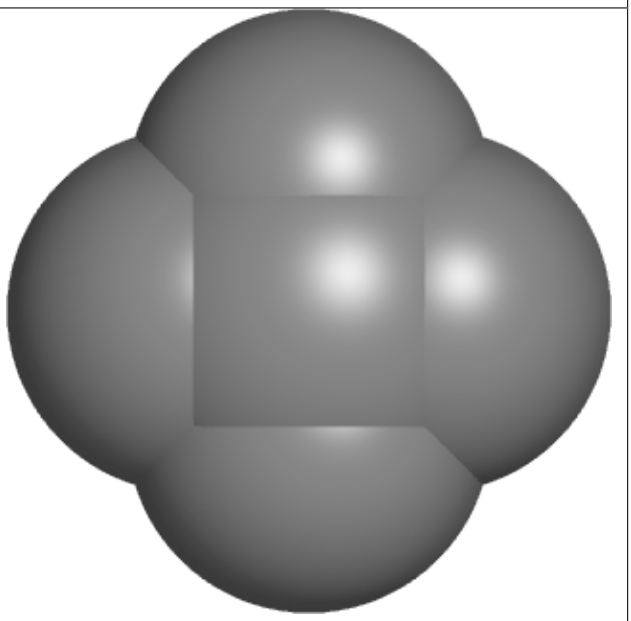
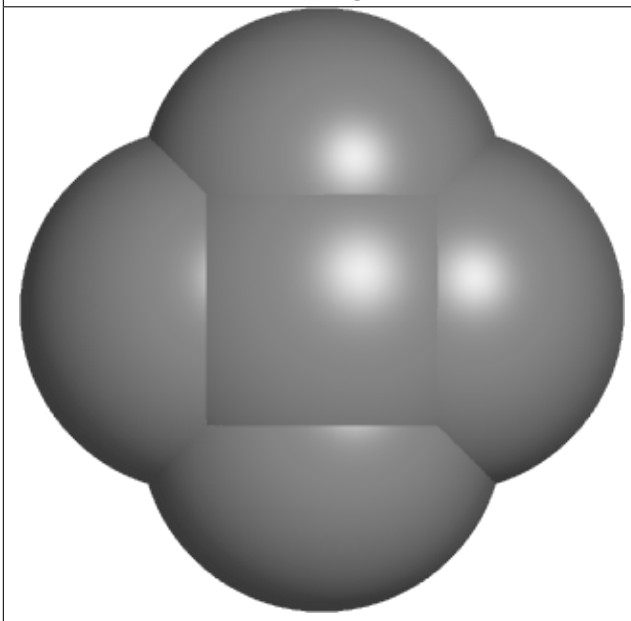
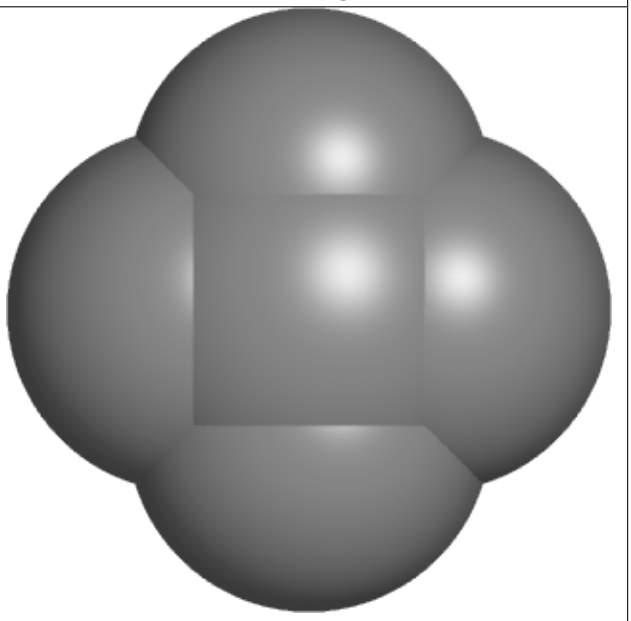
Torsions

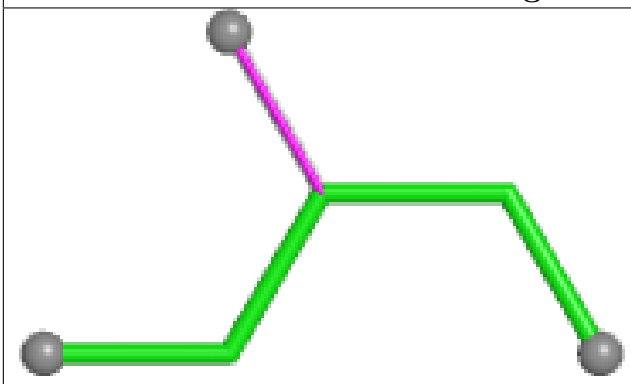
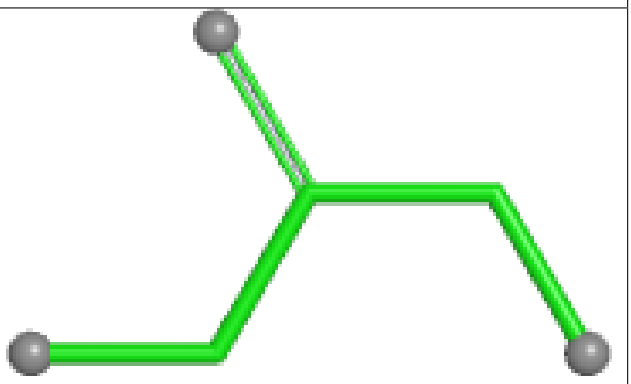
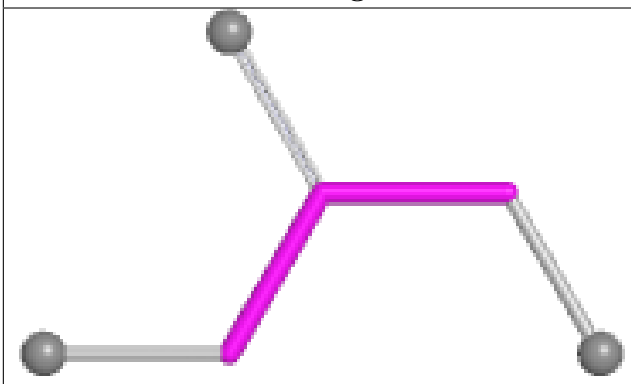
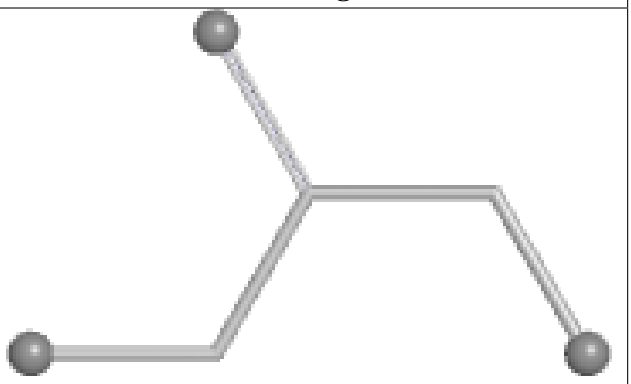


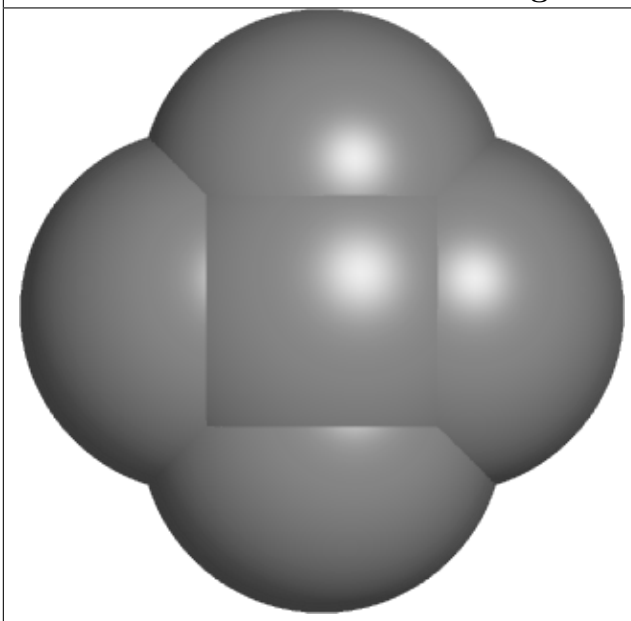
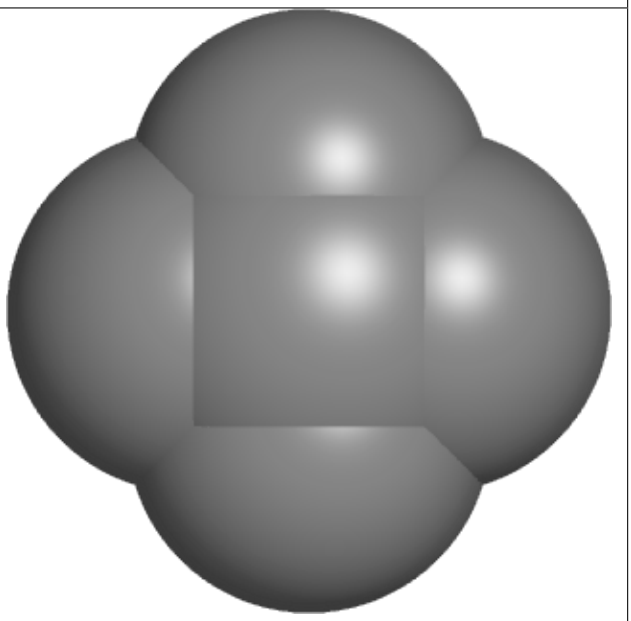
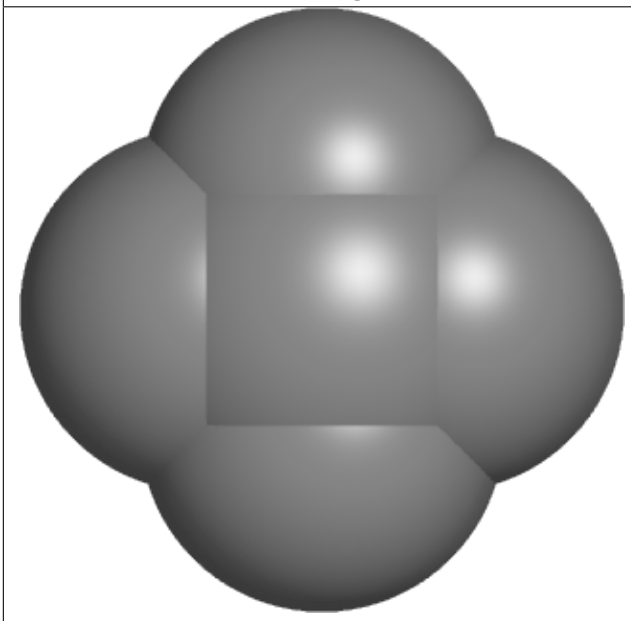
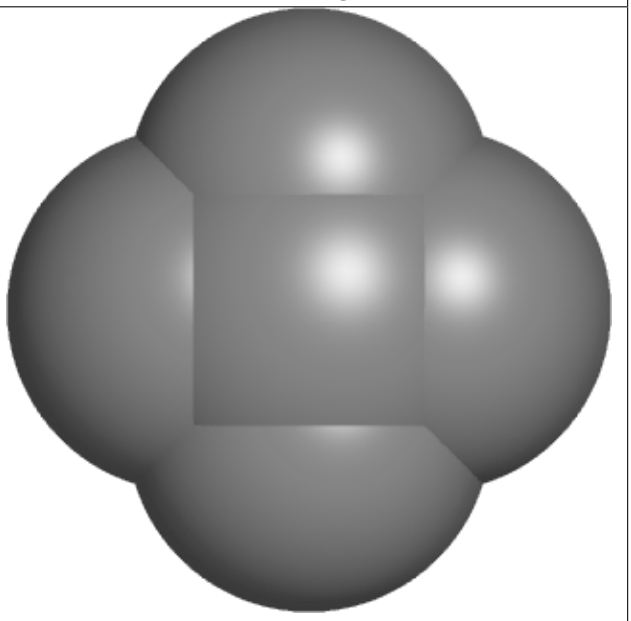
Rings

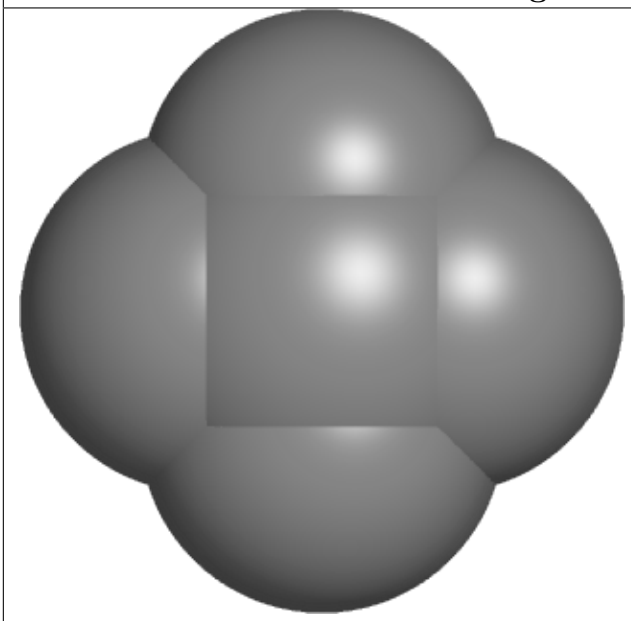
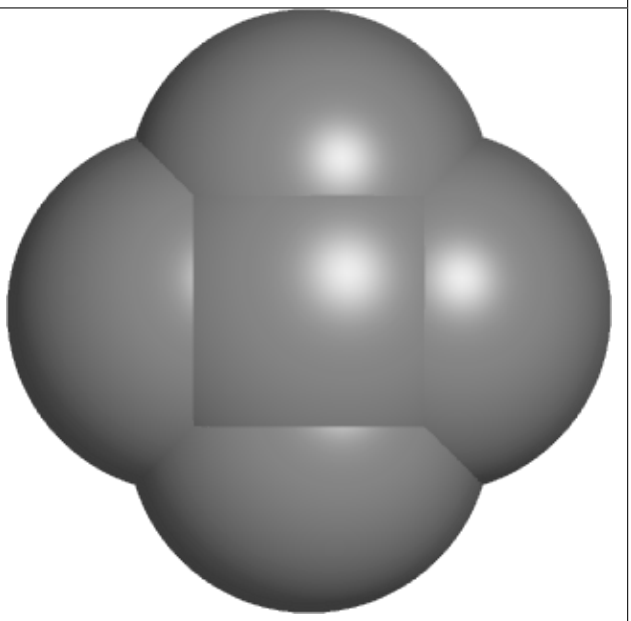
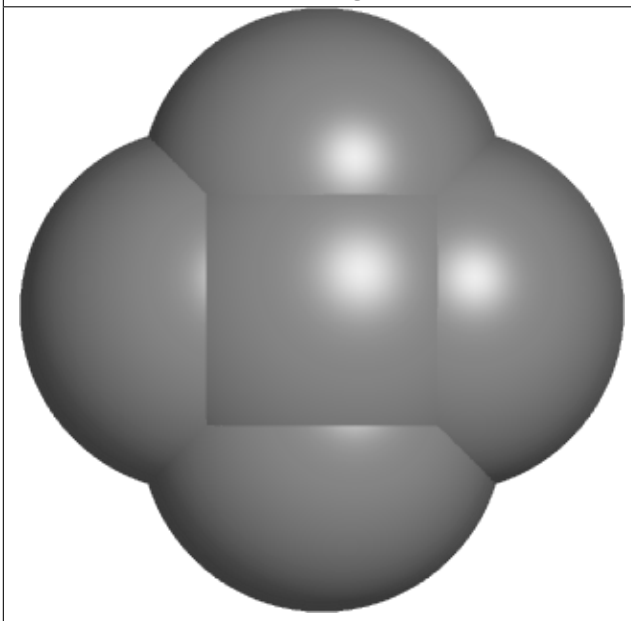
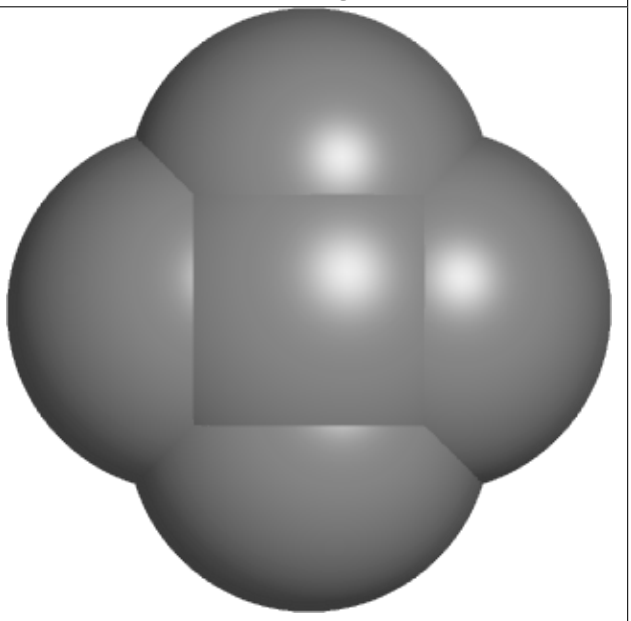
Ligand LFA B 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SO4 H 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

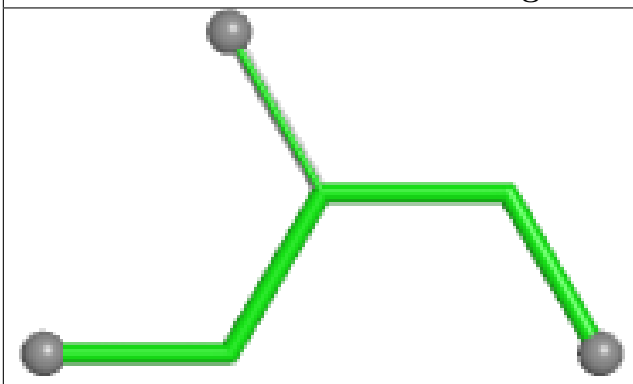
Ligand SO4 D 204	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand GOL B 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

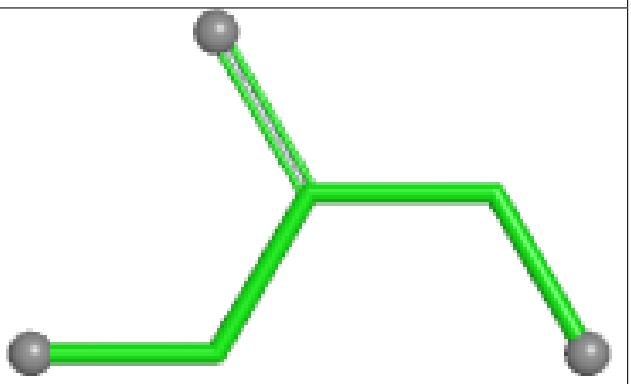
Ligand SO4 F 202	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SO4 B 201	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

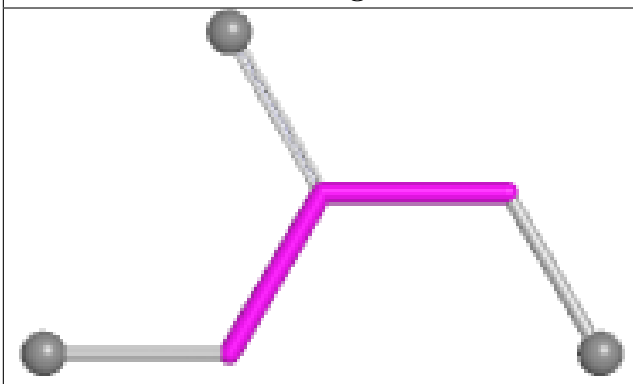
Ligand GOL G 201



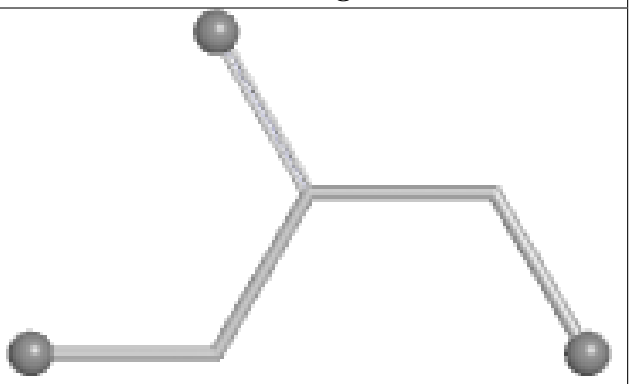
Bond lengths



Bond angles

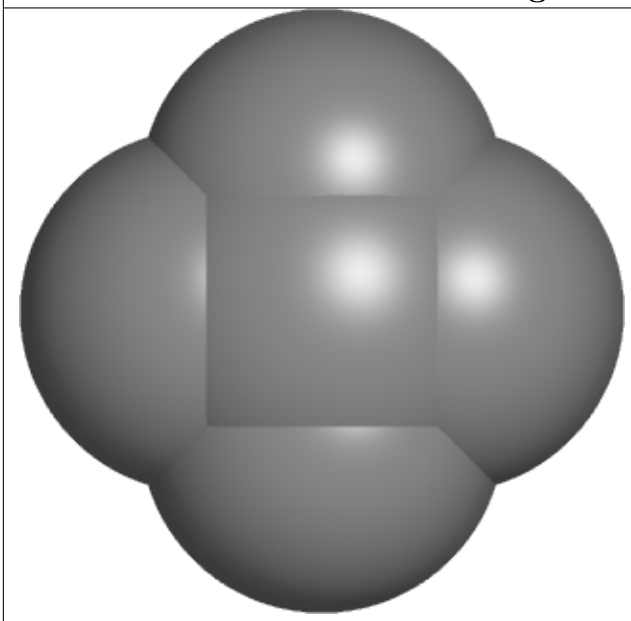


Torsions

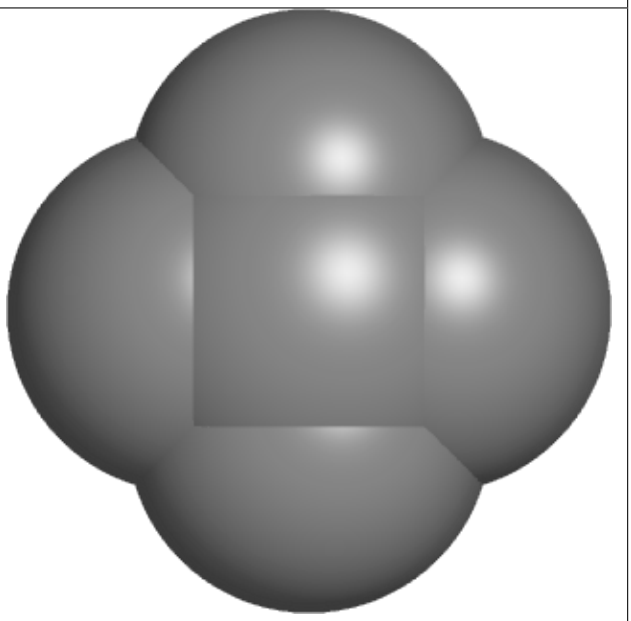


Rings

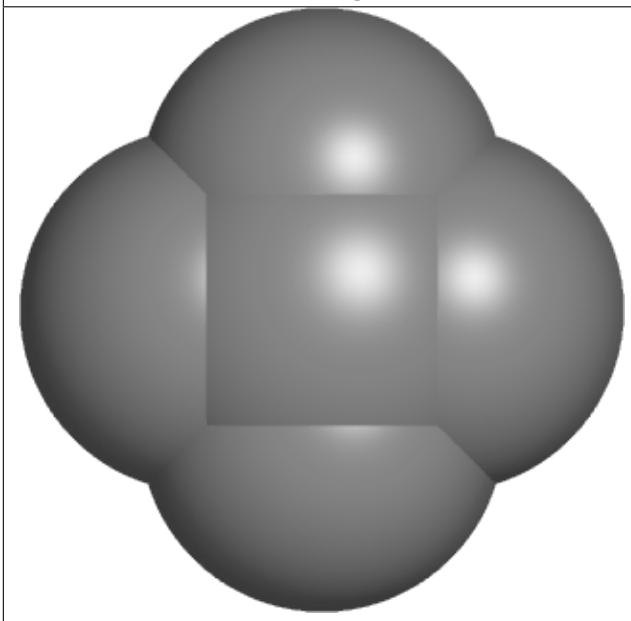
Ligand SO4 A 202



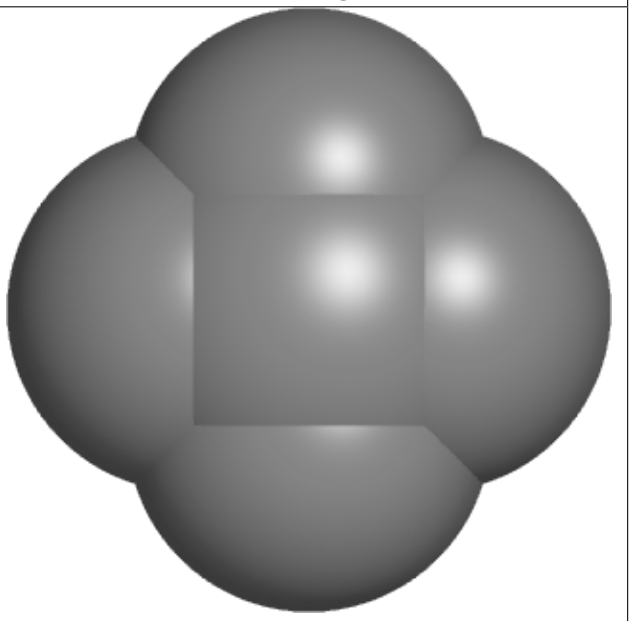
Bond lengths



Bond angles

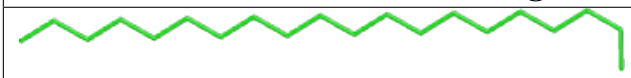


Torsions

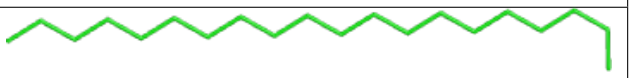


Rings

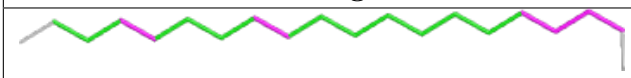
Ligand LFA D 203



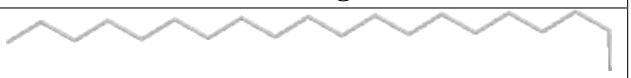
Bond lengths



Bond angles

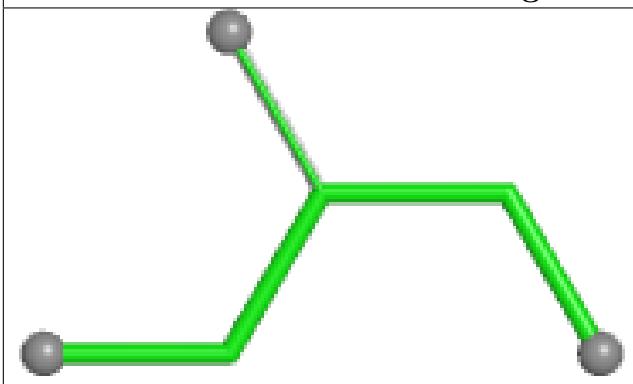


Torsions

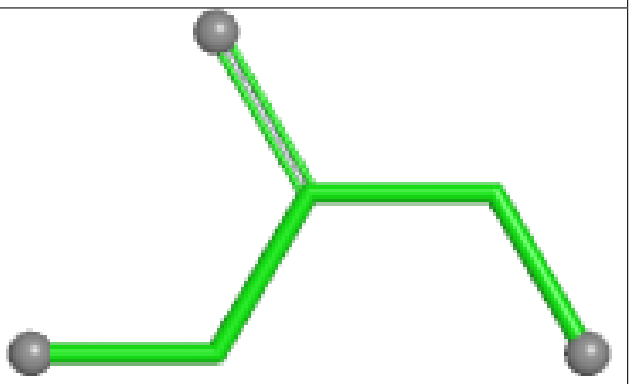


Rings

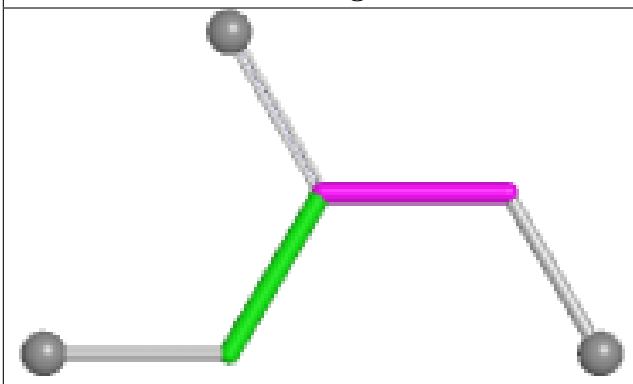
Ligand GOL H 202



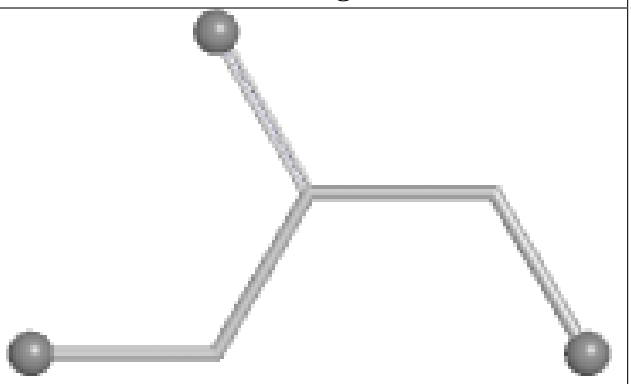
Bond lengths



Bond angles

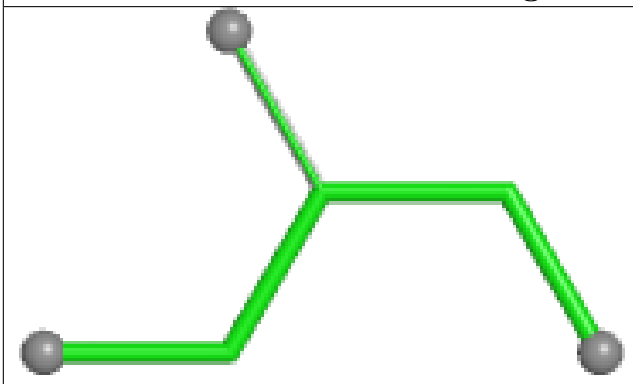


Torsions

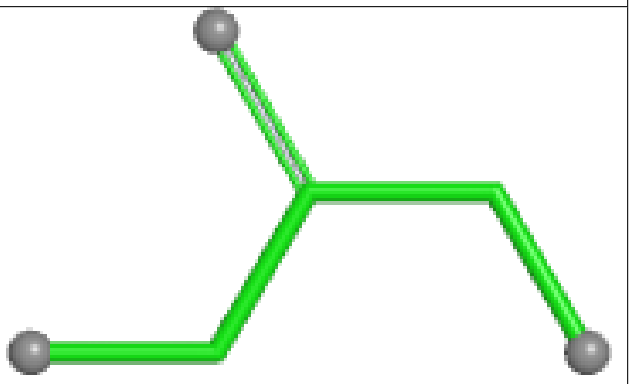


Rings

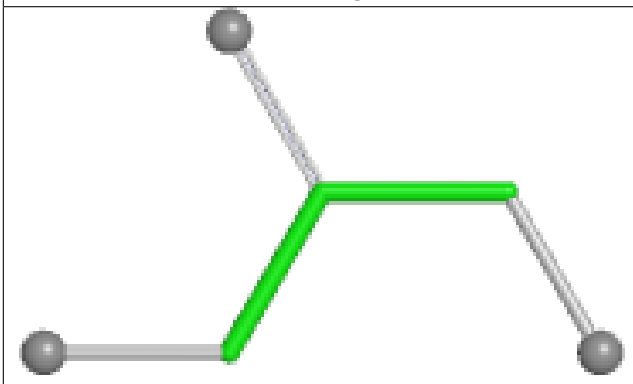
Ligand GOL D 201



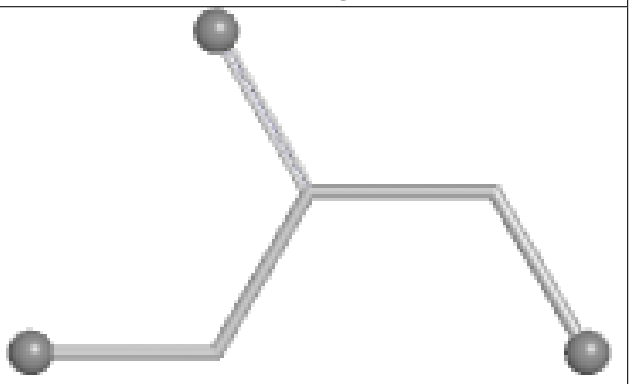
Bond lengths



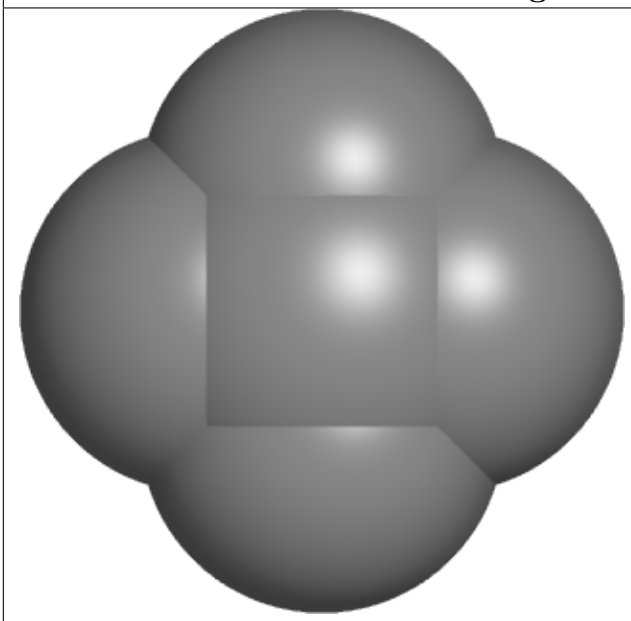
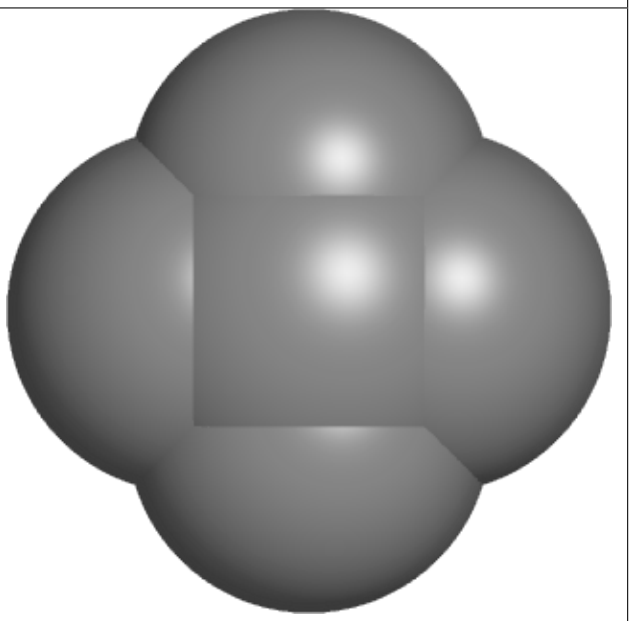
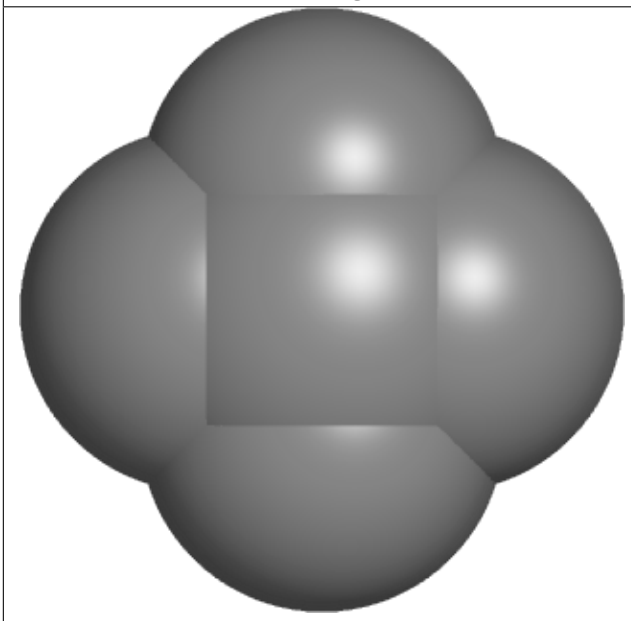
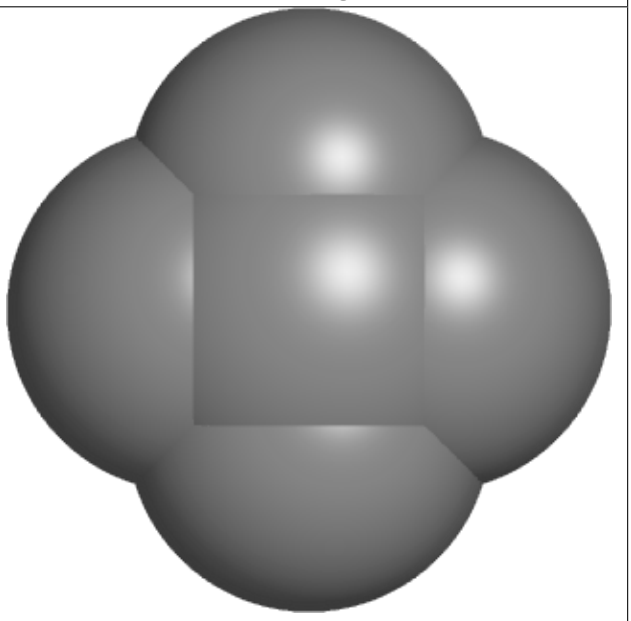
Bond angles



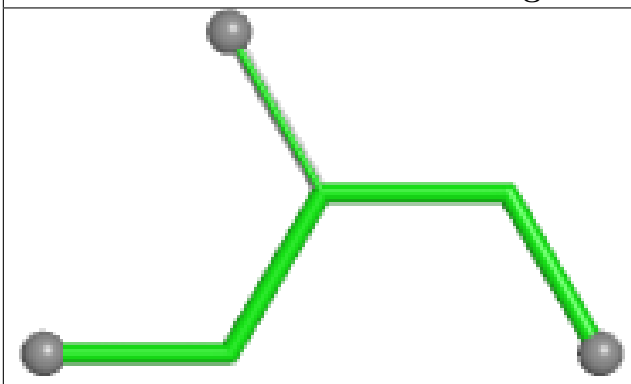
Torsions



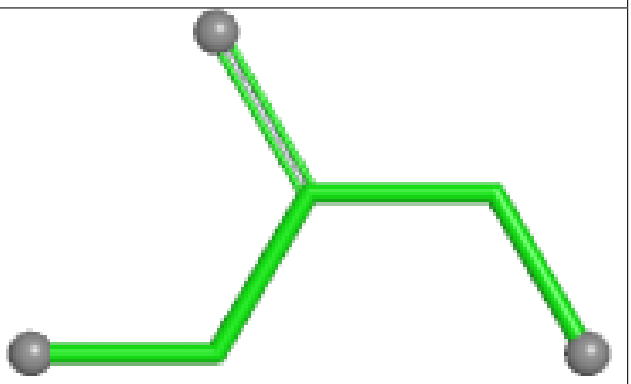
Rings

Ligand SO4 C 204	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

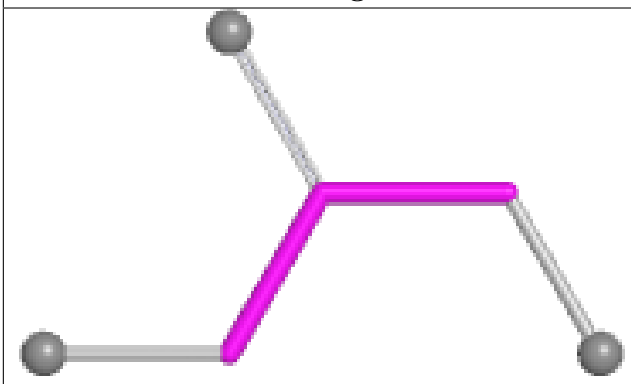
Ligand GOL C 201



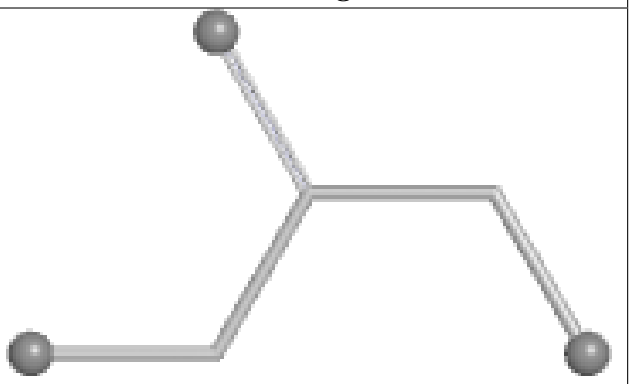
Bond lengths



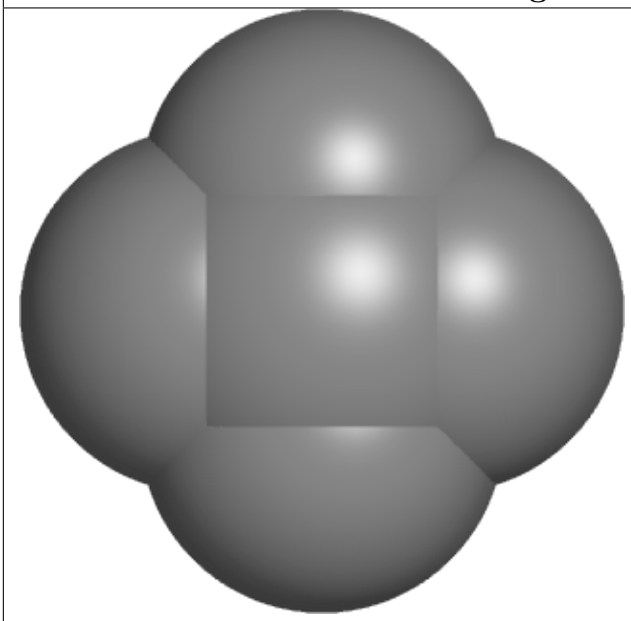
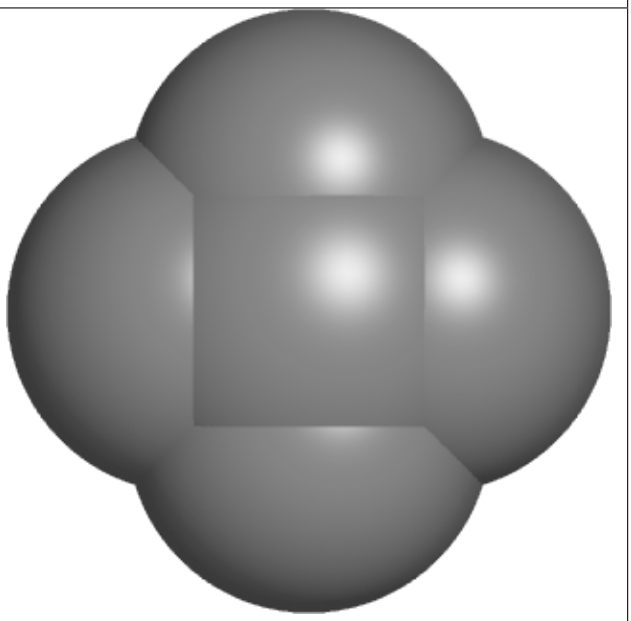
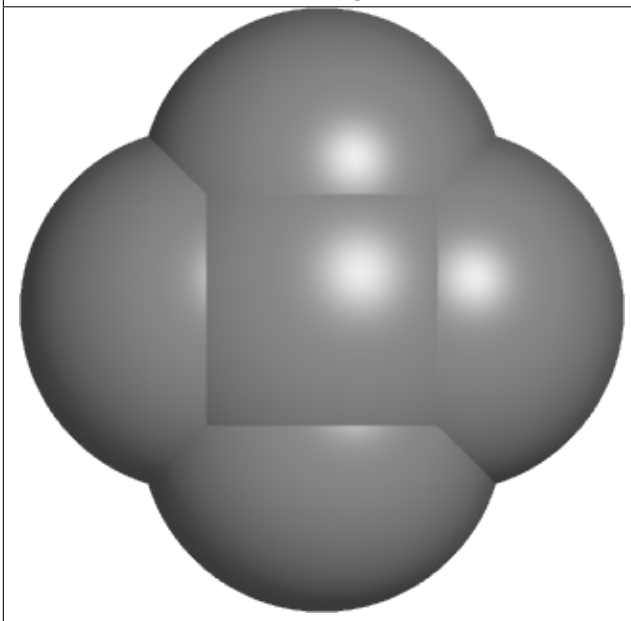
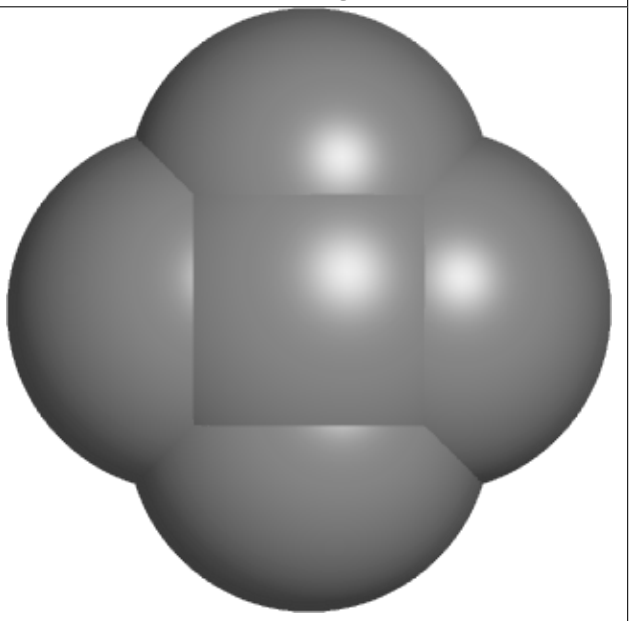
Bond angles

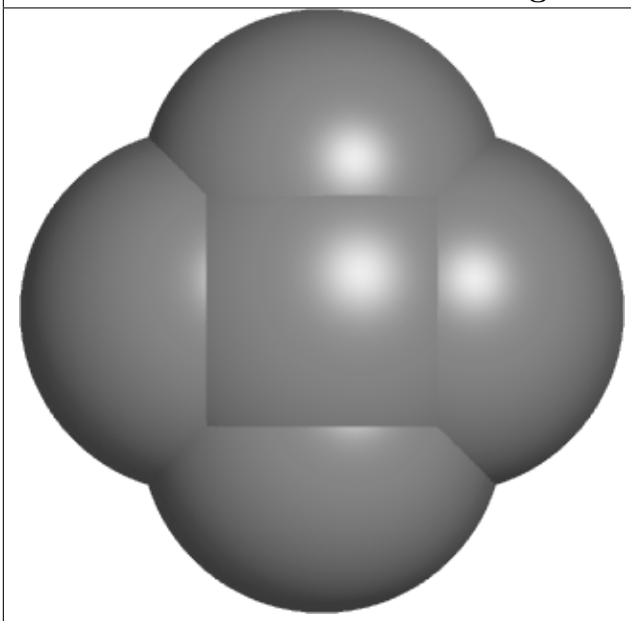
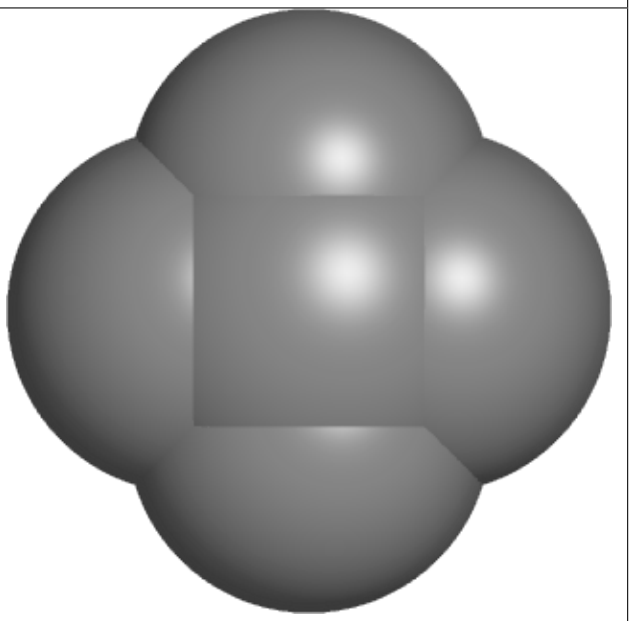
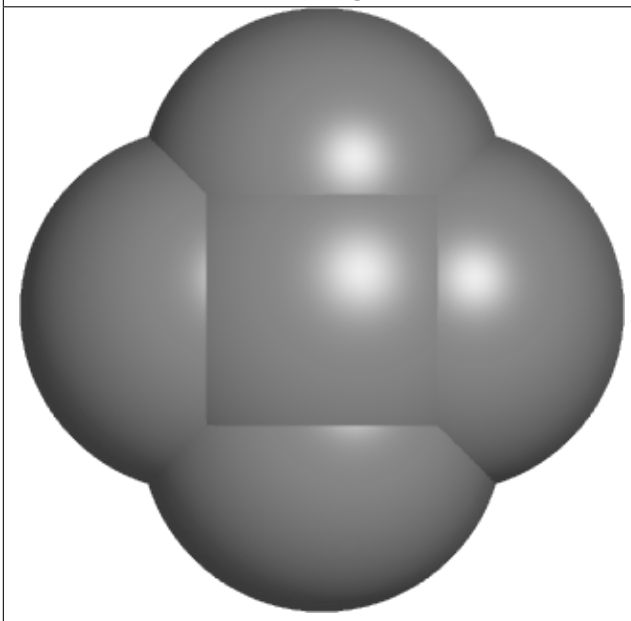
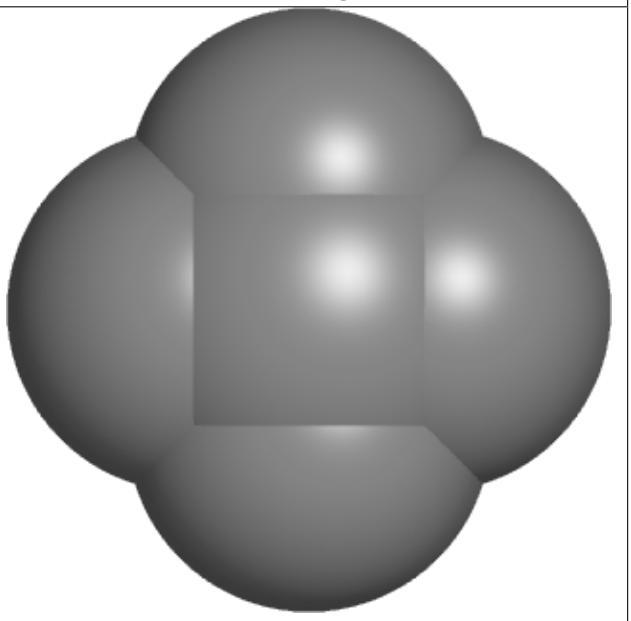


Torsions

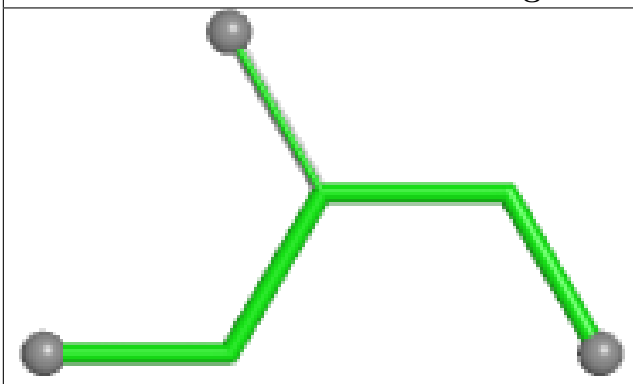


Rings

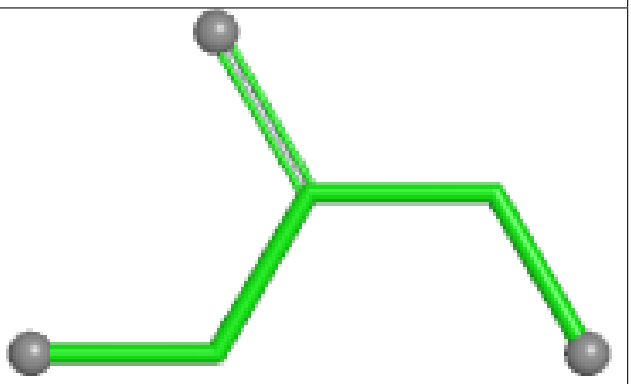
Ligand SO4 B 206	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SO4 B 203	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

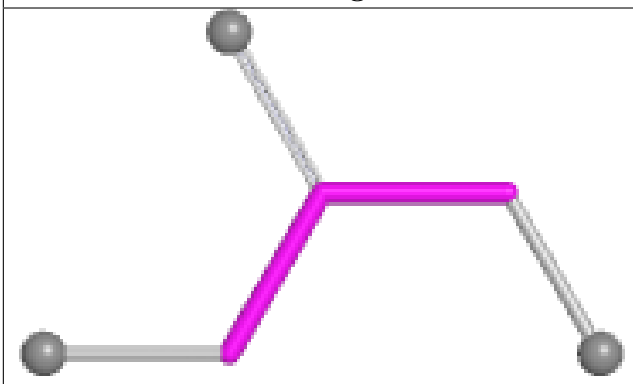
Ligand GOL B 204



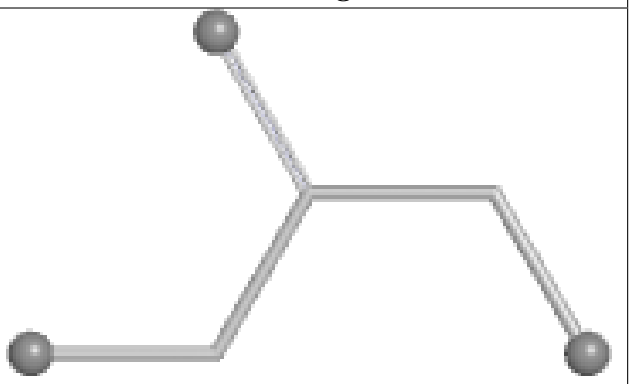
Bond lengths



Bond angles

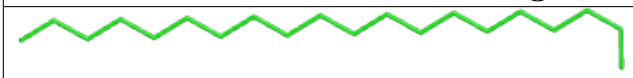


Torsions

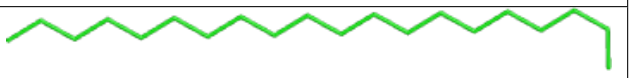


Rings

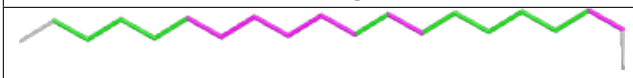
Ligand LFA E 203



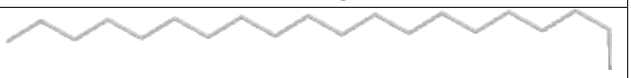
Bond lengths



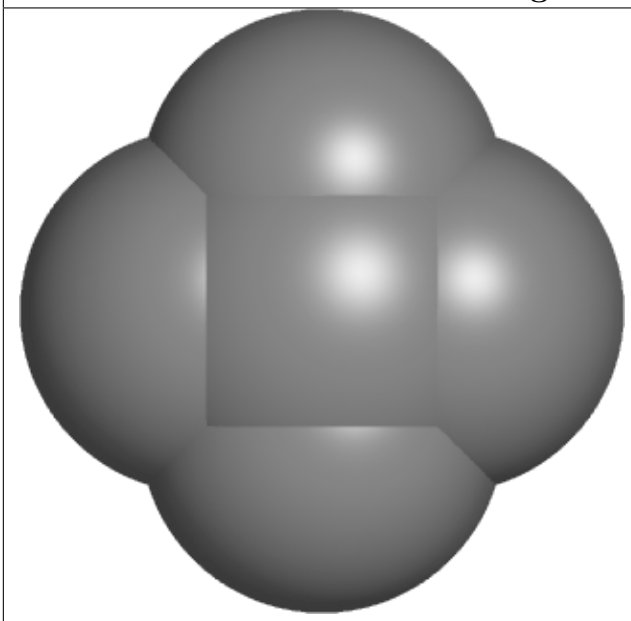
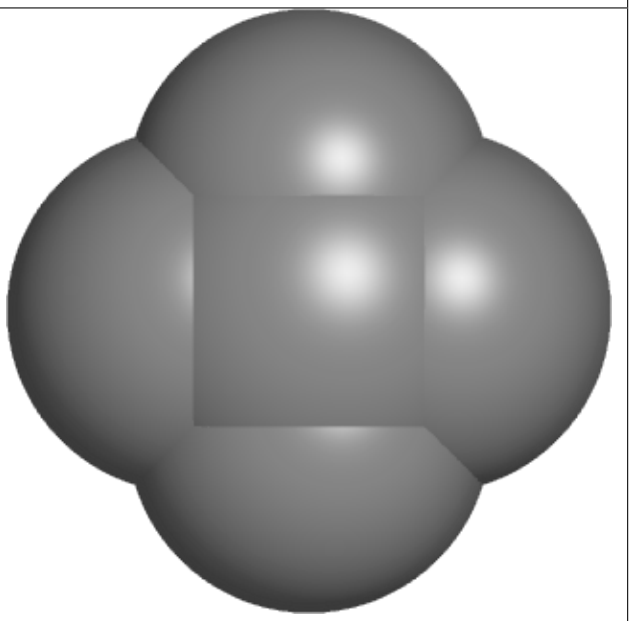
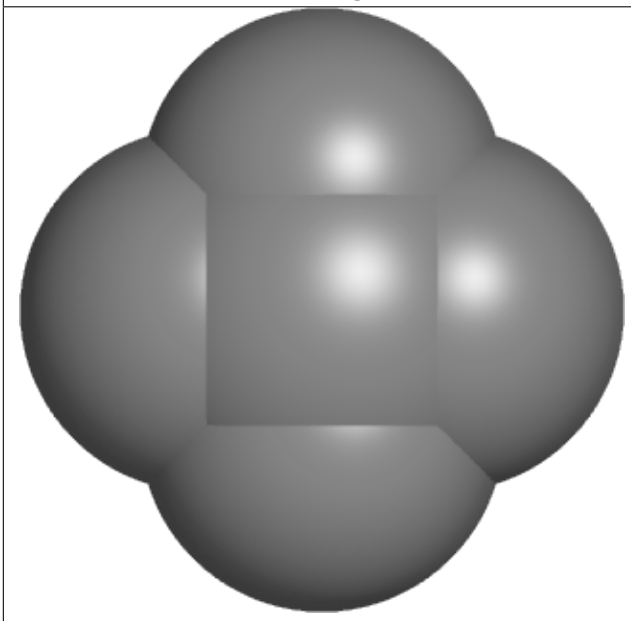
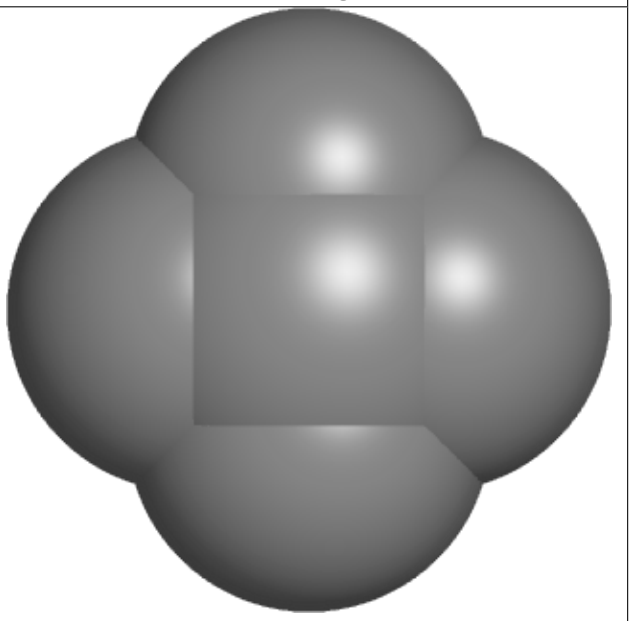
Bond angles

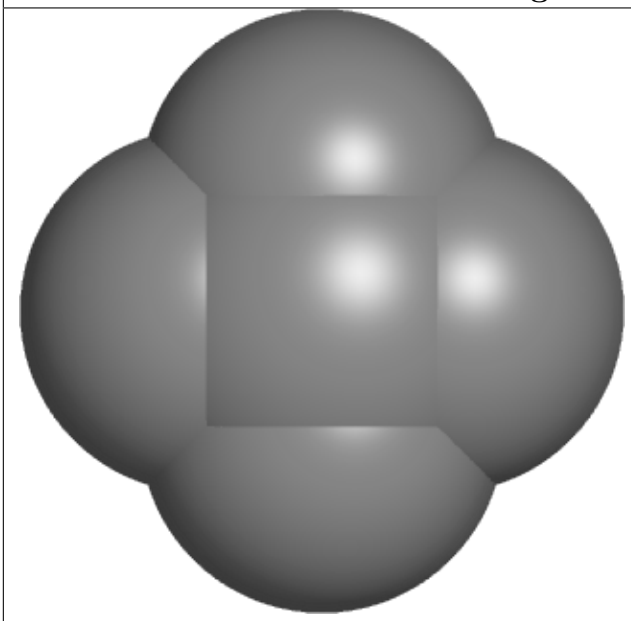
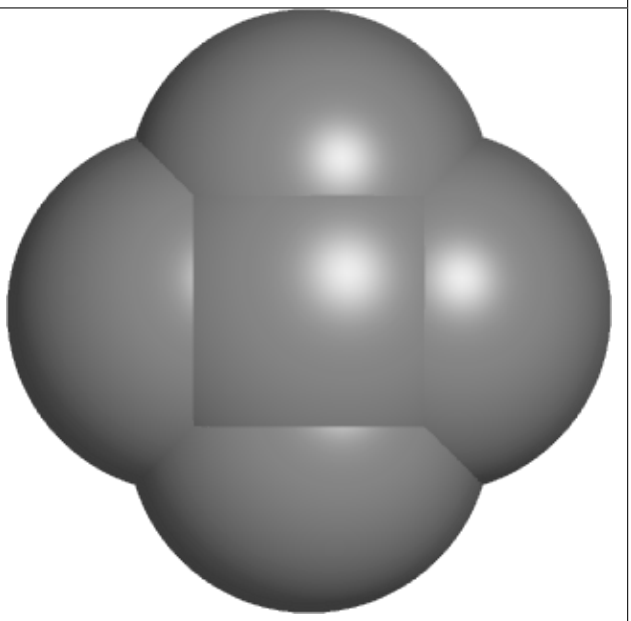
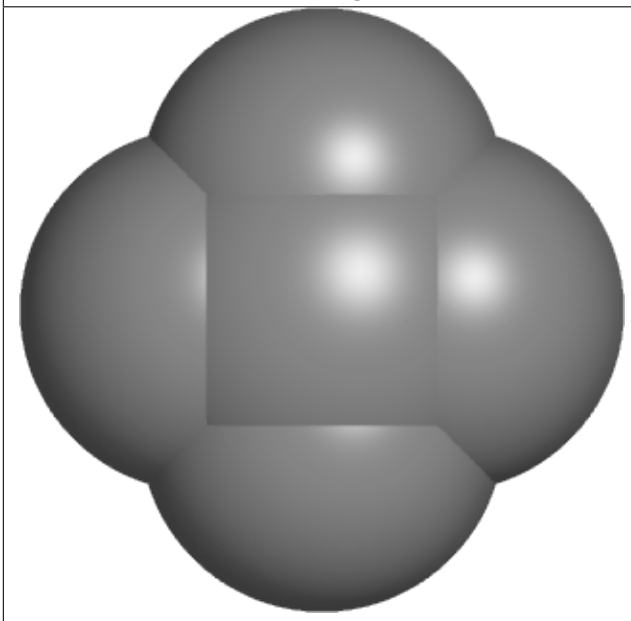
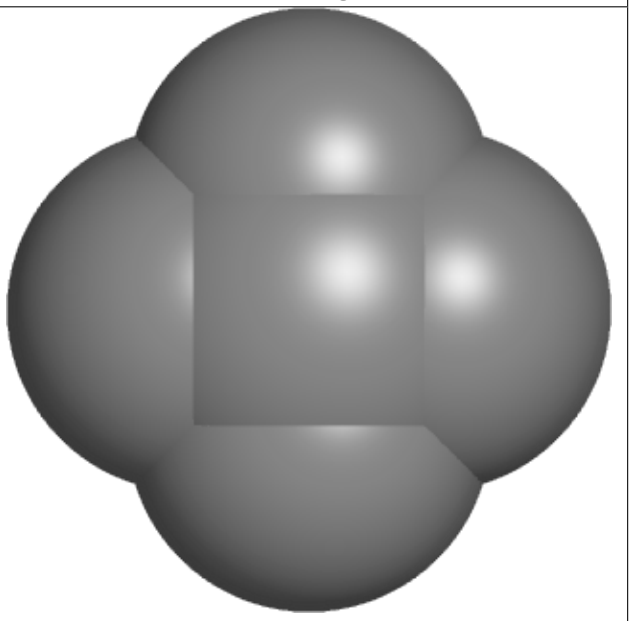


Torsions

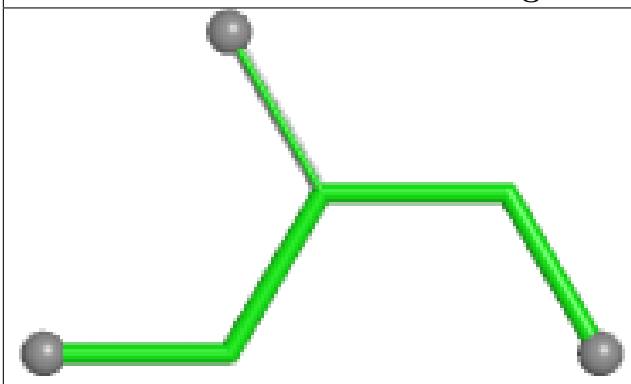


Rings

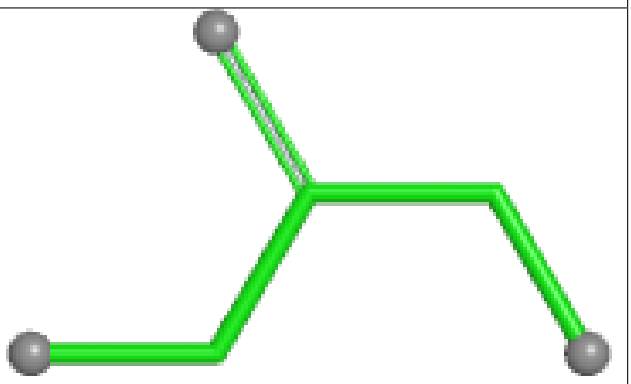
Ligand SO4 E 201	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SO4 F 201	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

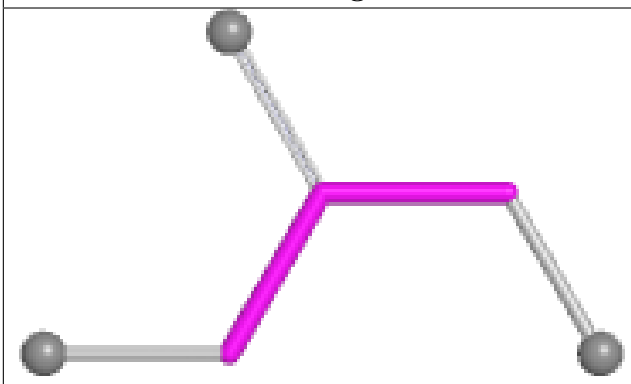
Ligand GOL D 202



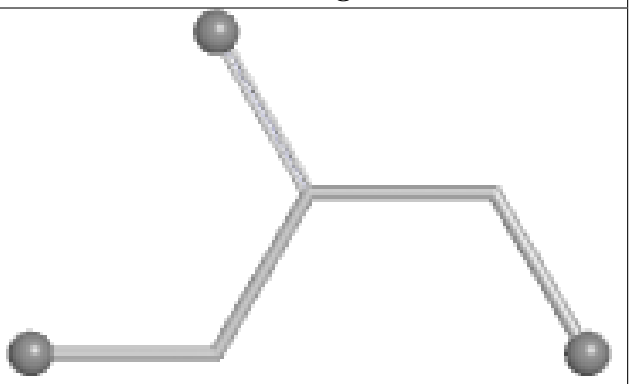
Bond lengths



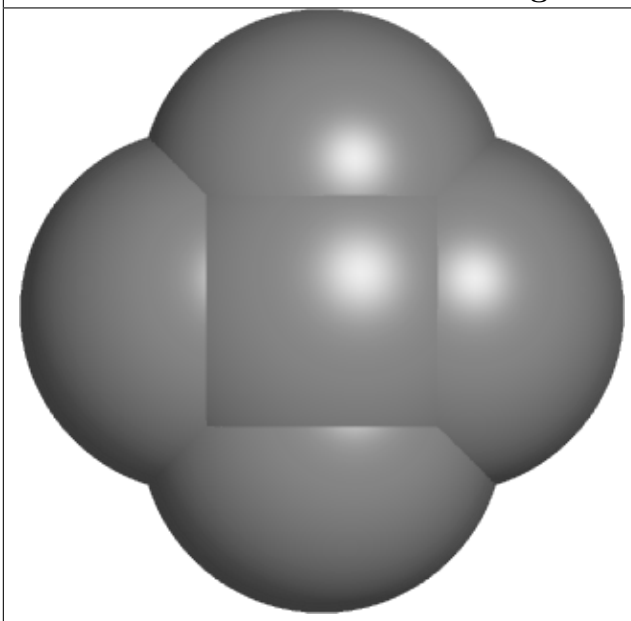
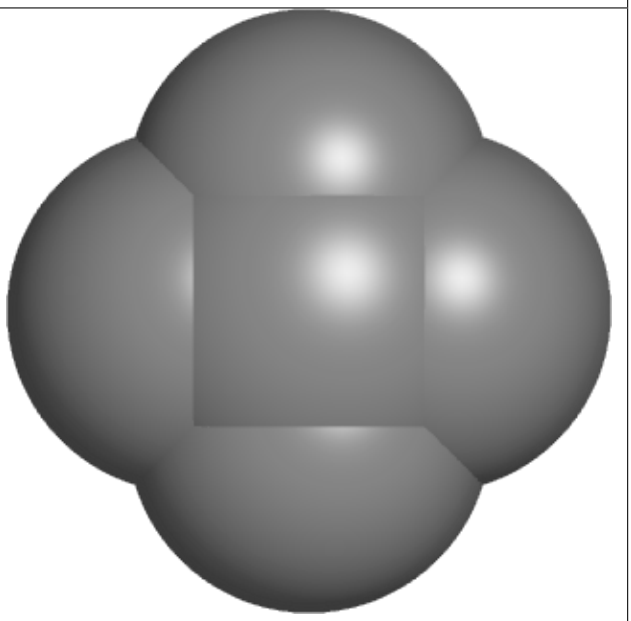
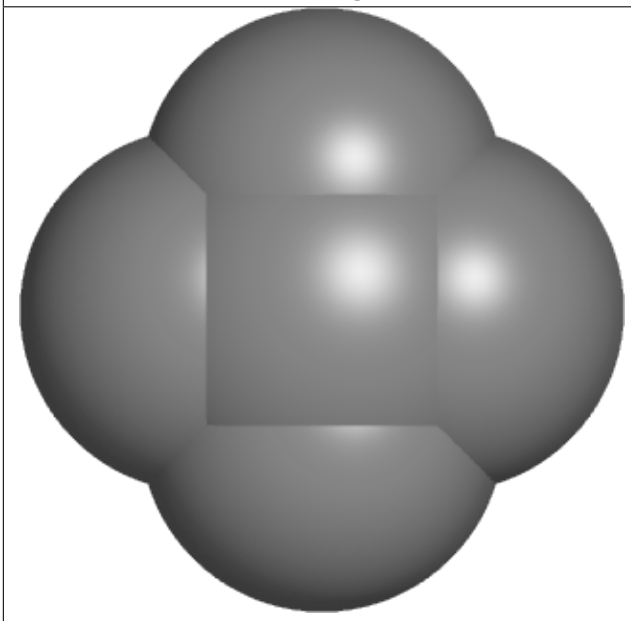
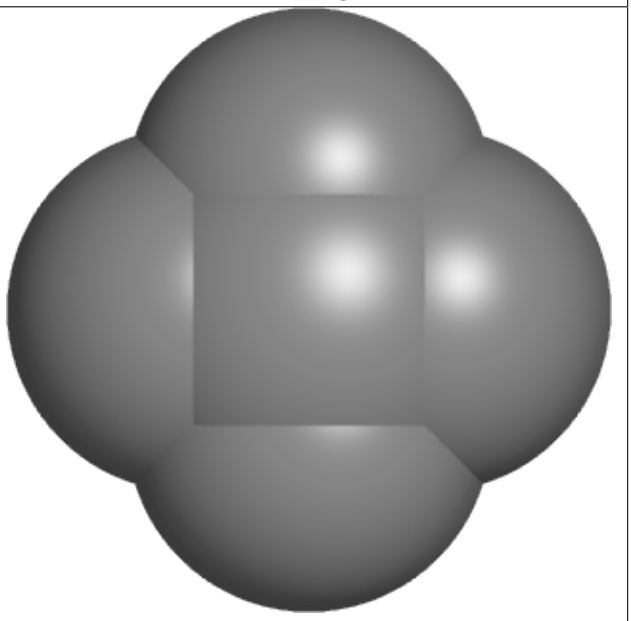
Bond angles

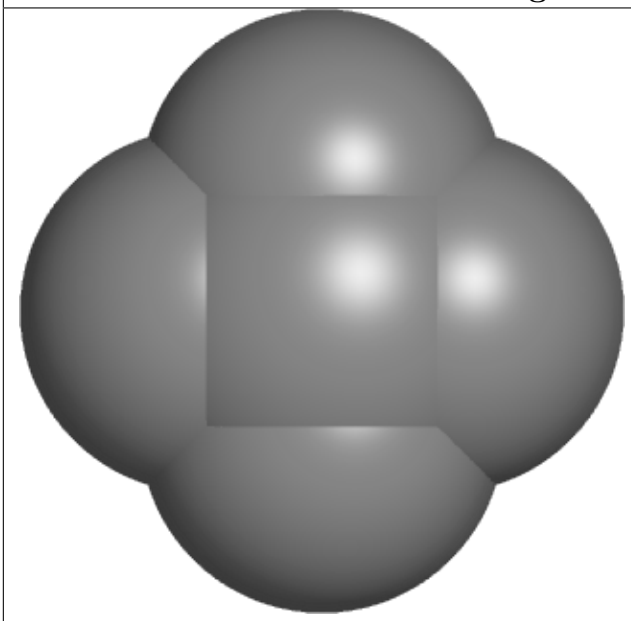
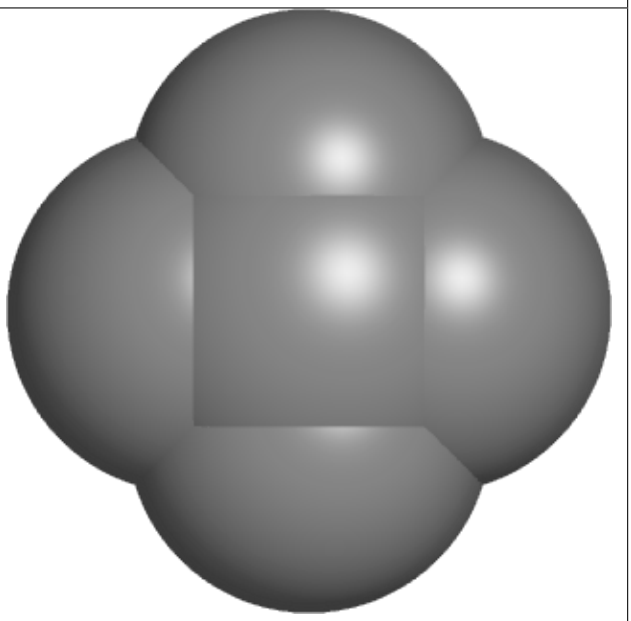
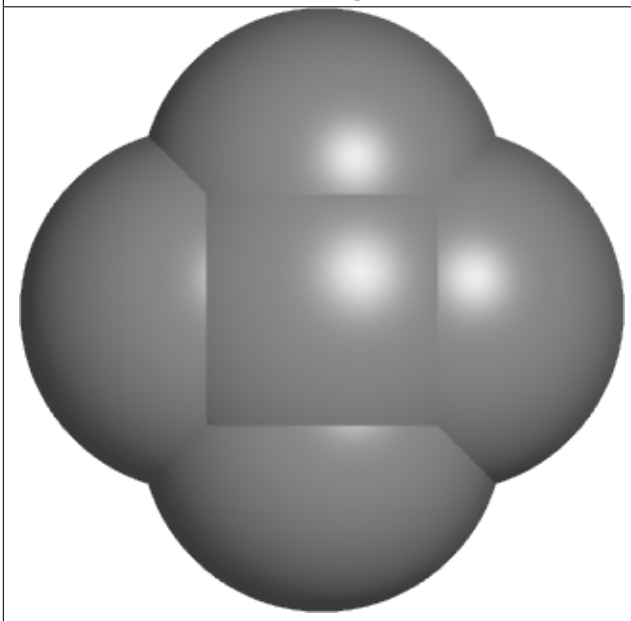
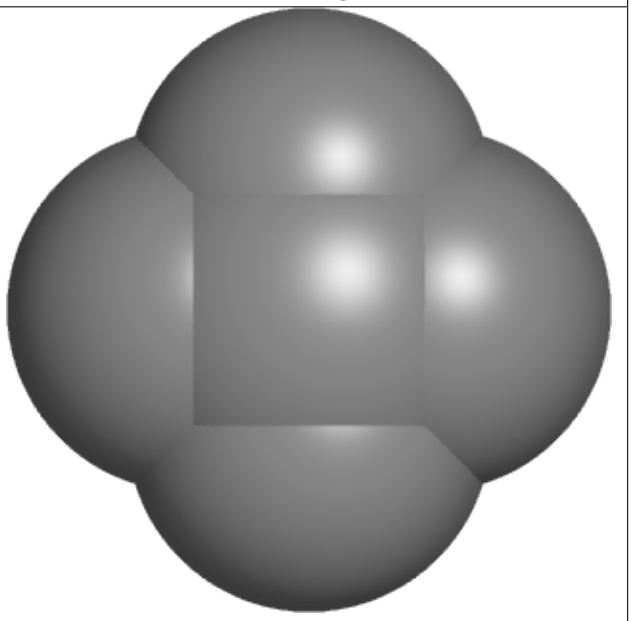


Torsions



Rings

Ligand SO4 E 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SO4 C 203	
 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	164/164 (100%)	0.26	1 (0%)	89	88	33, 43, 64, 102	0
1	B	164/164 (100%)	0.01	4 (2%)	59	57	33, 43, 66, 88	0
1	C	164/164 (100%)	0.04	5 (3%)	50	49	36, 47, 69, 91	0
1	D	164/164 (100%)	-0.01	3 (1%)	68	66	37, 47, 66, 95	0
1	E	164/164 (100%)	0.10	2 (1%)	79	78	35, 47, 65, 99	0
1	F	164/164 (100%)	0.40	13 (7%)	12	11	34, 54, 85, 101	0
1	G	164/164 (100%)	0.11	4 (2%)	59	57	41, 52, 79, 103	0
1	H	164/164 (100%)	0.21	10 (6%)	21	20	40, 55, 87, 105	0
All	All	1312/1312 (100%)	0.14	42 (3%)	47	46	33, 49, 75, 105	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	7.4
1	H	154	PHE	5.3
1	F	154	PHE	4.6
1	F	159	TYR	4.5
1	H	151	SER	4.3
1	H	1	MET	4.1
1	H	155[A]	GLN	4.0
1	D	1	MET	3.3
1	H	158	ARG	3.3
1	F	143	LEU	3.1
1	E	1	MET	3.0
1	G	162	GLN	3.0
1	F	158	ARG	3.0
1	C	159	TYR	3.0
1	H	152	VAL	3.0
1	H	150	MET	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	159	TYR	2.9
1	H	162	GLN	2.8
1	H	159	TYR	2.8
1	F	152	VAL	2.7
1	C	156	LEU	2.7
1	B	1	MET	2.7
1	F	162	GLN	2.6
1	C	1	MET	2.6
1	C	164	GLU	2.5
1	F	155[A]	GLN	2.5
1	F	142	LEU	2.4
1	G	158	ARG	2.4
1	F	41	PHE	2.4
1	F	146	ALA	2.3
1	B	155	GLN	2.3
1	F	164	GLU	2.3
1	F	148	GLY	2.3
1	F	151	SER	2.3
1	B	156	LEU	2.2
1	D	154	PHE	2.2
1	D	164	GLU	2.2
1	C	162	GLN	2.1
1	H	164	GLU	2.1
1	B	131[A]	GLU	2.1
1	G	155	GLN	2.0
1	G	164	GLU	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)

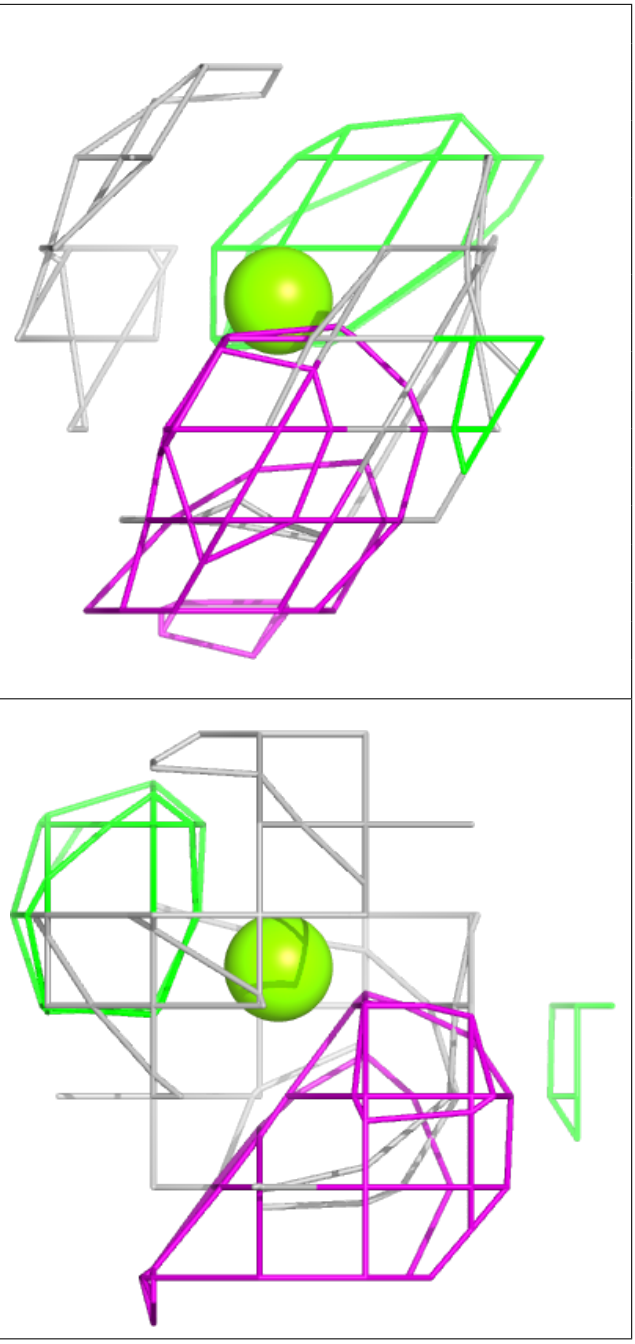
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	E	205	1/1	0.38	0.12	63,63,63,63	0
3	SO4	C	203	5/5	0.59	0.59	118,120,153,153	0
3	SO4	F	201	5/5	0.66	0.29	82,107,124,167	0
2	GOL	A	201	6/6	0.69	0.17	67,81,97,97	0
3	SO4	B	201	5/5	0.71	0.33	109,117,178,199	0
2	GOL	C	201	6/6	0.72	0.16	70,80,96,96	0
3	SO4	D	204	5/5	0.75	0.25	77,99,115,121	0
2	GOL	D	202	6/6	0.76	0.19	67,83,87,90	0
2	GOL	B	204	6/6	0.76	0.28	66,80,96,96	0
2	GOL	D	201	6/6	0.76	0.32	72,86,96,98	0
3	SO4	C	204	5/5	0.77	0.43	98,98,102,117	0
2	GOL	H	202	6/6	0.78	0.28	81,91,117,117	0
4	MG	G	203	1/1	0.79	0.06	58,58,58,58	0
5	LFA	G	202	20/20	0.79	0.30	46,69,95,105	0
3	SO4	B	206	5/5	0.80	0.41	76,87,95,110	0
2	GOL	C	202	6/6	0.82	0.24	57,74,79,89	0
4	MG	F	203	1/1	0.83	0.16	57,57,57,57	0
2	GOL	G	201	6/6	0.83	0.18	54,71,89,89	0
3	SO4	E	204	5/5	0.83	0.23	107,111,144,214	0
3	SO4	E	201	5/5	0.84	0.25	69,89,127,158	0
4	MG	H	203	1/1	0.88	0.26	30,30,30,30	0
4	MG	C	205	1/1	0.88	0.09	60,60,60,60	0
3	SO4	A	202	5/5	0.89	0.22	73,85,100,116	0
3	SO4	F	202	5/5	0.89	0.34	90,95,108,111	0
5	LFA	D	203	20/20	0.89	0.18	45,63,88,89	0
3	SO4	H	201	5/5	0.89	0.16	82,85,98,121	0
4	MG	D	205	1/1	0.90	0.08	58,58,58,58	0
5	LFA	B	205	20/20	0.90	0.17	40,61,87,98	0
5	LFA	E	203	20/20	0.91	0.18	41,65,85,90	0
2	GOL	E	202	6/6	0.92	0.19	63,69,85,87	0
2	GOL	B	202	6/6	0.94	0.11	52,62,63,65	0
4	MG	A	203	1/1	0.94	0.08	56,56,56,56	0
3	SO4	B	203	5/5	0.96	0.39	80,83,91,92	0
4	MG	B	207	1/1	0.97	0.09	47,47,47,47	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.

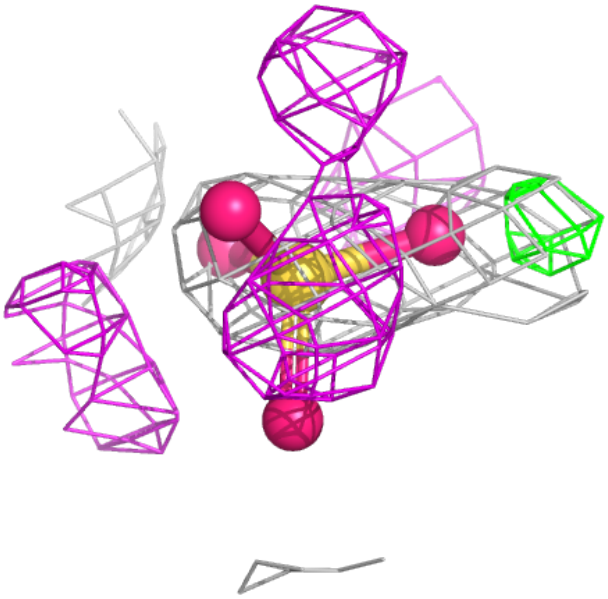
Electron density around MG E 205:

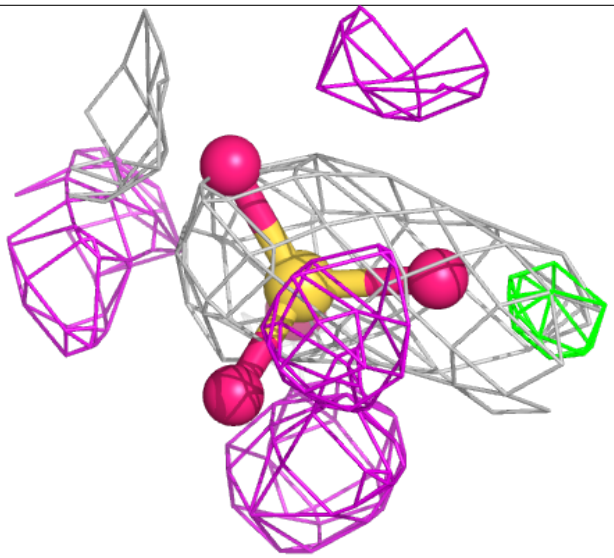
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

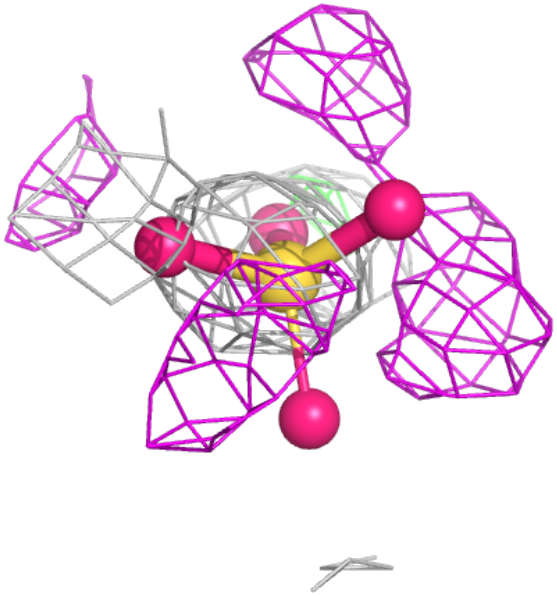


Electron density around SO4 C 203:

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

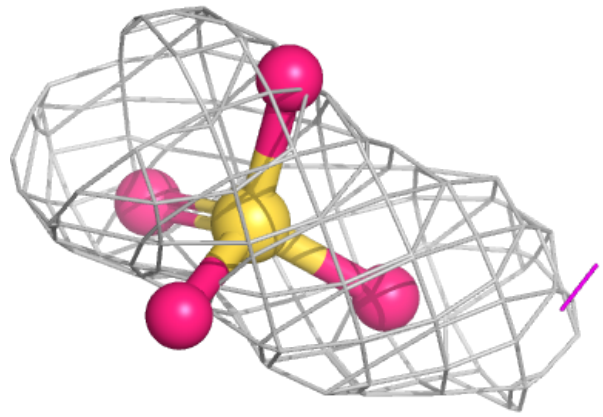


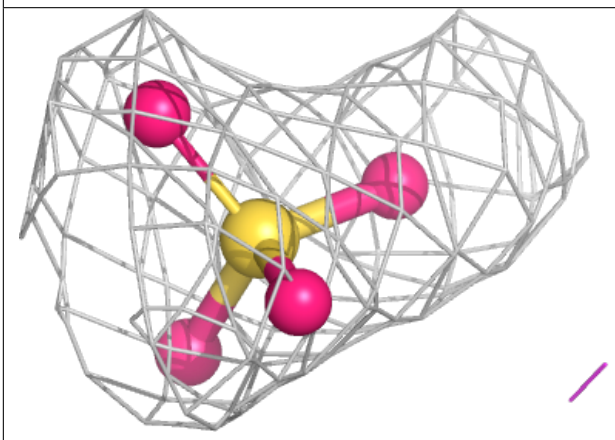


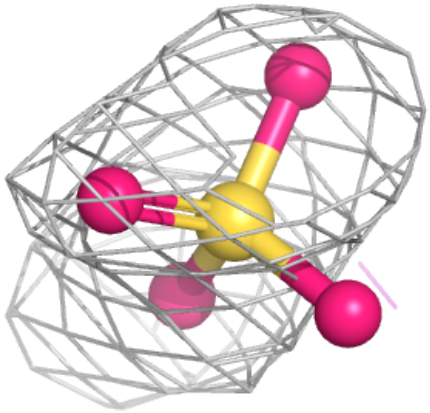


Electron density around SO4 F 201:

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

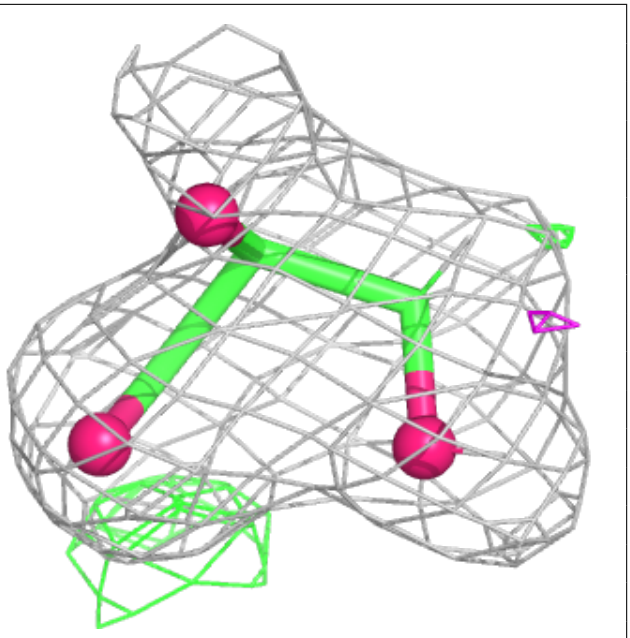


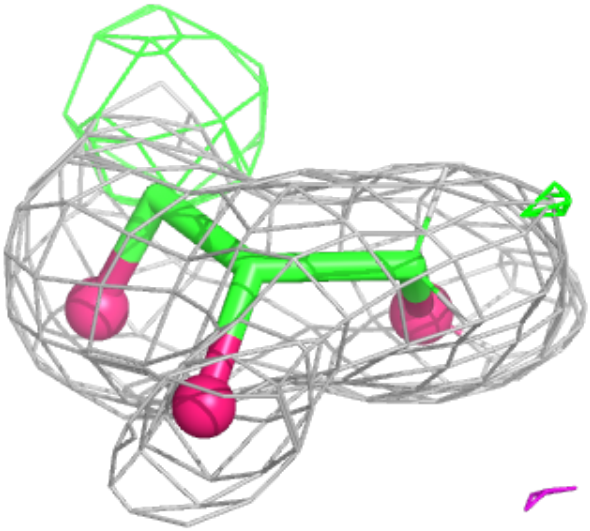


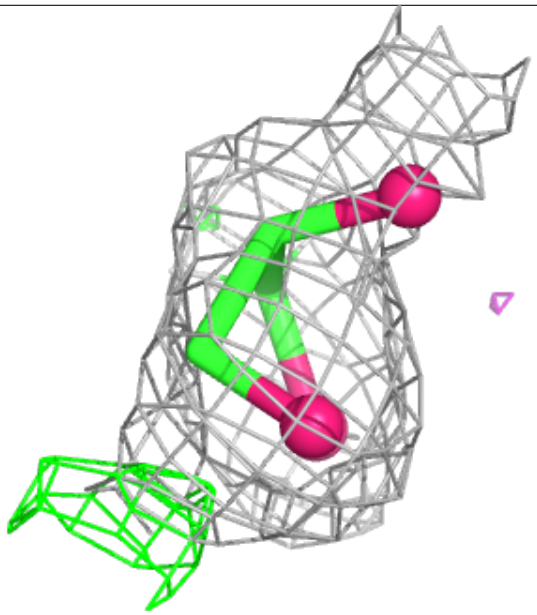


Electron density around GOL A 201:

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

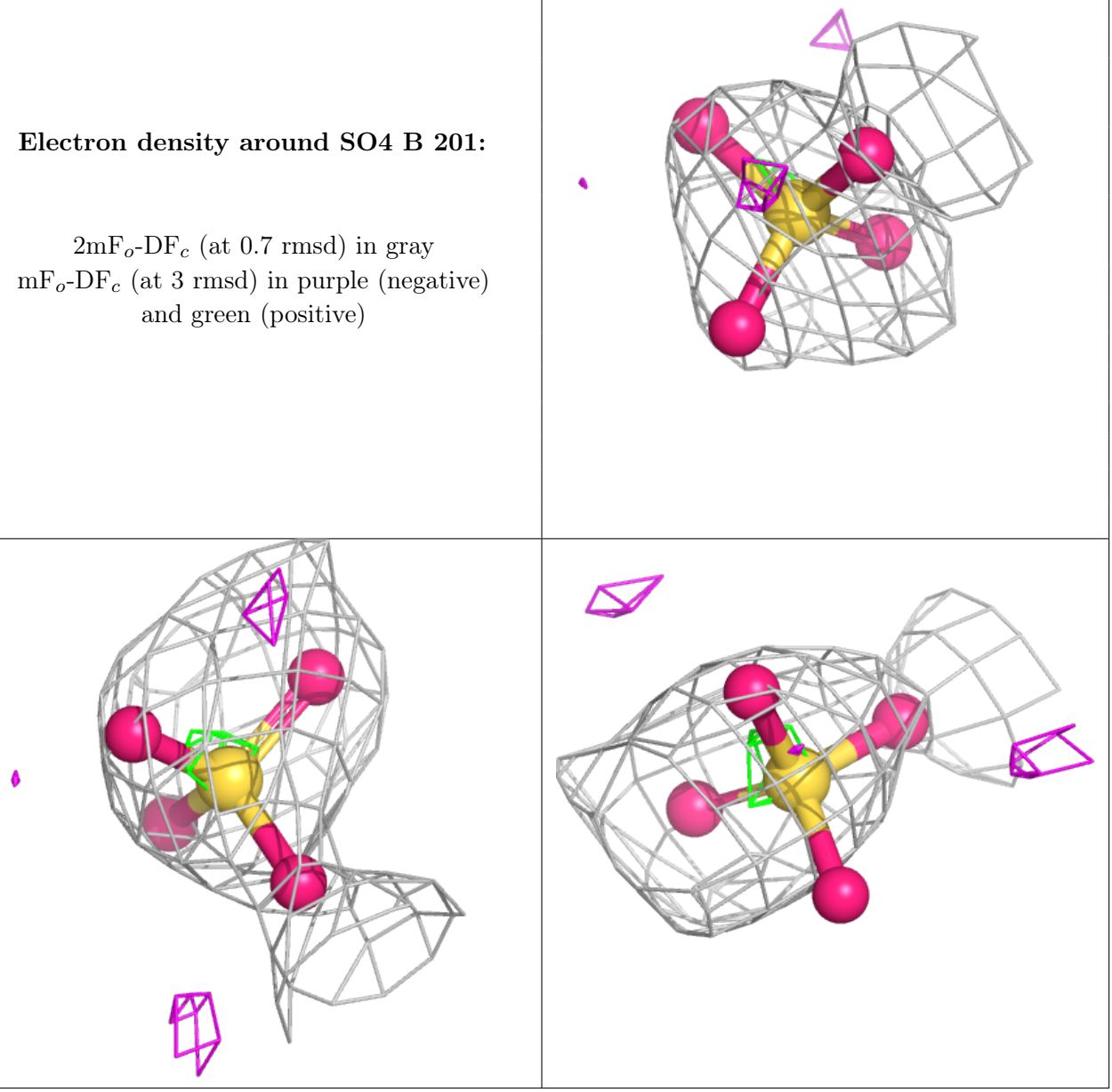






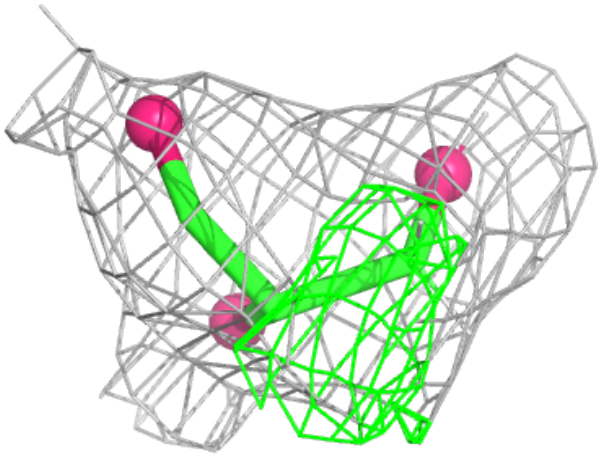
Electron density around SO4 B 201:

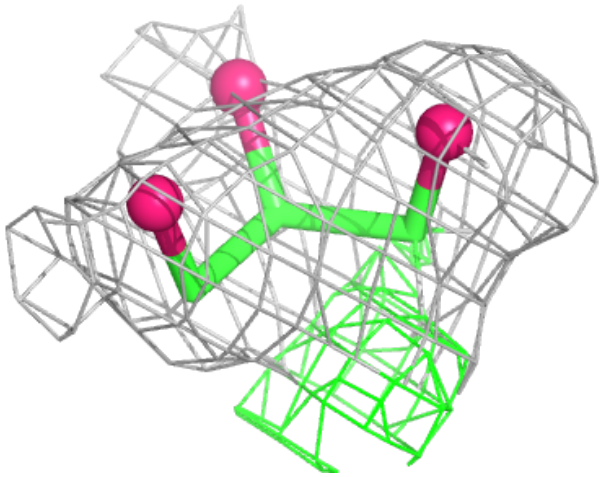
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

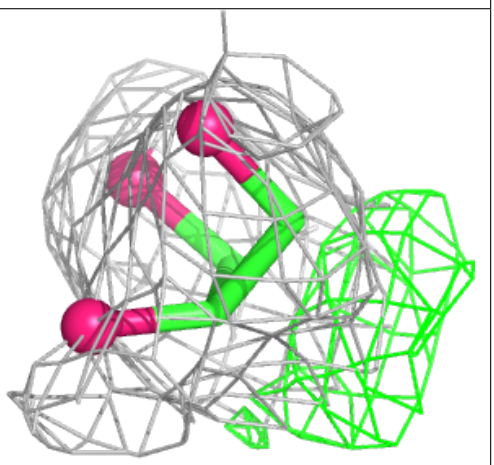


Electron density around GOL C 201:

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

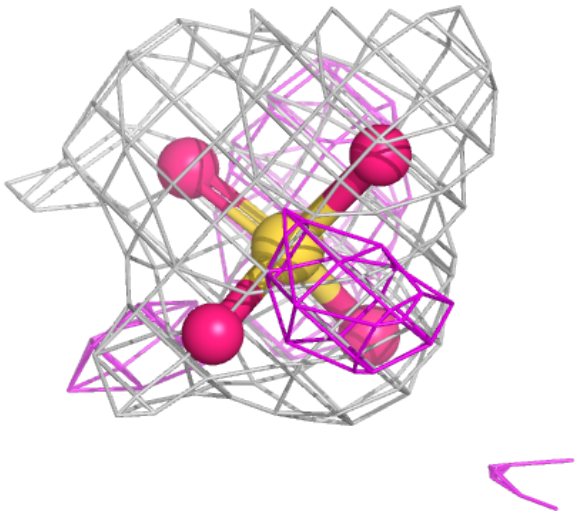


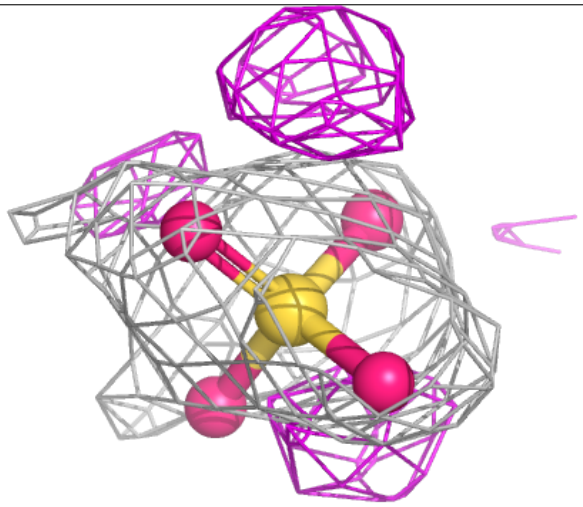


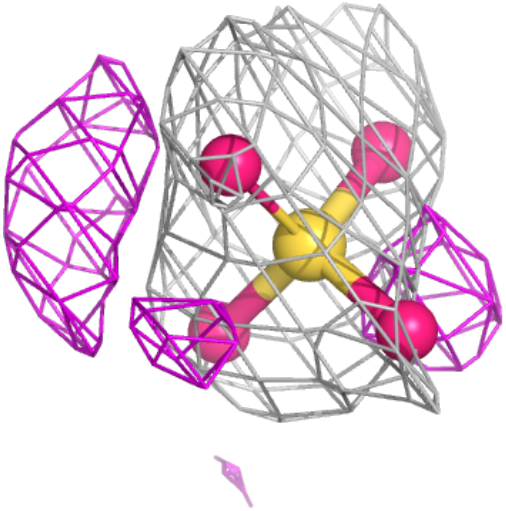


Electron density around SO4 D 204:

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

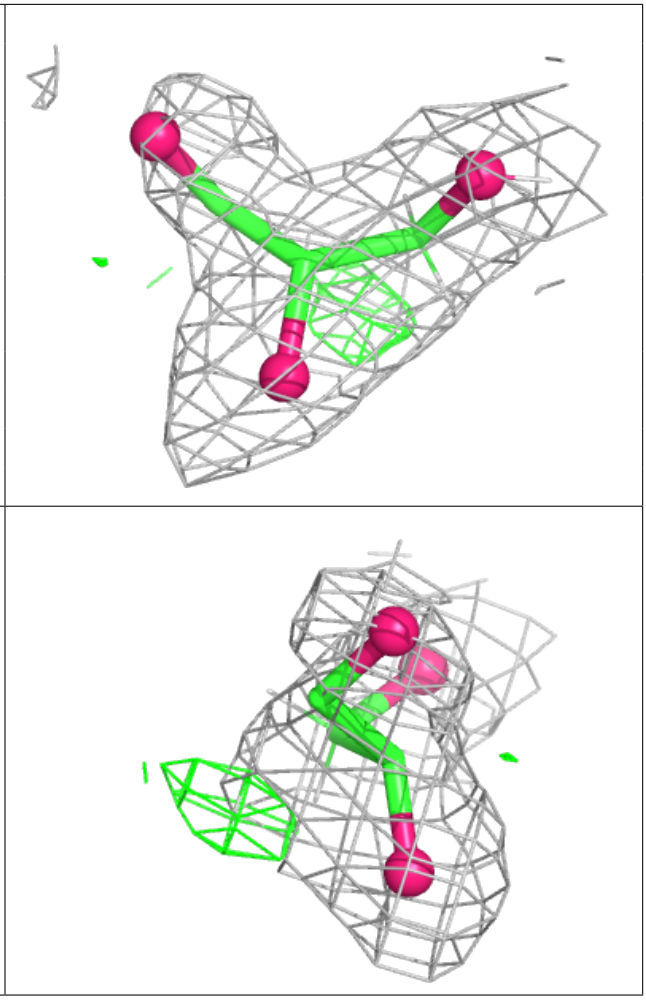






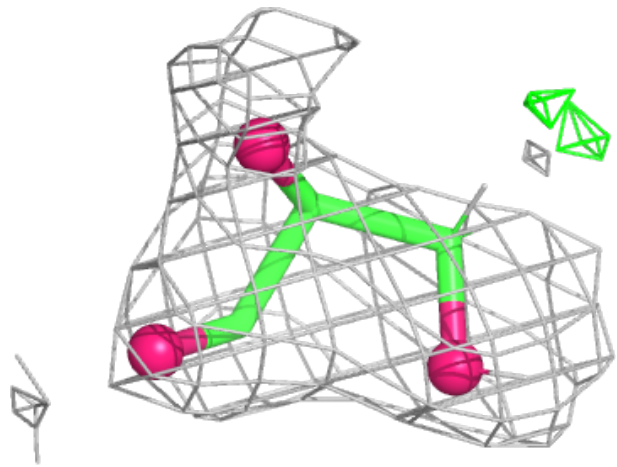
Electron density around GOL D 202:

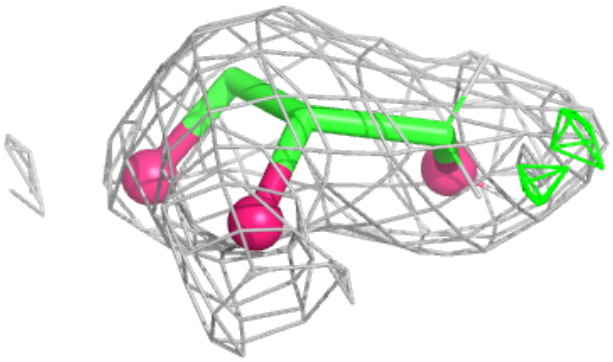
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

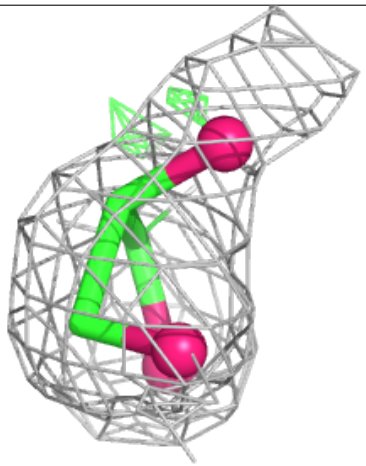


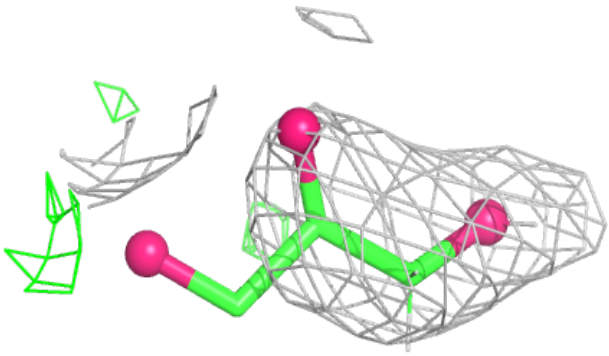
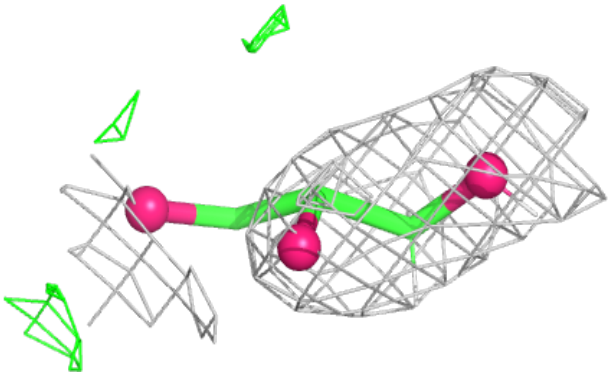
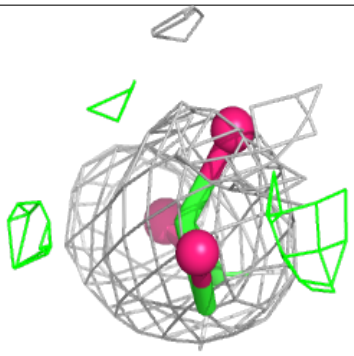
Electron density around GOL B 204:

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



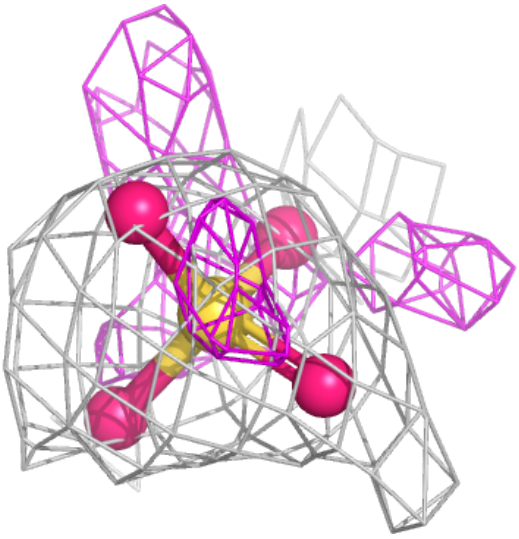


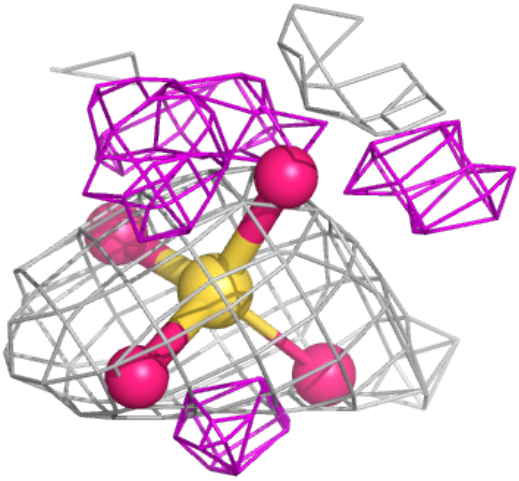


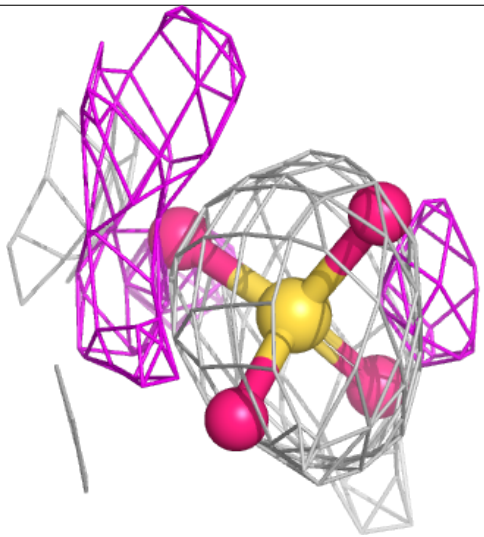
Electron density around GOL D 201: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around SO4 C 204:

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

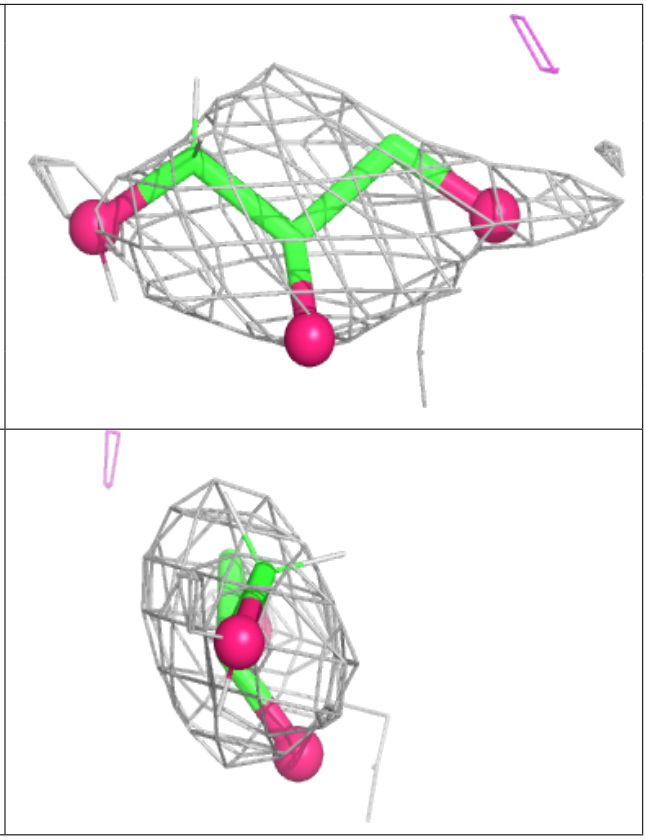


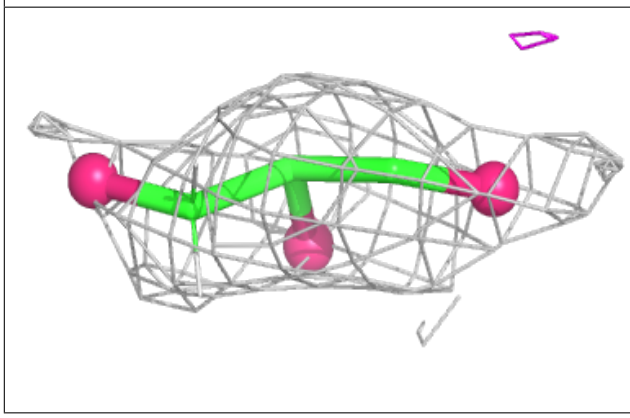




Electron density around GOL H 202:

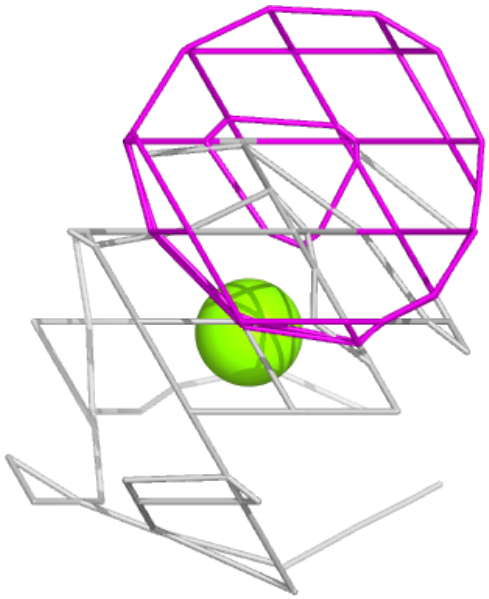
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

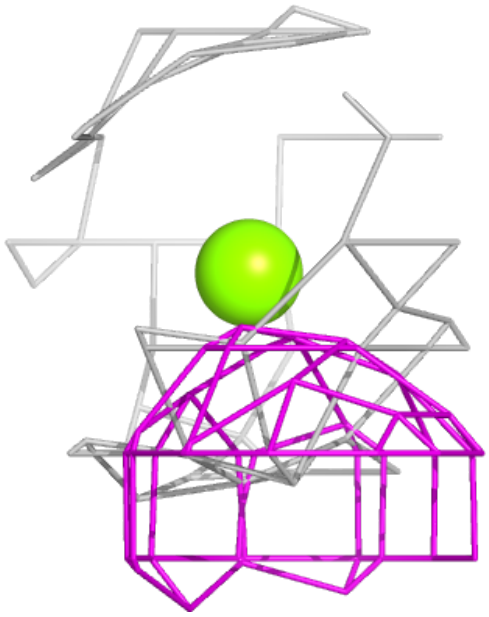


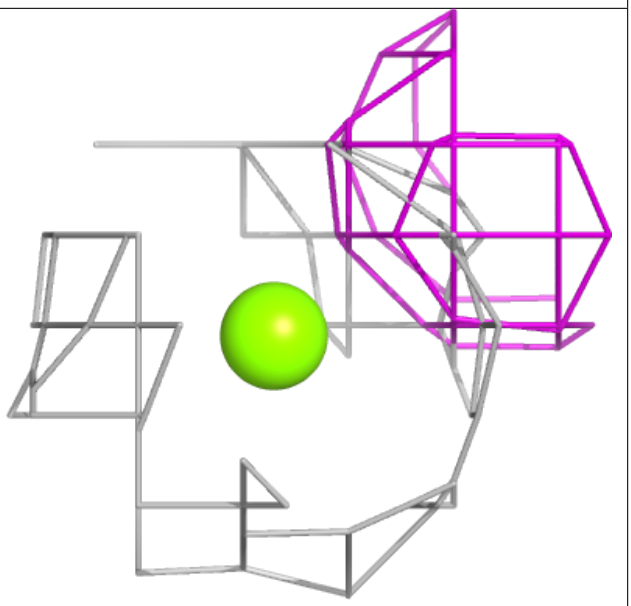


Electron density around MG G 203:

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

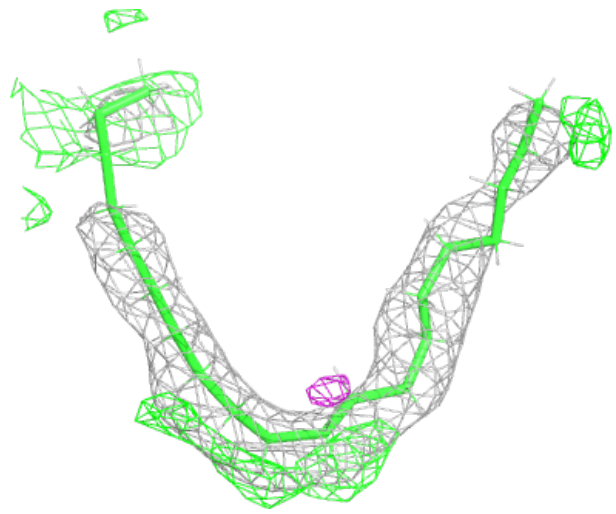


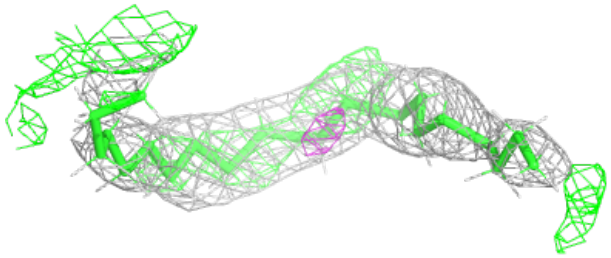




Electron density around LFA G 202:

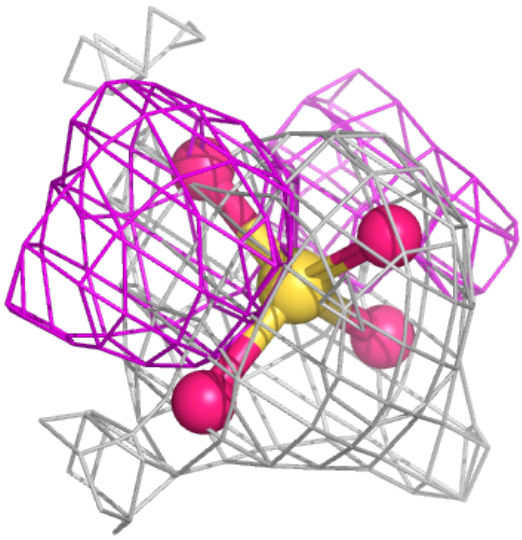
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

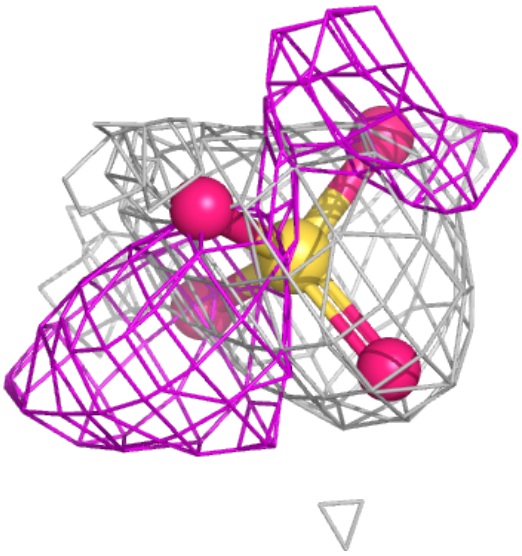


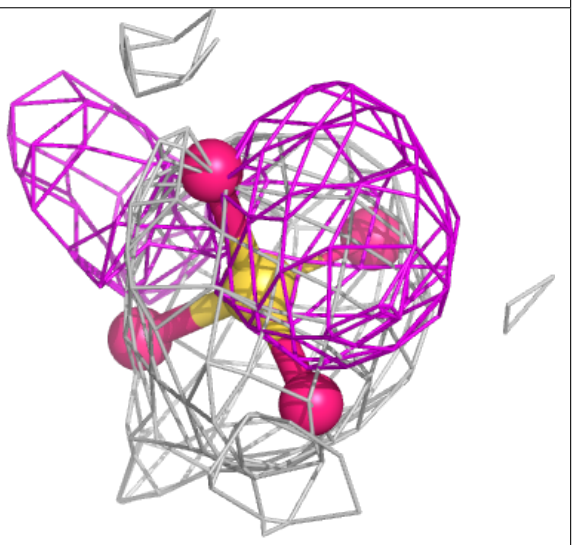


Electron density around SO4 B 206:

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

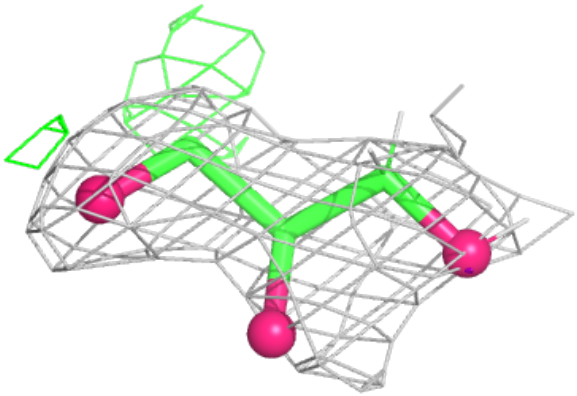


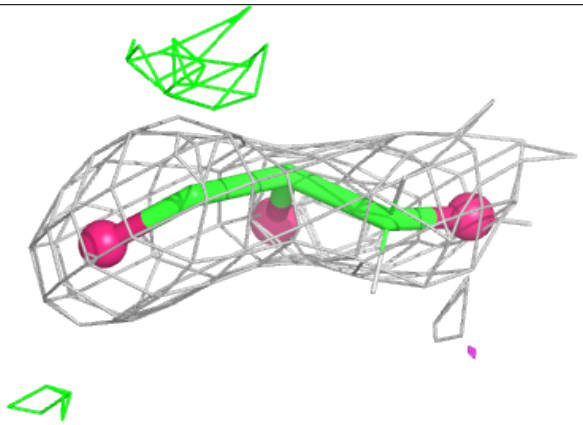


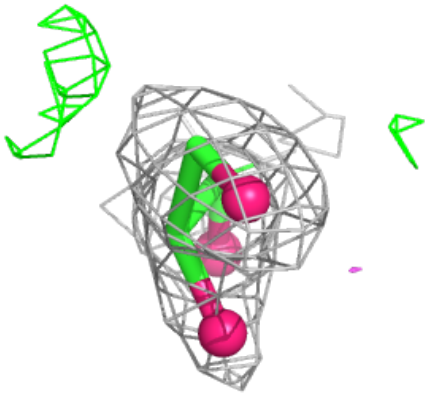


Electron density around GOL C 202:

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

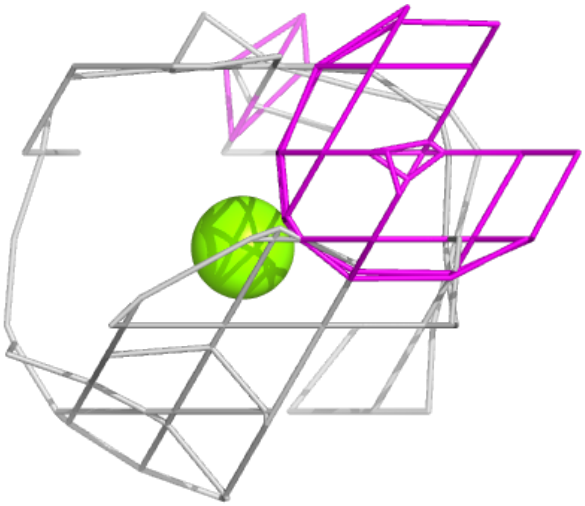


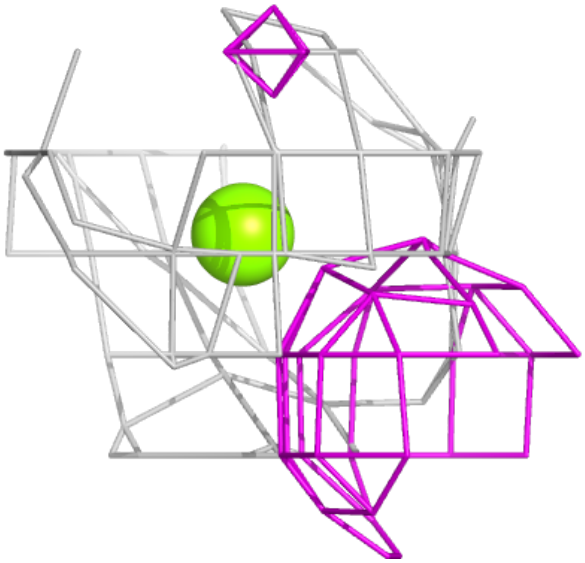


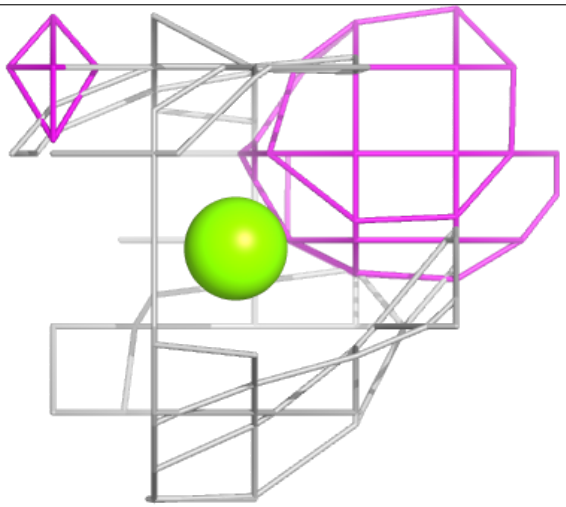


Electron density around MG F 203:

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

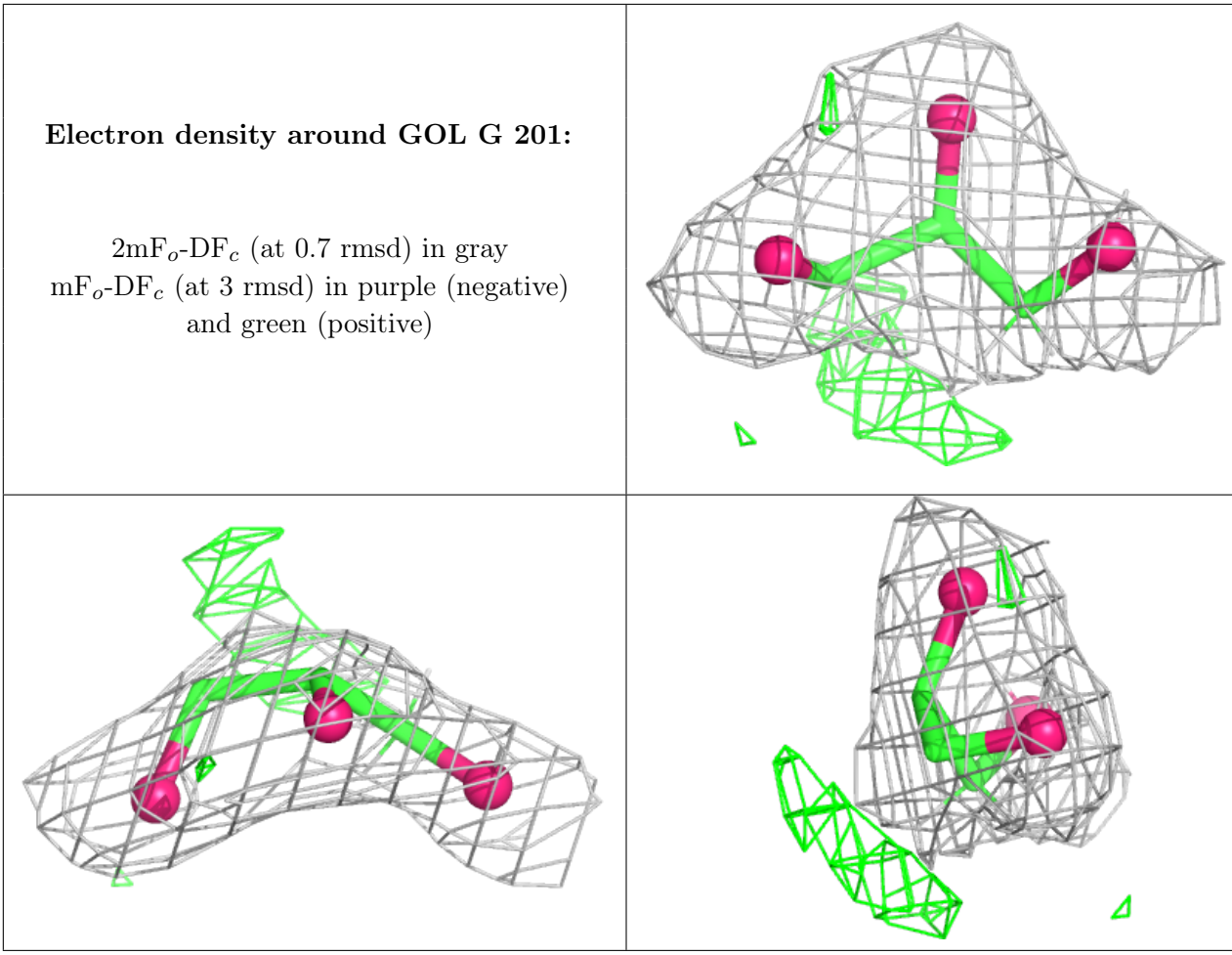






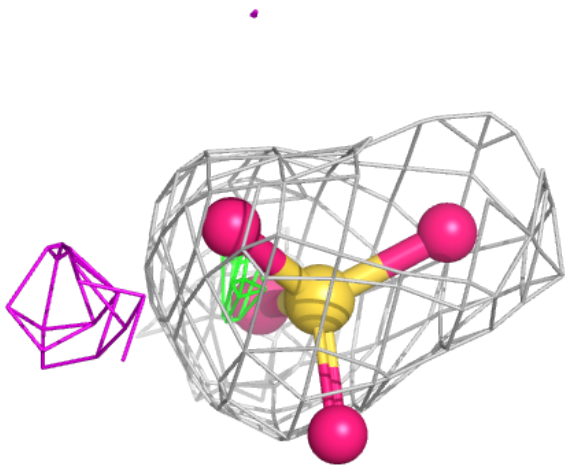
Electron density around GOL G 201:

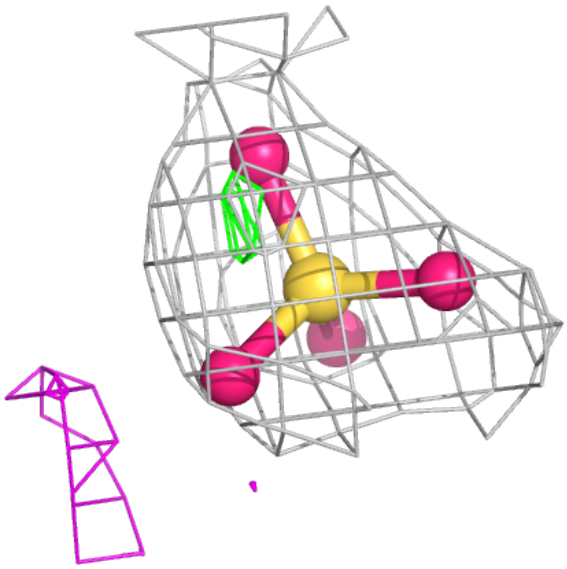
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

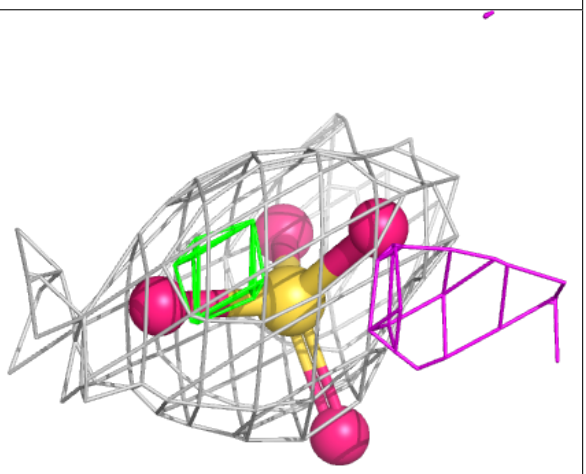


Electron density around SO4 E 204:

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

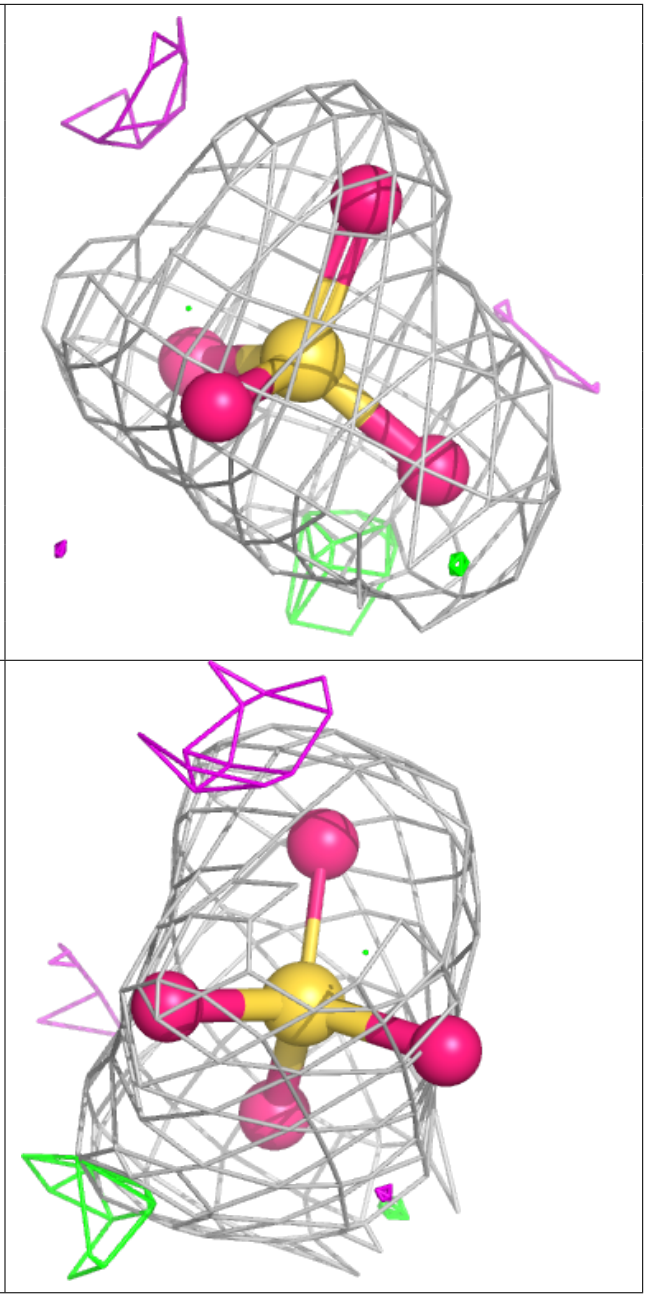






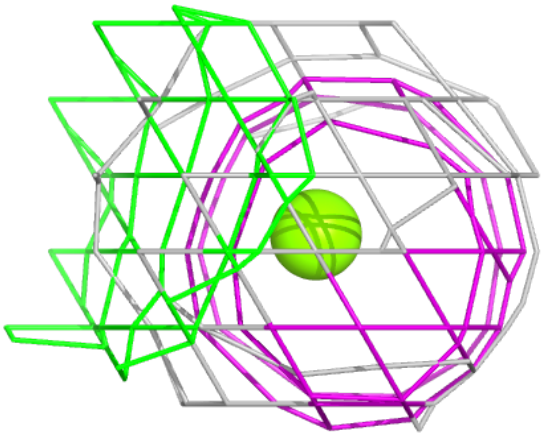
Electron density around SO4 E 201:

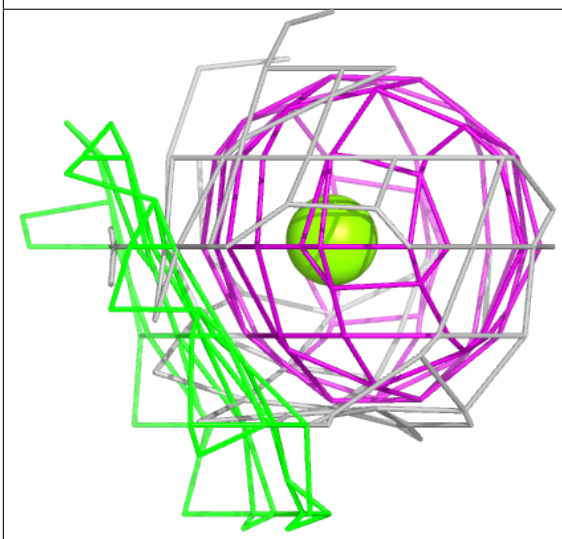
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

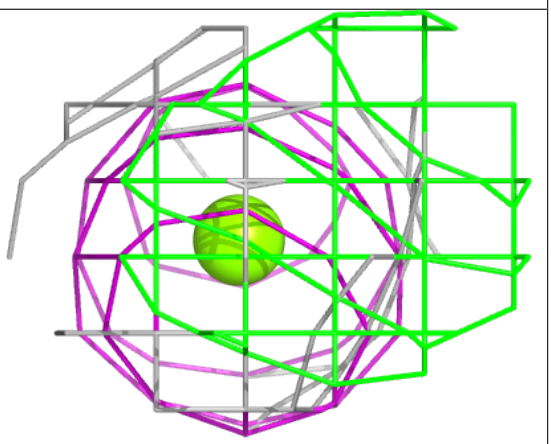


Electron density around MG H 203:

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

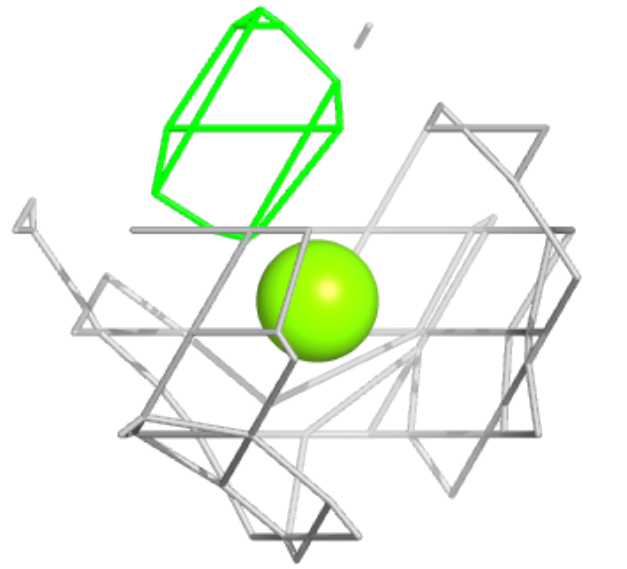


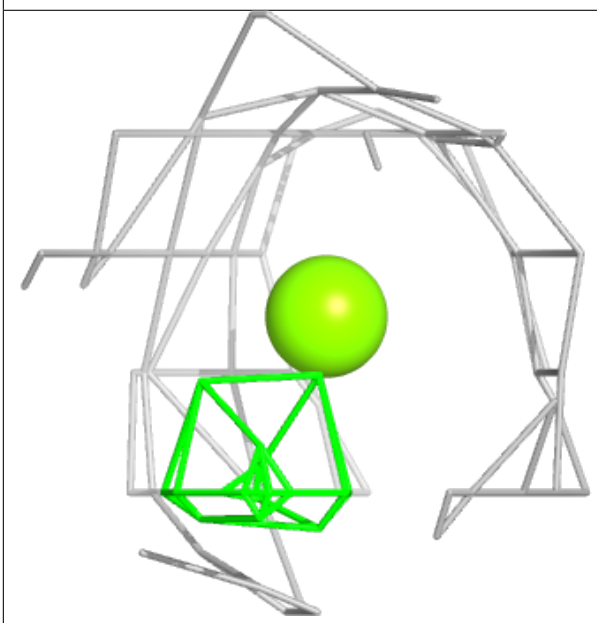


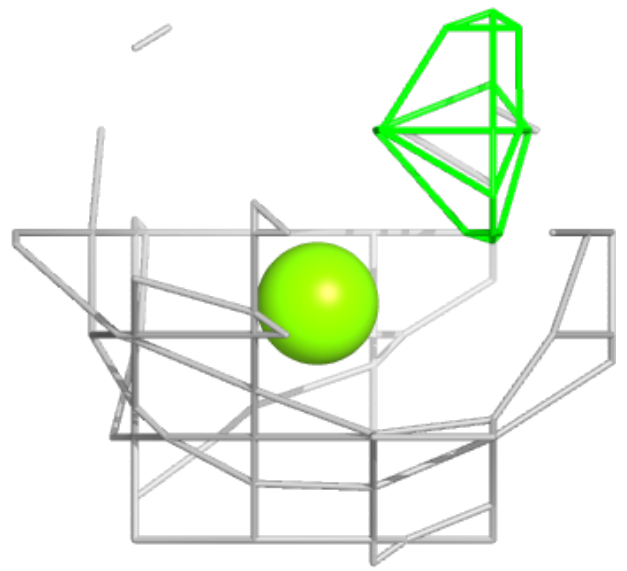


Electron density around MG C 205:

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

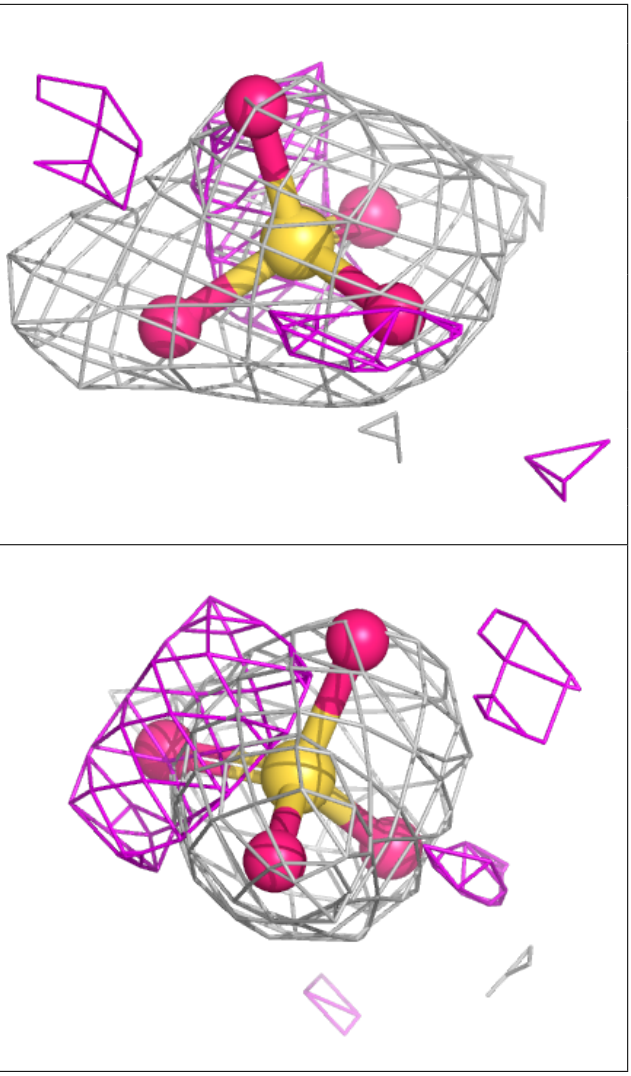






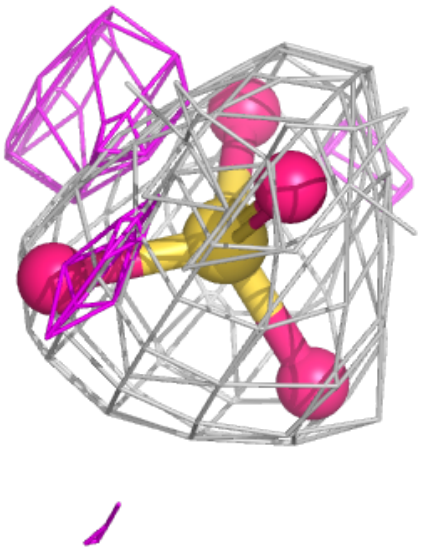
Electron density around SO4 A 202:

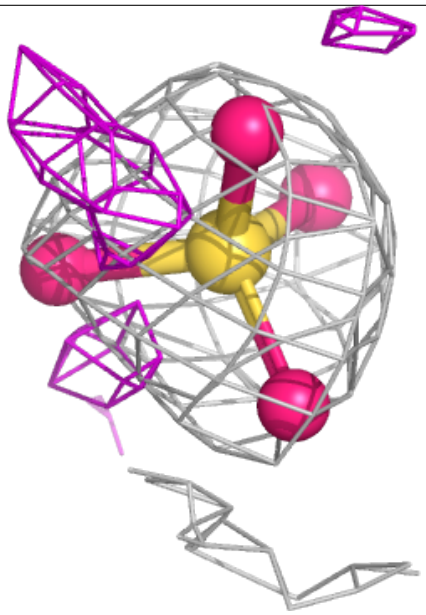
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

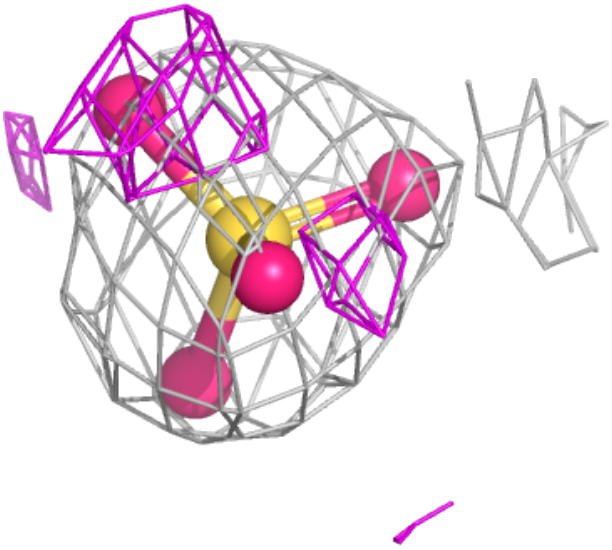


Electron density around SO4 F 202:

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

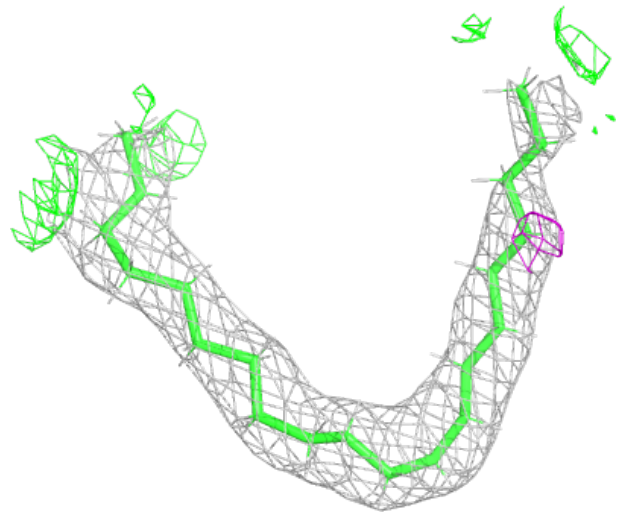


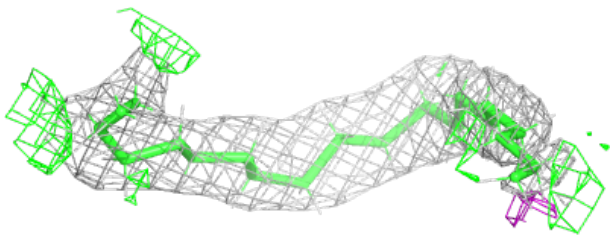




Electron density around LFA D 203:

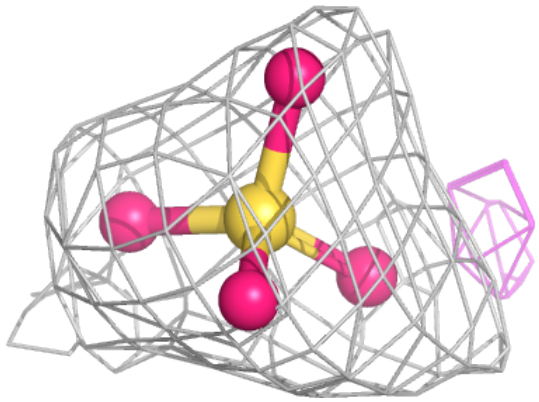
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

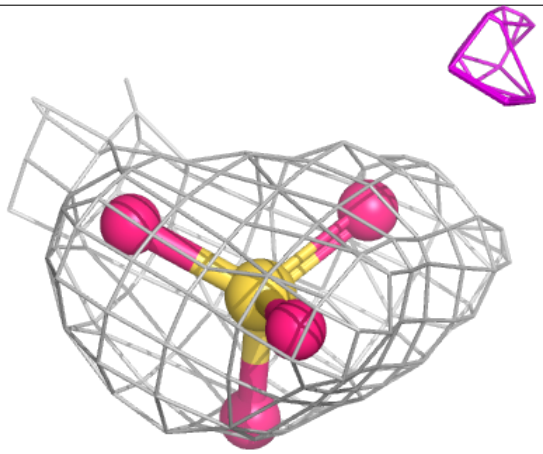


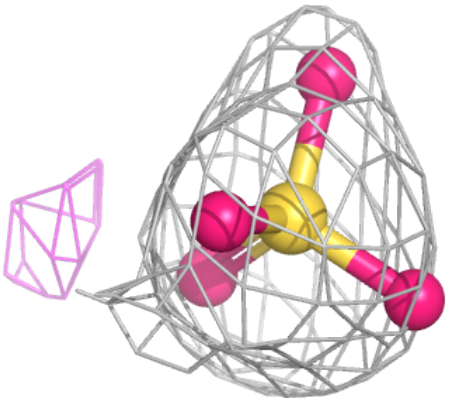


Electron density around SO4 H 201:

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

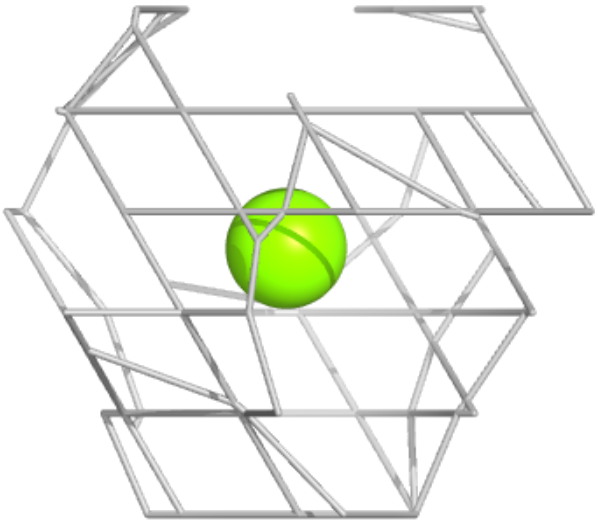


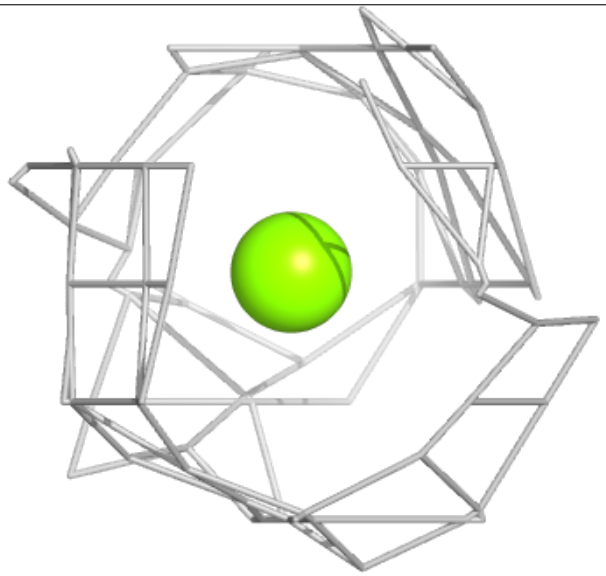


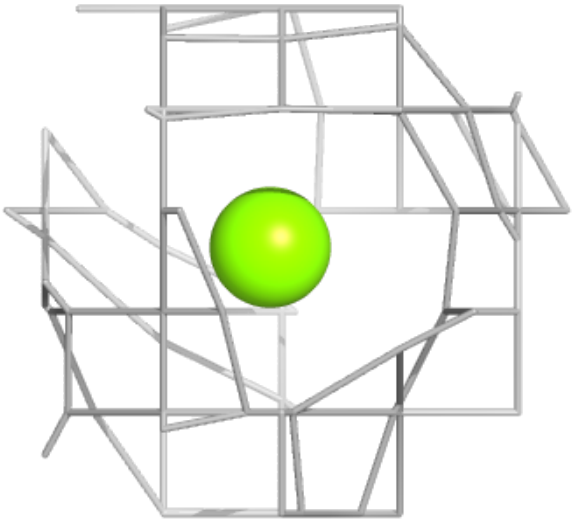


Electron density around MG D 205:

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

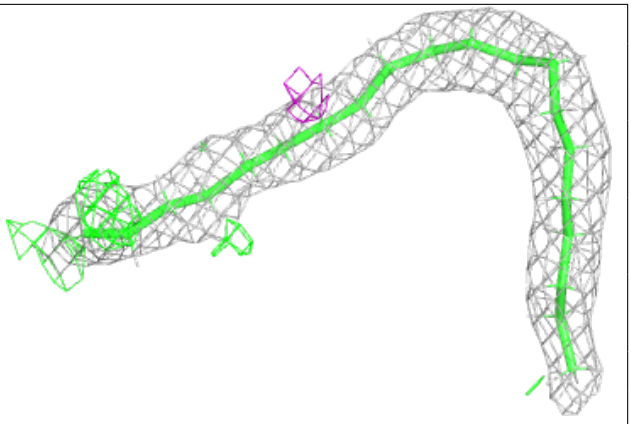


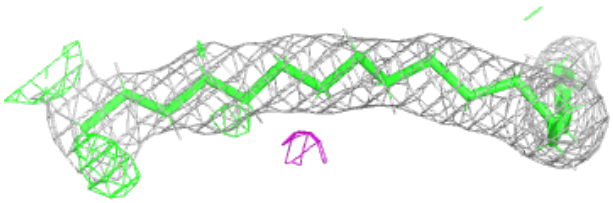


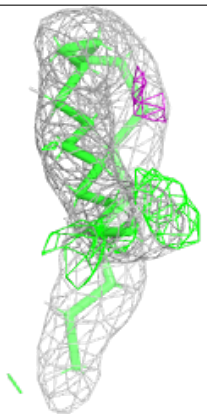


Electron density around LFA B 205:

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

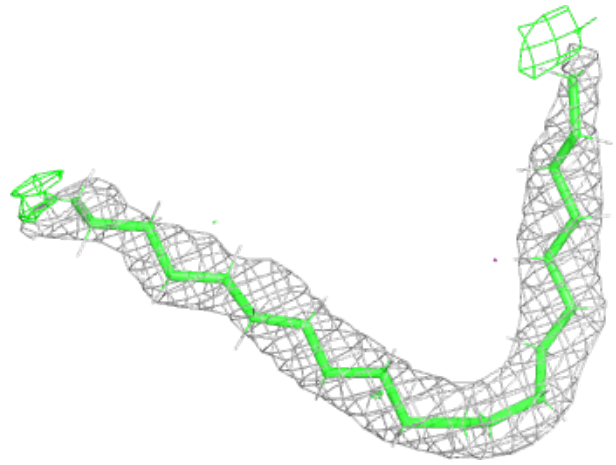


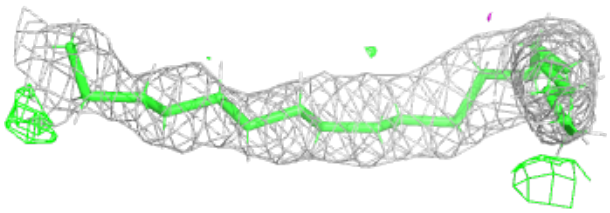


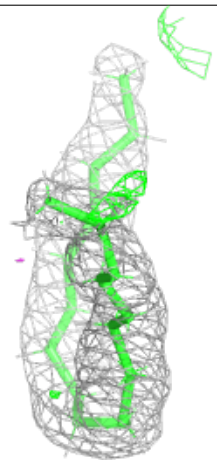


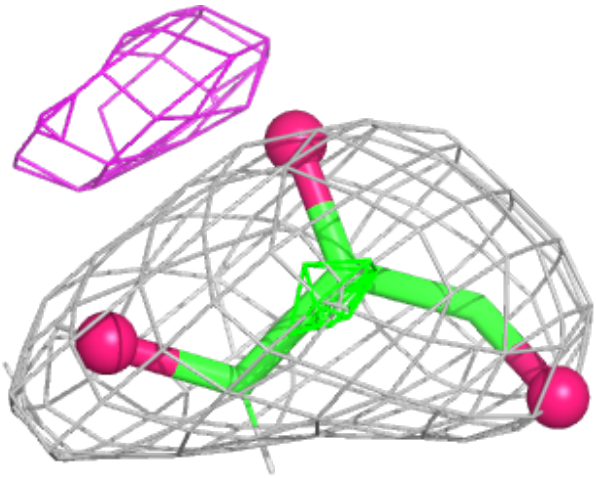
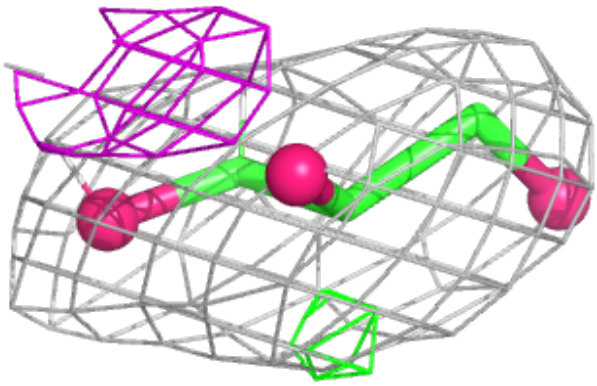
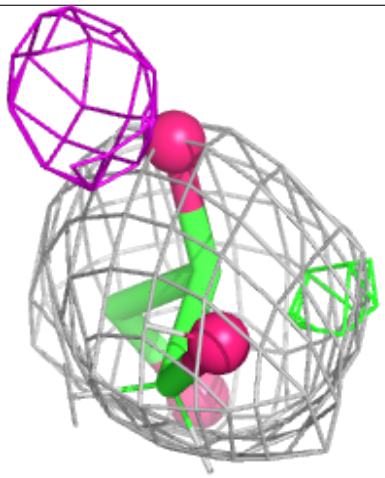
Electron density around LFA E 203:

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



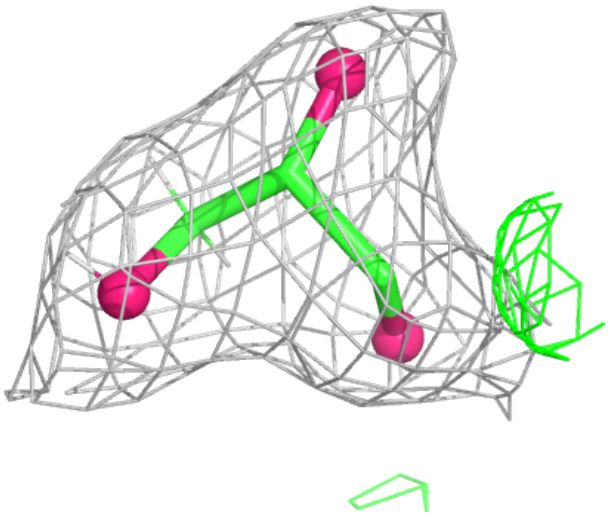


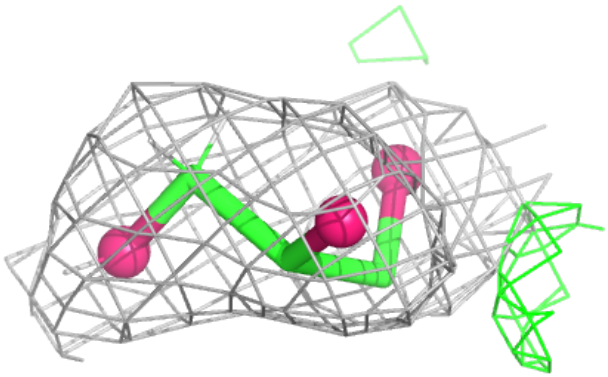


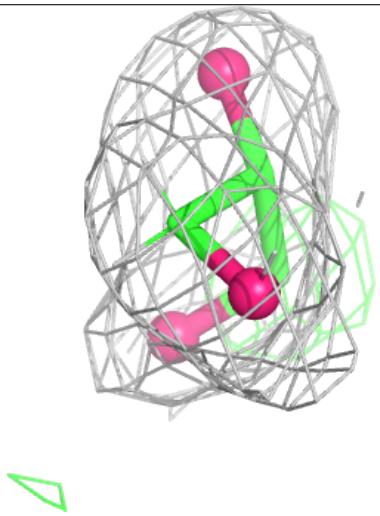
Electron density around GOL E 202: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around GOL B 202:

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

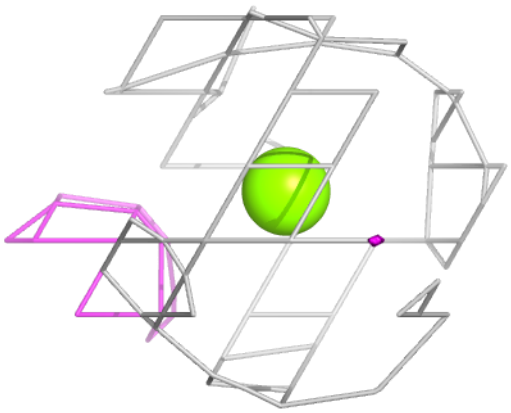


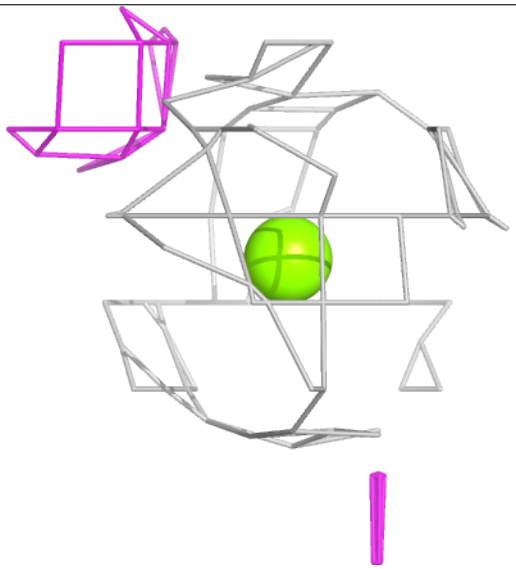


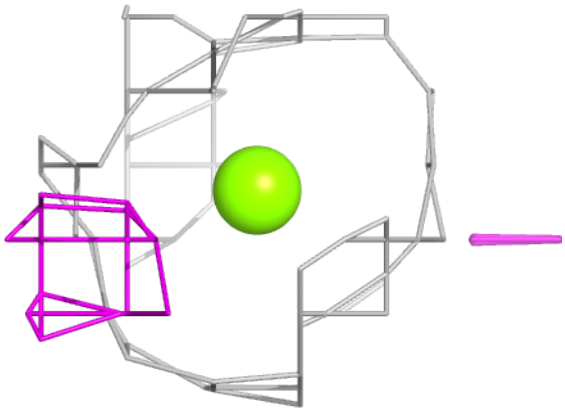


Electron density around MG A 203:

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

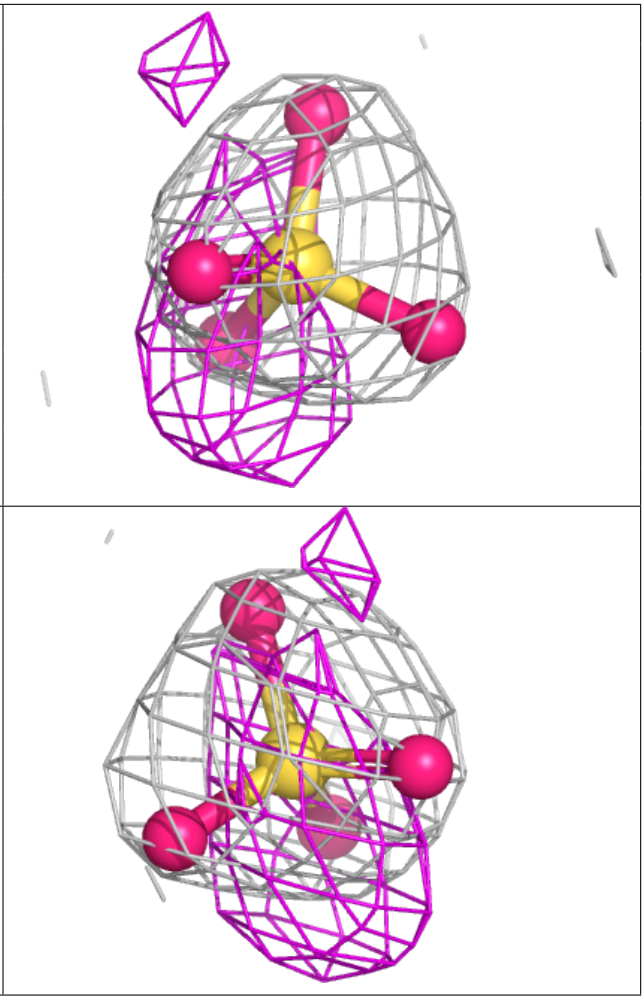






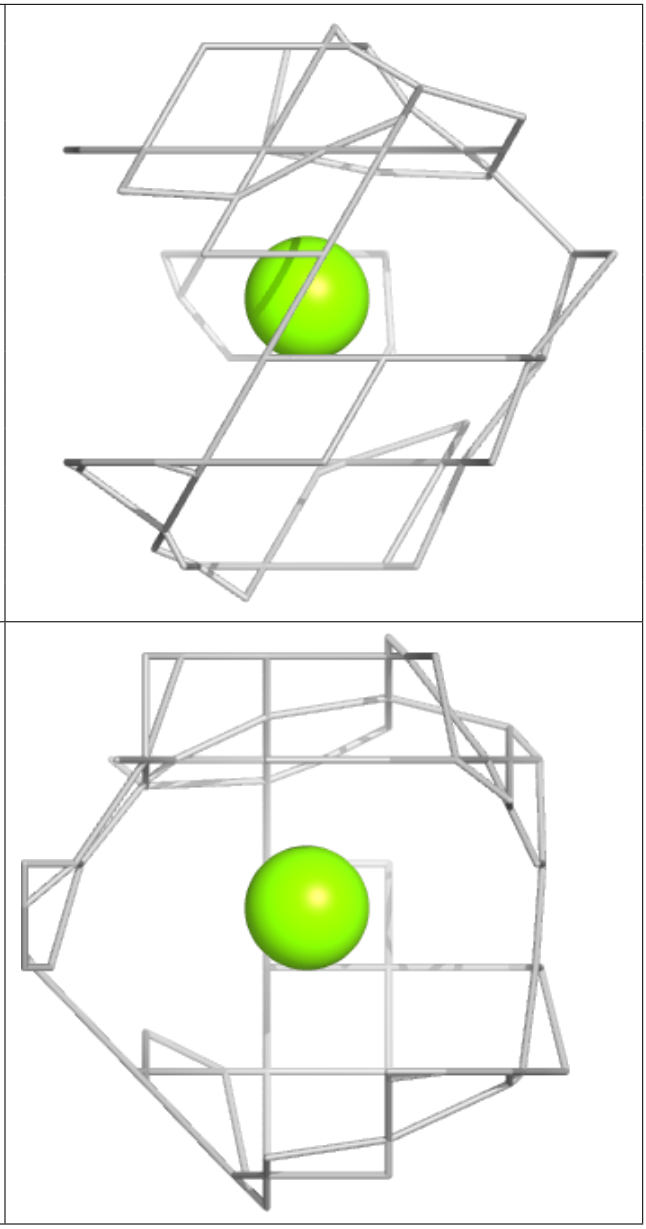
Electron density around SO4 B 203:

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



Electron density around MG B 207:

$2mF_o$-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.