Full wwPDB X-ray Structure Validation Report ⓘ

Nov 29, 2023 – 06:51 pm GMT

PDB ID	:	7NP8
Title	:	Crystal structure of the Coenzyme F420-dependent sulfite reductase from Methanocaldococcus jannaschii at 2.3-A resolution
Authors	:	Jespersen, M.; Wagner, T.
Deposited on	:	2021-02-26
Resolution	:	2.30 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:

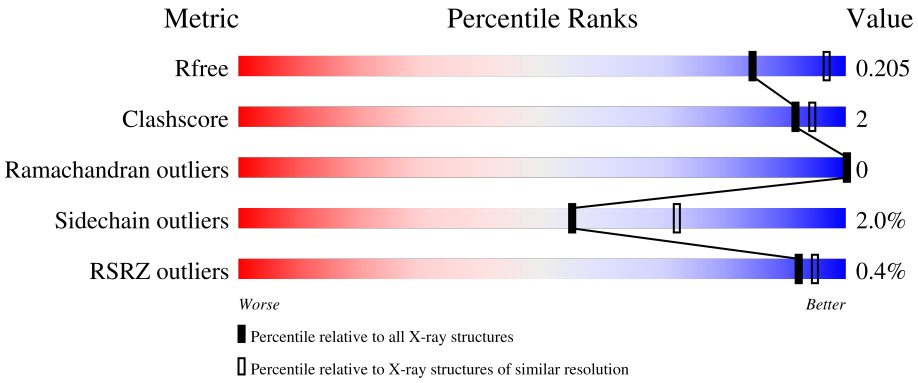
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	620	95% 5%
1	B	620	% 95% 5%
1	C	620	94% 6%
1	D	620	96% .

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
4	SO3	B	1013	-	-	X	-
5	SRM	A	1109	X	-	-	-
5	SRM	B	1008	X	-	-	-
5	SRM	C	1108	X	-	-	-
5	SRM	D	1109	X	-	-	-
6	GOL	A	1114	-	-	-	X
6	GOL	D	1117	-	-	-	X

2 Entry composition

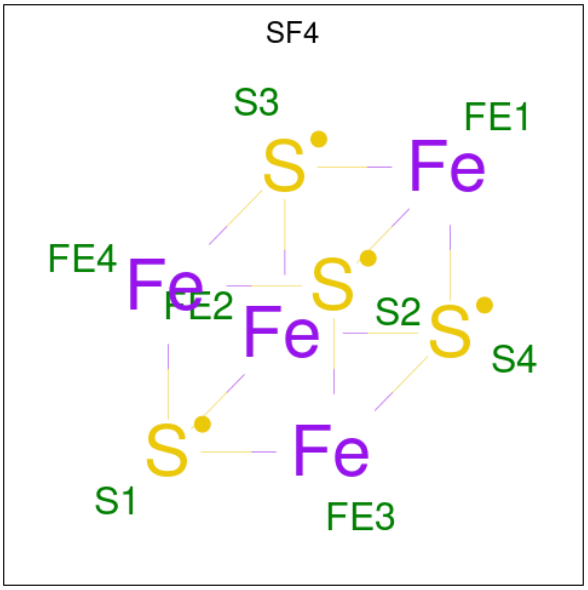
There are 11 unique types of molecules in this entry. The entry contains 21246 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Coenzyme F420-dependent sulfite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	619	Total	C	N	O	S	0	0	0
			4883	3102	834	911	36			
1	B	620	Total	C	N	O	S	0	1	0
			4895	3109	835	914	37			
1	C	619	Total	C	N	O	S	0	0	0
			4883	3102	834	911	36			
1	D	620	Total	C	N	O	S	0	1	0
			4893	3107	835	913	38			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0

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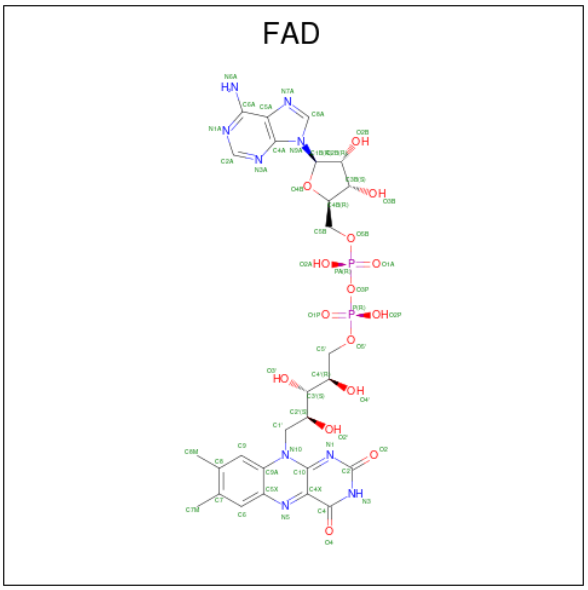
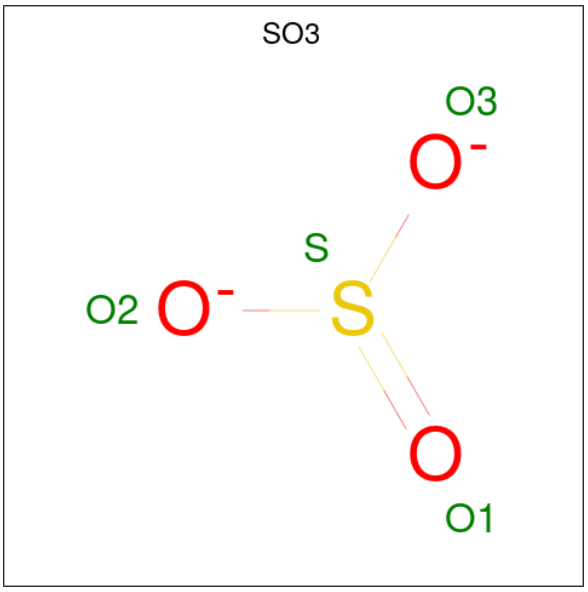
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



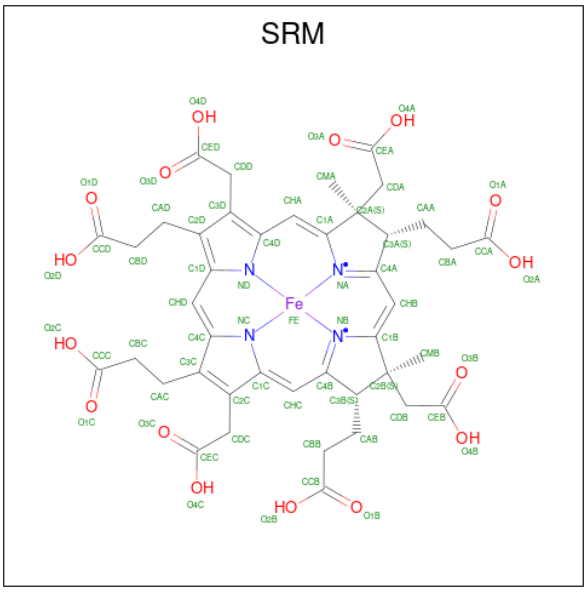
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is SULFITE ION (three-letter code: SO3) (formula: O_3S) (labeled as "Ligand of Interest" by depositor).



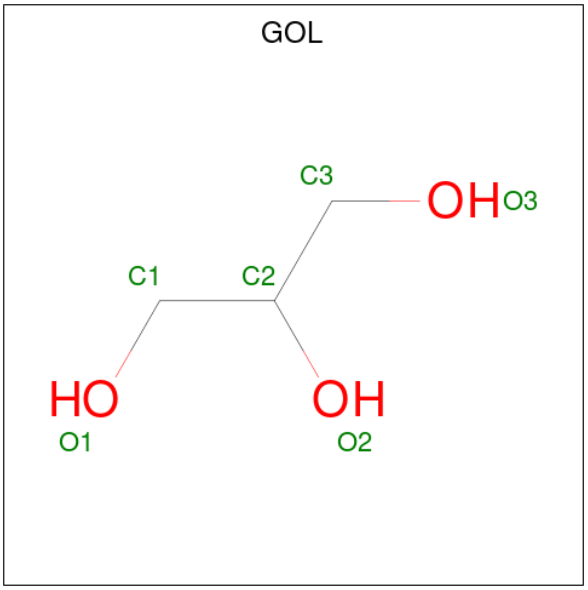
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 4 3 1	0	0
4	B	1	Total O S 4 3 1	0	0
4	C	1	Total O S 4 3 1	0	0
4	D	1	Total O S 4 3 1	0	0

- Molecule 5 is SIROHEME (three-letter code: SRM) (formula: $C_{42}H_{44}FeN_4O_{16}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	B	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	C	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	D	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

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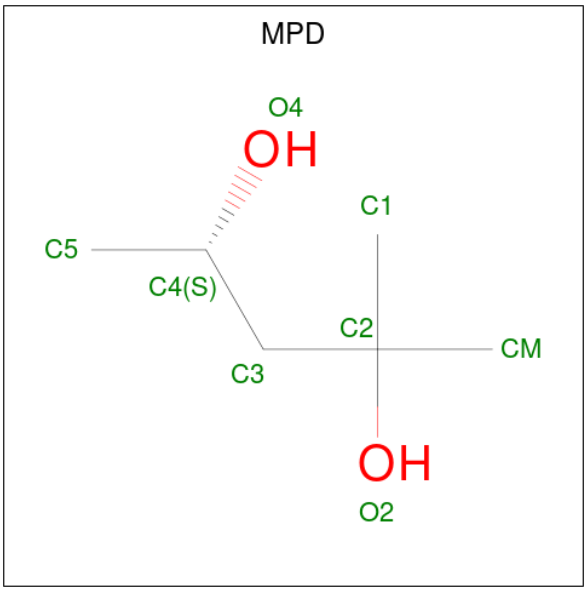
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 8 6 2	0	0
7	B	1	Total C O 8 6 2	0	0
7	C	1	Total C O 8 6 2	0	0
7	C	1	Total C O 8 6 2	0	0
7	D	1	Total C O 8 6 2	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	2	Total Ca 2 2	0	0
8	C	3	Total Ca 3 3	0	0
8	D	3	Total Ca 3 3	0	1

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total Cl 2 2	0	0
9	B	1	Total Cl 1 1	0	0
9	C	2	Total Cl 2 2	0	0
9	D	1	Total Cl 1 1	0	0

- Molecule 10 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	1	Total Fe 1 1	0	0

- Molecule 11 is water.

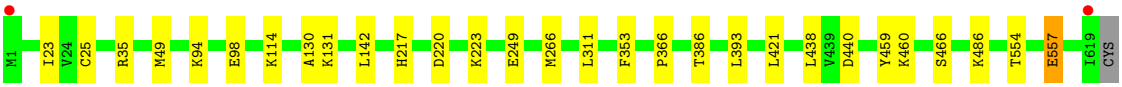
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	168	Total O 168 168	0	0
11	B	215	Total O 215 215	0	2
11	C	193	Total O 193 193	0	1
11	D	196	Total O 196 196	0	1

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.

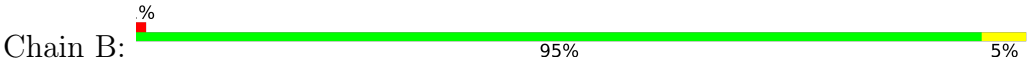
• Molecule 1: Coenzyme F420-dependent sulfite reductase

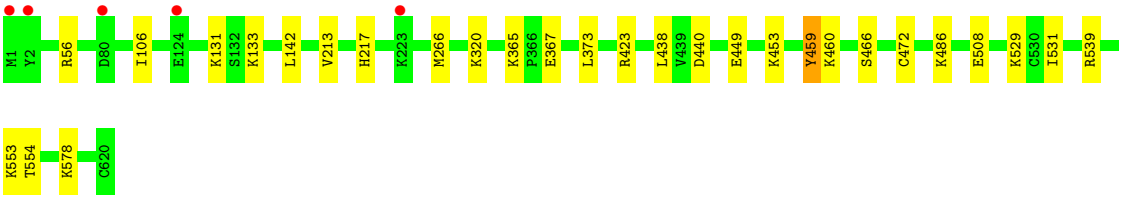
Chain A:



• Molecule 1: Coenzyme F420-dependent sulfite reductase

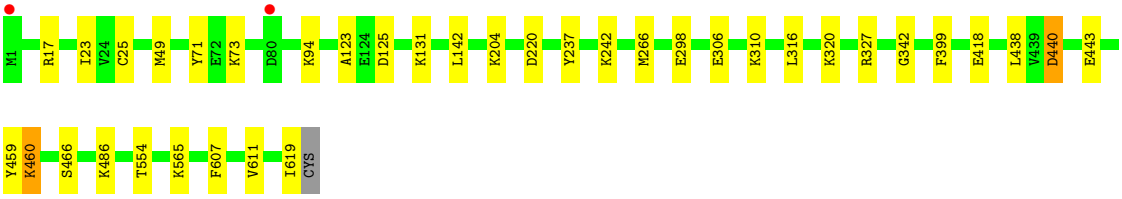
Chain B:





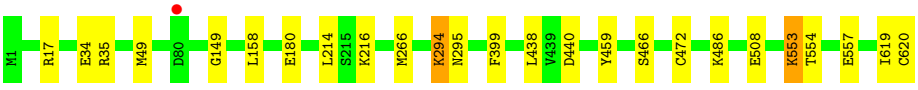
• Molecule 1: Coenzyme F420-dependent sulfite reductase

Chain C:



• Molecule 1: Coenzyme F420-dependent sulfite reductase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	167.26Å 172.20Å 195.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.82 – 2.30 78.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	83.2 (78.82-2.30) 83.2 (78.82-2.30)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.182 , 0.205 0.181 , 0.205	Depositor DCC
R_{free} test set	5170 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	38.5	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.118 for -k,-h,-l	Xtriage
Reported twinning fraction	0.050 for -k,-h,-l	Depositor
Outliers	1 of 104064 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21246	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: FAD, GOL, CL, MPD, CA, SRM, SF4, FE, SO3

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	0.25	0/4965	0.42	0/6663
1	B	0.24	0/4980	0.43	0/6683
1	C	0.25	0/4965	0.44	0/6663
1	D	0.25	0/4978	0.42	0/6679
All	All	0.25	0/19888	0.43	0/26688

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	4883	0	4949	12	0
1	B	4895	0	4960	17	0
1	C	4883	0	4948	18	0
1	D	4893	0	4957	10	0
2	A	48	0	0	1	0
2	B	48	0	0	0	0
2	C	48	0	0	1	0
2	D	48	0	0	0	0
3	A	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	53	0	31	0	0
3	C	53	0	31	1	0
3	D	53	0	31	1	0
4	A	4	0	0	1	0
4	B	4	0	0	2	0
4	C	4	0	0	1	0
4	D	4	0	0	0	0
5	A	63	0	34	6	0
5	B	63	0	34	3	0
5	C	63	0	34	4	0
5	D	63	0	34	2	0
6	A	36	0	48	0	0
6	B	42	0	56	0	0
6	C	36	0	48	2	0
6	D	78	0	104	1	0
7	A	8	0	14	0	0
7	B	8	0	14	0	0
7	C	16	0	28	0	0
7	D	8	0	14	1	0
8	A	1	0	0	0	0
8	B	2	0	0	0	0
8	C	3	0	0	0	0
8	D	3	0	0	0	0
9	A	2	0	0	0	0
9	B	1	0	0	0	0
9	C	2	0	0	0	0
9	D	1	0	0	0	0
10	D	1	0	0	0	0
11	A	168	0	0	0	0
11	B	215	0	0	4	0
11	C	193	0	0	2	0
11	D	196	0	0	2	0
All	All	21246	0	20400	66	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 2.

All (66) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:LYS:NZ	4:B:1013:SO3:O3	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:LYS:NZ	11:B:1101:HOH:O	2.32	0.62
1:D:294:LYS:HG2	1:D:295:ASN:N	2.18	0.58
1:C:565:LYS:NZ	11:C:1201:HOH:O	2.35	0.58
1:B:213:VAL:O	1:B:217:HIS:ND1	2.35	0.56
1:D:180:GLU:HB2	11:D:1324:HOH:O	2.06	0.56
1:C:607:PHE:O	1:C:611:VAL:HG23	2.06	0.55
1:B:423:ARG:NH2	4:B:1013:SO3:O1	2.39	0.55
1:C:460:LYS:NZ	4:C:1117:SO3:O2	2.40	0.55
5:B:1008:SRM:HBC2	5:B:1008:SRM:HCD1	1.90	0.54
1:C:418:GLU:HG3	6:C:1111:GOL:H32	1.90	0.53
1:A:94:LYS:NZ	1:A:98:GLU:OE1	2.40	0.52
1:C:298:GLU:HA	11:C:1208:HOH:O	2.09	0.52
1:A:460:LYS:NZ	4:A:1108:SO3:O3	2.31	0.51
5:A:1109:SRM:HBC2	5:A:1109:SRM:CDC	2.41	0.51
1:C:316:LEU:HG	1:C:320:LYS:HE3	1.93	0.51
5:B:1008:SRM:HBC2	5:B:1008:SRM:CDC	2.41	0.50
5:D:1109:SRM:HBC2	5:D:1109:SRM:HCD1	1.95	0.49
5:A:1109:SRM:HBC2	5:A:1109:SRM:HCD1	1.94	0.48
1:A:366:PRO:HB3	1:B:373:LEU:HD11	1.96	0.47
5:D:1109:SRM:HBC2	5:D:1109:SRM:CDC	2.45	0.47
1:C:237:TYR:CE2	1:C:242:LYS:HE2	2.50	0.46
5:C:1108:SRM:HBC2	5:C:1108:SRM:CDC	2.46	0.46
5:A:1109:SRM:HDB1	1:B:472:CYS:HB3	1.97	0.46
1:A:386:THR:HB	5:A:1109:SRM:HBB2	1.98	0.45
5:C:1108:SRM:HBC2	5:C:1108:SRM:HCD1	1.98	0.45
1:B:459:TYR:OH	5:B:1008:SRM:O4D	2.31	0.45
1:D:553:LYS:HE3	1:D:557:GLU:HG2	1.99	0.45
1:B:365:LYS:NZ	11:B:1117:HOH:O	2.49	0.44
1:D:399:PHE:O	7:D:1113:MPD:H12	2.18	0.44
1:A:130:ALA:O	1:A:131:LYS:HG3	2.18	0.44
1:B:508:GLU:HA	11:B:1274:HOH:O	2.17	0.43
1:B:56:ARG:HA	1:B:56:ARG:HD3	1.88	0.43
1:D:438:LEU:HD22	1:D:486:LYS:HE3	2.00	0.43
1:C:438:LEU:HD22	1:C:486:LYS:HE3	2.00	0.43
1:D:149:GLY:HA2	6:D:1125:GOL:H11	1.99	0.43
1:A:438:LEU:HD22	1:A:486:LYS:HE3	1.99	0.43
1:C:327:ARG:HD3	1:C:399:PHE:CE2	2.54	0.43
1:D:508:GLU:HB3	11:D:1298:HOH:O	2.18	0.43
1:A:217:HIS:NE2	1:A:249:GLU:OE1	2.52	0.43
5:C:1108:SRM:C4C	1:D:472:CYS:HA	2.49	0.42
1:B:320:LYS:NZ	11:B:1111:HOH:O	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:GLU:O	1:B:453:LYS:HB3	2.19	0.42
1:A:353:PHE:HA	1:A:393:LEU:O	2.19	0.42
1:D:158:LEU:HD21	3:D:1106:FAD:HM83	2.00	0.42
1:A:23:ILE:HD13	1:A:142:LEU:HD23	2.01	0.41
1:B:106:ILE:HG13	1:B:142:LEU:HD13	2.01	0.41
5:C:1108:SRM:HMA1	5:C:1108:SRM:HAA1	1.92	0.41
1:C:71:TYR:CE1	1:C:73:LYS:HE2	2.55	0.41
5:A:1109:SRM:C4C	1:B:472:CYS:HA	2.50	0.41
1:C:17:ARG:HB2	1:C:204:LYS:HE3	2.03	0.41
1:C:23:ILE:HD13	1:C:142:LEU:HD23	2.02	0.41
1:A:557:GLU:CD	1:A:557:GLU:N	2.74	0.41
1:C:440:ASP:OD1	1:C:443:GLU:HB2	2.21	0.41
1:D:17:ARG:NH1	1:D:34:GLU:O	2.53	0.41
1:A:25:CYS:HA	2:A:1102:SF4:S3	2.61	0.41
5:A:1109:SRM:HAB1	5:A:1109:SRM:HMB3	1.75	0.41
1:B:131:LYS:O	1:B:133:LYS:HD2	2.20	0.41
1:A:220:ASP:HB2	1:A:223:LYS:HD3	2.02	0.41
1:C:342:GLY:HA2	6:C:1111:GOL:H12	2.02	0.41
1:B:438:LEU:HD22	1:B:486:LYS:HE3	2.02	0.40
1:C:306:GLU:O	1:C:310:LYS:HG3	2.21	0.40
1:C:25:CYS:HA	2:C:1102:SF4:S3	2.62	0.40
1:B:531:ILE:HA	1:B:539:ARG:HB2	2.04	0.40
1:C:94:LYS:HG3	1:C:123:ALA:HB1	2.04	0.40
1:C:131:LYS:O	3:C:1107:FAD:H8A	2.21	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	617/620 (100%)	608 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	619/620 (100%)	608 (98%)	11 (2%)	0	100	100
1	C	617/620 (100%)	608 (98%)	9 (2%)	0	100	100
1	D	619/620 (100%)	609 (98%)	10 (2%)	0	100	100
All	All	2472/2480 (100%)	2433 (98%)	39 (2%)	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	526/527 (100%)	515 (98%)	11 (2%)	53	70
1	B	528/527 (100%)	520 (98%)	8 (2%)	65	79
1	C	526/527 (100%)	516 (98%)	10 (2%)	57	73
1	D	528/527 (100%)	515 (98%)	13 (2%)	47	65
All	All	2108/2108 (100%)	2066 (98%)	42 (2%)	55	72

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	49	MET
1	A	114	LYS
1	A	266	MET
1	A	311	LEU
1	A	421	LEU
1	A	440	ASP
1	A	459	TYR
1	A	466	SER
1	A	554	THR
1	A	557	GLU
1	B	266	MET
1	B	367	GLU

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Mol	Chain	Res	Type
1	B	440	ASP
1	B	459	TYR
1	B	466	SER
1	B	553	LYS
1	B	554	THR
1	B	578	LYS
1	C	49	MET
1	C	125	ASP
1	C	220	ASP
1	C	266	MET
1	C	440	ASP
1	C	459	TYR
1	C	460	LYS
1	C	466	SER
1	C	554	THR
1	C	619	ILE
1	D	35	ARG
1	D	49	MET
1	D	214	LEU
1	D	216	LYS
1	D	266	MET
1	D	294	LYS
1	D	440	ASP
1	D	459	TYR
1	D	466	SER
1	D	553	LYS
1	D	554	THR
1	D	619	ILE
1	D	620	CYS

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 89 ligands modelled in this entry, 16 are monoatomic - leaving 73 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	$\#\|Z\| > 2$
4	SO3	B	1013	-	1,3,3	1.32	0	0,3,3	-	-
4	SO3	C	1117	5	1,3,3	1.34	0	0,3,3	-	-
2	SF4	B	1004	1	0,12,12	-	-	-		
6	GOL	D	1120	-	5,5,5	0.32	0	5,5,5	0.34	0
6	GOL	C	1110	-	5,5,5	0.09	0	5,5,5	0.32	0
7	MPD	C	1113	-	7,7,7	0.29	0	9,10,10	0.28	0
6	GOL	B	1016	-	5,5,5	0.29	0	5,5,5	0.29	0
6	GOL	A	1111	-	5,5,5	0.43	0	5,5,5	0.38	0
6	GOL	D	1112	-	5,5,5	0.40	0	5,5,5	0.26	0
2	SF4	B	1007	1	0,12,12	-	-	-		
2	SF4	C	1103	1	0,12,12	-	-	-		
2	SF4	C	1104	1	0,12,12	-	-	-		
6	GOL	A	1115	-	5,5,5	0.33	0	5,5,5	0.31	0
6	GOL	D	1124	-	5,5,5	0.08	0	5,5,5	0.32	0
2	SF4	A	1107	1	0,12,12	-	-	-		
6	GOL	B	1018	-	5,5,5	0.08	0	5,5,5	0.59	0
6	GOL	B	1015	-	5,5,5	0.35	0	5,5,5	0.33	0
2	SF4	B	1005	1	0,12,12	-	-	-		
2	SF4	A	1103	1	0,12,12	-	-	-		
2	SF4	A	1104	1	0,12,12	-	-	-		
5	SRM	D	1109	1,4	68,70,70	2.44	14 (20%)	81,112,112	1.72	12 (14%)
4	SO3	D	1108	5	1,3,3	1.29	0	0,3,3	-	-
6	GOL	C	1111	-	5,5,5	0.08	0	5,5,5	0.32	0
2	SF4	D	1105	1	0,12,12	-	-	-		
6	GOL	D	1111	-	5,5,5	0.43	0	5,5,5	0.32	0
6	GOL	D	1125	-	5,5,5	0.08	0	5,5,5	0.32	0
6	GOL	D	1126	-	5,5,5	0.15	0	5,5,5	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SF4	D	1101	1	0,12,12	-	-	-		
6	GOL	A	1116	-	5,5,5	0.37	0	5,5,5	0.32	0
2	SF4	A	1105	1	0,12,12	-	-	-		
3	FAD	B	1006	-	53,58,58	0.67	0	68,89,89	0.70	1 (1%)
5	SRM	C	1108	1,4	68,70,70	2.38	12 (17%)	81,112,112	1.68	12 (14%)
2	SF4	A	1101	1	0,12,12	-	-	-		
6	GOL	C	1109	-	5,5,5	0.42	0	5,5,5	0.45	0
6	GOL	B	1009	-	5,5,5	0.09	0	5,5,5	0.32	0
2	SF4	C	1105	1	0,12,12	-	-	-		
6	GOL	C	1120	-	5,5,5	0.19	0	5,5,5	0.49	0
6	GOL	D	1110	-	5,5,5	0.36	0	5,5,5	0.49	0
6	GOL	B	1017	-	5,5,5	0.09	0	5,5,5	0.32	0
3	FAD	C	1107	-	53,58,58	1.31	5 (9%)	68,89,89	1.29	11 (16%)
2	SF4	D	1107	1	0,12,12	-	-	-		
7	MPD	A	1112	-	7,7,7	0.30	0	9,10,10	0.52	0
3	FAD	D	1106	-	53,58,58	0.66	0	68,89,89	0.68	2 (2%)
2	SF4	C	1106	1	0,12,12	-	-	-		
6	GOL	A	1114	-	5,5,5	0.30	0	5,5,5	0.27	0
2	SF4	D	1104	1	0,12,12	-	-	-		
7	MPD	C	1112	-	7,7,7	0.30	0	9,10,10	0.47	0
2	SF4	B	1001	1	0,12,12	-	-	-		
6	GOL	A	1110	-	5,5,5	0.15	0	5,5,5	0.53	0
2	SF4	D	1103	1	0,12,12	-	-	-		
2	SF4	A	1102	1	0,12,12	-	-	-		
6	GOL	B	1019	-	5,5,5	0.08	0	5,5,5	0.27	0
6	GOL	C	1118	-	5,5,5	0.36	0	5,5,5	0.15	0
6	GOL	D	1119	-	5,5,5	0.10	0	5,5,5	0.33	0
2	SF4	B	1003	1	0,12,12	-	-	-		
6	GOL	D	1122	-	5,5,5	0.09	0	5,5,5	0.32	0
7	MPD	B	1010	-	7,7,7	0.12	0	9,10,10	0.32	0
2	SF4	C	1102	1	0,12,12	-	-	-		
2	SF4	D	1102	1	0,12,12	-	-	-		
7	MPD	D	1113	-	7,7,7	0.12	0	9,10,10	0.33	0
6	GOL	D	1123	-	5,5,5	0.09	0	5,5,5	0.32	0
6	GOL	D	1117	-	5,5,5	0.39	0	5,5,5	0.47	0
5	SRM	B	1008	1	68,70,70	2.39	11 (16%)	81,112,112	1.68	15 (18%)
6	GOL	B	1014	-	5,5,5	0.36	0	5,5,5	0.24	0
2	SF4	C	1101	1	0,12,12	-	-	-		
3	FAD	A	1106	-	53,58,58	0.66	0	68,89,89	0.71	1 (1%)
6	GOL	D	1121	-	5,5,5	0.09	0	5,5,5	0.32	0
4	SO3	A	1108	5	1,3,3	1.33	0	0,3,3	-	-
6	GOL	C	1119	-	5,5,5	0.31	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SRM	A	1109	1,4	68,70,70	2.45	11 (16%)	81,112,112	1.68	14 (17%)
6	GOL	A	1117	-	5,5,5	0.10	0	5,5,5	0.34	0
2	SF4	B	1002	1	0,12,12	-	-	-		
6	GOL	D	1118	-	5,5,5	0.14	0	5,5,5	0.26	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	SF4	B	1004	1	-	-	0/6/5/5
6	GOL	D	1120	-	-	4/4/4/4	-
6	GOL	C	1110	-	-	2/4/4/4	-
7	MPD	C	1113	-	-	0/5/5/5	-
6	GOL	B	1016	-	-	0/4/4/4	-
6	GOL	A	1111	-	-	2/4/4/4	-
6	GOL	D	1112	-	-	4/4/4/4	-
6	GOL	D	1124	-	-	1/4/4/4	-
6	GOL	A	1115	-	-	2/4/4/4	-
2	SF4	B	1007	1	-	-	0/6/5/5
2	SF4	C	1103	1	-	-	0/6/5/5
2	SF4	C	1104	1	-	-	0/6/5/5
2	SF4	A	1107	1	-	-	0/6/5/5
6	GOL	B	1018	-	-	2/4/4/4	-
6	GOL	B	1015	-	-	2/4/4/4	-
2	SF4	B	1005	1	-	-	0/6/5/5
2	SF4	A	1103	1	-	-	0/6/5/5
2	SF4	A	1104	1	-	-	0/6/5/5
5	SRM	D	1109	1,4	1/1/19/23	15/38/126/126	-
6	GOL	D	1111	-	-	2/4/4/4	-
6	GOL	C	1111	-	-	3/4/4/4	-
6	GOL	D	1126	-	-	0/4/4/4	-
6	GOL	D	1125	-	-	3/4/4/4	-
2	SF4	D	1105	1	-	-	0/6/5/5
2	SF4	D	1101	1	-	-	0/6/5/5
6	GOL	A	1116	-	-	1/4/4/4	-
5	SRM	C	1108	1,4	1/1/19/23	14/38/126/126	-
3	FAD	B	1006	-	-	2/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	A	1105	1	-	-	0/6/5/5
2	SF4	A	1101	1	-	-	0/6/5/5
6	GOL	C	1109	-	-	0/4/4/4	-
6	GOL	B	1009	-	-	4/4/4/4	-
2	SF4	C	1105	1	-	-	0/6/5/5
6	GOL	C	1120	-	-	2/4/4/4	-
6	GOL	D	1110	-	-	0/4/4/4	-
6	GOL	B	1017	-	-	3/4/4/4	-
3	FAD	C	1107	-	-	1/30/50/50	0/6/6/6
7	MPD	A	1112	-	-	2/5/5/5	-
2	SF4	D	1107	1	-	-	0/6/5/5
3	FAD	D	1106	-	-	1/30/50/50	0/6/6/6
2	SF4	C	1106	1	-	-	0/6/5/5
6	GOL	A	1114	-	-	0/4/4/4	-
7	MPD	C	1112	-	-	2/5/5/5	-
2	SF4	D	1104	1	-	-	0/6/5/5
6	GOL	A	1110	-	-	2/4/4/4	-
6	GOL	B	1019	-	-	0/4/4/4	-
6	GOL	C	1118	-	-	2/4/4/4	-
6	GOL	D	1122	-	-	3/4/4/4	-
7	MPD	B	1010	-	-	4/5/5/5	-
6	GOL	D	1119	-	-	4/4/4/4	-
2	SF4	A	1102	1	-	-	0/6/5/5
2	SF4	B	1001	1	-	-	0/6/5/5
7	MPD	D	1113	-	-	4/5/5/5	-
2	SF4	B	1003	1	-	-	0/6/5/5
2	SF4	C	1102	1	-	-	0/6/5/5
2	SF4	D	1102	1	-	-	0/6/5/5
6	GOL	D	1123	-	-	2/4/4/4	-
6	GOL	D	1117	-	-	3/4/4/4	-
5	SRM	B	1008	1	1/1/19/23	17/38/126/126	-
6	GOL	B	1014	-	-	0/4/4/4	-
2	SF4	D	1103	1	-	-	0/6/5/5
3	FAD	A	1106	-	-	1/30/50/50	0/6/6/6
2	SF4	C	1101	1	-	-	0/6/5/5
6	GOL	D	1121	-	-	3/4/4/4	-
6	GOL	C	1119	-	-	0/4/4/4	-
5	SRM	A	1109	1,4	1/1/19/23	16/38/126/126	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	1117	-	-	2/4/4/4	-
2	SF4	B	1002	1	-	-	0/6/5/5
6	GOL	D	1118	-	-	4/4/4/4	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1109	SRM	C4A-NA	-11.74	1.26	1.35
5	D	1109	SRM	C4A-NA	-11.46	1.27	1.35
5	B	1008	SRM	C4A-NA	-11.22	1.27	1.35
5	C	1108	SRM	C4A-NA	-11.07	1.27	1.35
5	A	1109	SRM	CHD-C4C	9.23	1.48	1.35
5	B	1008	SRM	CHD-C4C	9.13	1.48	1.35
5	C	1108	SRM	CHD-C4C	8.95	1.47	1.35
5	D	1109	SRM	CHD-C4C	8.92	1.47	1.35
3	C	1107	FAD	C9A-C5X	5.19	1.49	1.41
5	D	1109	SRM	C3C-C2C	5.16	1.47	1.36
5	A	1109	SRM	C3C-C2C	4.98	1.47	1.36
5	B	1008	SRM	C3C-C2C	4.86	1.47	1.36
5	C	1108	SRM	C3C-C2C	4.85	1.47	1.36
5	D	1109	SRM	CHC-C1C	4.62	1.47	1.38
5	A	1109	SRM	CHC-C1C	4.61	1.47	1.38
5	B	1008	SRM	CHC-C1C	4.51	1.47	1.38
5	C	1108	SRM	CHC-C1C	4.43	1.47	1.38
5	D	1109	SRM	C3D-C2D	3.83	1.48	1.39
5	B	1008	SRM	FE-NC	3.73	2.10	1.95
5	C	1108	SRM	FE-NC	3.71	2.10	1.95
5	C	1108	SRM	C3D-C2D	3.70	1.47	1.39
5	A	1109	SRM	FE-NC	3.68	2.10	1.95
5	B	1008	SRM	C3D-C2D	3.65	1.47	1.39
3	C	1107	FAD	C8-C7	3.62	1.49	1.40
5	D	1109	SRM	FE-NC	3.61	2.09	1.95
5	A	1109	SRM	C3D-C2D	3.56	1.47	1.39
5	C	1108	SRM	C1C-NC	-3.07	1.33	1.39
5	A	1109	SRM	C1C-NC	-2.94	1.34	1.39
5	B	1008	SRM	C1C-NC	-2.93	1.34	1.39
5	D	1109	SRM	C1C-NC	-2.92	1.34	1.39
5	A	1109	SRM	C1D-CHD	2.65	1.48	1.41
5	C	1108	SRM	C4C-NC	-2.65	1.34	1.39
5	C	1108	SRM	C1D-CHD	2.62	1.48	1.41
5	D	1109	SRM	C4C-NC	-2.59	1.34	1.39
3	C	1107	FAD	C5A-C4A	2.57	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1107	FAD	C4X-N5	2.55	1.35	1.30
5	A	1109	SRM	C4C-NC	-2.55	1.34	1.39
5	B	1008	SRM	CHB-C4A	2.49	1.46	1.39
5	D	1109	SRM	C1D-CHD	2.46	1.47	1.41
5	B	1008	SRM	C1D-CHD	2.44	1.47	1.41
3	C	1107	FAD	C4-N3	-2.43	1.34	1.38
5	B	1008	SRM	C4C-NC	-2.42	1.35	1.39
5	D	1109	SRM	CHB-C4A	2.32	1.45	1.39
5	A	1109	SRM	CHB-C4A	2.32	1.45	1.39
5	C	1108	SRM	CHB-C4A	2.30	1.45	1.39
5	C	1108	SRM	C4D-CHA	2.26	1.47	1.41
5	A	1109	SRM	C4D-CHA	2.18	1.47	1.41
5	B	1008	SRM	C4D-CHA	2.16	1.47	1.41
5	D	1109	SRM	C4D-CHA	2.14	1.47	1.41
5	C	1108	SRM	CHC-C4B	-2.12	1.33	1.39
5	D	1109	SRM	O2C-CCC	-2.06	1.23	1.30
5	D	1109	SRM	C1C-C2C	2.01	1.48	1.45
5	D	1109	SRM	CHC-C4B	-2.00	1.33	1.39

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1108	SRM	C2C-C1C-NC	5.42	115.60	110.32
5	D	1109	SRM	C2C-C1C-NC	5.35	115.53	110.32
5	A	1109	SRM	C2C-C1C-NC	5.27	115.45	110.32
5	B	1008	SRM	C2C-C1C-NC	5.12	115.31	110.32
5	A	1109	SRM	CHC-C1C-NC	-4.88	119.16	124.44
5	D	1109	SRM	CHC-C1C-NC	-4.85	119.20	124.44
5	D	1109	SRM	C3C-C4C-NC	4.75	114.95	110.32
5	C	1108	SRM	C3C-C4C-NC	4.75	114.94	110.32
5	B	1008	SRM	CHC-C1C-NC	-4.65	119.41	124.44
5	B	1008	SRM	C3C-C4C-NC	4.53	114.73	110.32
5	C	1108	SRM	CHC-C1C-NC	-4.50	119.57	124.44
5	A	1109	SRM	C3C-C4C-NC	4.37	114.58	110.32
5	A	1109	SRM	C1C-C2C-C3C	-3.99	102.25	106.86
5	D	1109	SRM	C1C-C2C-C3C	-3.99	102.25	106.86
5	C	1108	SRM	C1C-C2C-C3C	-3.88	102.37	106.86
5	B	1008	SRM	C1C-C2C-C3C	-3.87	102.39	106.86
5	B	1008	SRM	C2A-C1A-CHA	-3.83	120.04	123.54
5	A	1109	SRM	C2A-C1A-CHA	-3.70	120.16	123.54
5	D	1109	SRM	C2A-C1A-CHA	-3.64	120.21	123.54
3	C	1107	FAD	N3A-C2A-N1A	-3.54	123.15	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1108	SRM	C4C-C3C-C2C	-3.49	102.83	106.86
5	D	1109	SRM	C4C-C3C-C2C	-3.47	102.85	106.86
5	C	1108	SRM	C2A-C1A-CHA	-3.39	120.45	123.54
5	A	1109	SRM	CBD-CAD-C2D	-3.25	107.08	112.62
5	B	1008	SRM	C4C-C3C-C2C	-3.22	103.13	106.86
5	A	1109	SRM	C4C-C3C-C2C	-3.22	103.14	106.86
5	D	1109	SRM	CBD-CAD-C2D	-3.09	107.35	112.62
5	B	1008	SRM	CBD-CAD-C2D	-3.02	107.46	112.62
3	C	1107	FAD	C4-C4X-N5	2.83	122.26	118.23
5	A	1109	SRM	C4D-CHA-C1A	-2.80	124.56	130.12
5	B	1008	SRM	C4A-CHB-C1B	-2.76	121.80	125.88
3	C	1107	FAD	C4A-C5A-N7A	-2.71	106.57	109.40
5	D	1109	SRM	CDD-C3D-C2D	2.67	131.25	126.49
5	C	1108	SRM	CAC-CBC-CCC	-2.60	108.00	113.60
5	C	1108	SRM	CHD-C4C-NC	-2.60	121.61	124.43
5	D	1109	SRM	CHD-C4C-NC	-2.57	121.64	124.43
5	C	1108	SRM	C4A-CHB-C1B	-2.56	122.10	125.88
5	C	1108	SRM	C4D-CHA-C1A	-2.55	125.08	130.12
3	C	1107	FAD	C4X-C10-N1	-2.53	118.87	124.73
5	D	1109	SRM	C4A-CHB-C1B	-2.53	122.16	125.88
5	B	1008	SRM	C4D-CHA-C1A	-2.52	125.13	130.12
3	C	1107	FAD	O2-C2-N1	-2.48	117.72	121.83
5	A	1109	SRM	C4A-CHB-C1B	-2.48	122.22	125.88
3	C	1107	FAD	P-O3P-PA	-2.47	124.35	132.83
5	D	1109	SRM	C4D-CHA-C1A	-2.40	125.36	130.12
5	A	1109	SRM	CDD-C3D-C2D	2.39	130.76	126.49
5	B	1008	SRM	CDD-C3D-C2D	2.39	130.75	126.49
3	B	1006	FAD	C5A-C6A-N6A	2.38	123.97	120.35
5	C	1108	SRM	CAC-C3C-C4C	2.34	129.31	124.89
3	C	1107	FAD	O4-C4-C4X	-2.34	120.39	126.60
3	A	1106	FAD	C5A-C6A-N6A	2.34	123.91	120.35
5	A	1109	SRM	CHD-C4C-NC	-2.33	121.91	124.43
3	D	1106	FAD	C5A-C6A-N6A	2.31	123.86	120.35
5	B	1008	SRM	CAC-CBC-CCC	-2.30	108.66	113.60
5	C	1108	SRM	CBD-CAD-C2D	-2.26	108.76	112.62
3	C	1107	FAD	C10-N1-C2	2.17	121.25	116.90
3	C	1107	FAD	C4X-C4-N3	2.17	118.69	113.19
5	A	1109	SRM	CAC-CBC-CCC	-2.15	108.98	113.60
5	B	1008	SRM	O3D-CED-CDD	-2.13	116.96	123.04
5	B	1008	SRM	CAC-C3C-C4C	2.11	128.87	124.89
5	A	1109	SRM	O3D-CED-CDD	-2.05	117.19	123.04
5	B	1008	SRM	C1A-NA-C4A	2.04	107.55	105.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1107	FAD	C3B-C2B-C1B	2.03	104.03	100.98
5	A	1109	SRM	CAC-C3C-C4C	2.03	128.71	124.89
5	D	1109	SRM	O3D-CED-CDD	-2.02	117.26	123.04
5	B	1008	SRM	CHD-C4C-NC	-2.02	122.25	124.43
3	D	1106	FAD	C4-N3-C2	-2.01	121.93	125.64
3	C	1107	FAD	C2A-N1A-C6A	2.01	122.19	118.75

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1109	SRM	NC
5	B	1008	SRM	NC
5	C	1108	SRM	NC
5	D	1109	SRM	NC

All (141) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1109	SRM	C1A-C2A-CDA-CEA
5	A	1109	SRM	CMA-C2A-CDA-CEA
5	A	1109	SRM	C2C-C3C-CAC-CBC
5	A	1109	SRM	C4C-C3C-CAC-CBC
5	B	1008	SRM	C1A-C2A-CDA-CEA
5	B	1008	SRM	CMA-C2A-CDA-CEA
5	B	1008	SRM	C4A-C3A-CAA-CBA
5	B	1008	SRM	C2C-C3C-CAC-CBC
5	C	1108	SRM	C1A-C2A-CDA-CEA
5	C	1108	SRM	CMA-C2A-CDA-CEA
5	C	1108	SRM	C3A-C2A-CDA-CEA
5	C	1108	SRM	C4A-C3A-CAA-CBA
5	C	1108	SRM	C2C-C3C-CAC-CBC
5	D	1109	SRM	C1A-C2A-CDA-CEA
5	D	1109	SRM	CMA-C2A-CDA-CEA
5	D	1109	SRM	C3A-C2A-CDA-CEA
5	D	1109	SRM	C2A-C3A-CAA-CBA
5	D	1109	SRM	C4A-C3A-CAA-CBA
5	D	1109	SRM	C2C-C3C-CAC-CBC
5	D	1109	SRM	C4C-C3C-CAC-CBC
6	A	1110	GOL	O1-C1-C2-C3
6	A	1115	GOL	O1-C1-C2-C3
6	A	1117	GOL	C1-C2-C3-O3
6	A	1117	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	B	1009	GOL	O1-C1-C2-C3
6	B	1009	GOL	C1-C2-C3-O3
6	B	1009	GOL	O2-C2-C3-O3
6	B	1017	GOL	O1-C1-C2-C3
6	B	1018	GOL	O1-C1-C2-C3
6	D	1111	GOL	O1-C1-C2-C3
6	D	1118	GOL	O1-C1-C2-C3
6	D	1118	GOL	C1-C2-C3-O3
6	D	1118	GOL	O2-C2-C3-O3
6	D	1122	GOL	C1-C2-C3-O3
6	D	1123	GOL	O1-C1-C2-C3
6	D	1125	GOL	O1-C1-C2-C3
7	D	1113	MPD	C1-C2-C3-C4
5	B	1008	SRM	C4C-C3C-CAC-CBC
5	C	1108	SRM	C4C-C3C-CAC-CBC
5	B	1008	SRM	C2A-C3A-CAA-CBA
5	C	1108	SRM	C2A-C3A-CAA-CBA
5	A	1109	SRM	C4A-C3A-CAA-CBA
5	D	1109	SRM	C3A-CAA-CBA-CCA
6	A	1110	GOL	O1-C1-C2-O2
6	A	1115	GOL	O1-C1-C2-O2
6	B	1018	GOL	O1-C1-C2-O2
6	C	1110	GOL	O2-C2-C3-O3
6	D	1111	GOL	O1-C1-C2-O2
6	D	1118	GOL	O1-C1-C2-O2
6	D	1123	GOL	O1-C1-C2-O2
5	B	1008	SRM	C4B-C3B-CAB-CBB
5	A	1109	SRM	C2A-C3A-CAA-CBA
5	A	1109	SRM	C4B-C3B-CAB-CBB
5	A	1109	SRM	C3A-C2A-CDA-CEA
6	A	1116	GOL	O1-C1-C2-C3
6	B	1015	GOL	O1-C1-C2-C3
6	C	1110	GOL	C1-C2-C3-O3
6	C	1111	GOL	O1-C1-C2-C3
6	C	1118	GOL	O1-C1-C2-C3
6	C	1120	GOL	C1-C2-C3-O3
6	D	1112	GOL	O1-C1-C2-C3
6	D	1117	GOL	C1-C2-C3-O3
6	D	1119	GOL	O1-C1-C2-C3
6	D	1119	GOL	C1-C2-C3-O3
6	D	1120	GOL	O1-C1-C2-C3
6	D	1120	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	D	1121	GOL	O1-C1-C2-C3
6	D	1125	GOL	C1-C2-C3-O3
6	B	1017	GOL	O1-C1-C2-O2
6	C	1111	GOL	O1-C1-C2-O2
6	C	1120	GOL	O2-C2-C3-O3
6	D	1119	GOL	O2-C2-C3-O3
6	D	1122	GOL	O2-C2-C3-O3
6	D	1125	GOL	O1-C1-C2-O2
6	B	1015	GOL	O1-C1-C2-O2
6	D	1112	GOL	O1-C1-C2-O2
6	D	1117	GOL	O2-C2-C3-O3
5	D	1109	SRM	C2B-CDB-CEB-O4B
5	B	1008	SRM	C3C-CAC-CBC-CCC
5	D	1109	SRM	C3C-CAC-CBC-CCC
5	C	1108	SRM	C4B-C3B-CAB-CBB
5	A	1109	SRM	C3C-CAC-CBC-CCC
5	C	1108	SRM	C3C-CAC-CBC-CCC
6	B	1009	GOL	O1-C1-C2-O2
6	B	1017	GOL	O2-C2-C3-O3
6	C	1118	GOL	O1-C1-C2-O2
6	D	1112	GOL	O2-C2-C3-O3
6	D	1121	GOL	O1-C1-C2-O2
7	D	1113	MPD	O2-C2-C3-C4
5	A	1109	SRM	C3A-CAA-CBA-CCA
5	C	1108	SRM	C3A-CAA-CBA-CCA
6	A	1111	GOL	O2-C2-C3-O3
6	C	1111	GOL	O2-C2-C3-O3
6	D	1117	GOL	O1-C1-C2-O2
6	D	1119	GOL	O1-C1-C2-O2
6	D	1120	GOL	O1-C1-C2-O2
6	D	1121	GOL	O2-C2-C3-O3
5	B	1008	SRM	C3A-CAA-CBA-CCA
6	A	1111	GOL	C1-C2-C3-O3
6	D	1122	GOL	O1-C1-C2-C3
5	C	1108	SRM	C2B-CDB-CEB-O4B
5	D	1109	SRM	C2B-CDB-CEB-O3B
7	B	1010	MPD	CM-C2-C3-C4
7	D	1113	MPD	CM-C2-C3-C4
5	D	1109	SRM	C4B-C3B-CAB-CBB
5	C	1108	SRM	C2B-CDB-CEB-O3B
5	D	1109	SRM	CAB-CBB-CCB-O2B
5	D	1109	SRM	CAB-CBB-CCB-O1B

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Mol	Chain	Res	Type	Atoms
5	A	1109	SRM	CAB-CBB-CCB-O2B
3	B	1006	FAD	PA-O3P-P-O1P
3	A	1106	FAD	O4B-C4B-C5B-O5B
5	A	1109	SRM	CAB-CBB-CCB-O1B
5	B	1008	SRM	C3D-CDD-CED-O4D
7	A	1112	MPD	O2-C2-C3-C4
7	B	1010	MPD	O2-C2-C3-C4
5	A	1109	SRM	C3D-CDD-CED-O4D
5	B	1008	SRM	CAB-CBB-CCB-O1B
5	B	1008	SRM	CAB-CBB-CCB-O2B
5	C	1108	SRM	CAB-CBB-CCB-O1B
5	C	1108	SRM	CAB-CBB-CCB-O2B
5	B	1008	SRM	C2B-C3B-CAB-CBB
3	D	1106	FAD	O4B-C4B-C5B-O5B
5	A	1109	SRM	C3D-CDD-CED-O3D
5	B	1008	SRM	C3D-CDD-CED-O3D
5	D	1109	SRM	C3D-CDD-CED-O3D
3	C	1107	FAD	O4B-C4B-C5B-O5B
5	B	1008	SRM	CAD-CBD-CCD-O1D
6	D	1112	GOL	C1-C2-C3-O3
6	D	1124	GOL	C1-C2-C3-O3
7	B	1010	MPD	C2-C3-C4-C5
7	C	1112	MPD	C2-C3-C4-C5
7	D	1113	MPD	C2-C3-C4-C5
3	B	1006	FAD	O4B-C4B-C5B-O5B
5	B	1008	SRM	CAC-CBC-CCC-O2C
5	A	1109	SRM	CAC-CBC-CCC-O2C
5	A	1109	SRM	CAC-CBC-CCC-O1C
6	D	1120	GOL	O2-C2-C3-O3
5	B	1008	SRM	CAD-CBD-CCD-O2D
7	A	1112	MPD	C2-C3-C4-O4
7	B	1010	MPD	C2-C3-C4-O4
7	C	1112	MPD	C2-C3-C4-O4

There are no ring outliers.

14 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1013	SO3	2	0
4	C	1117	SO3	1	0
5	D	1109	SRM	2	0
6	C	1111	GOL	2	0

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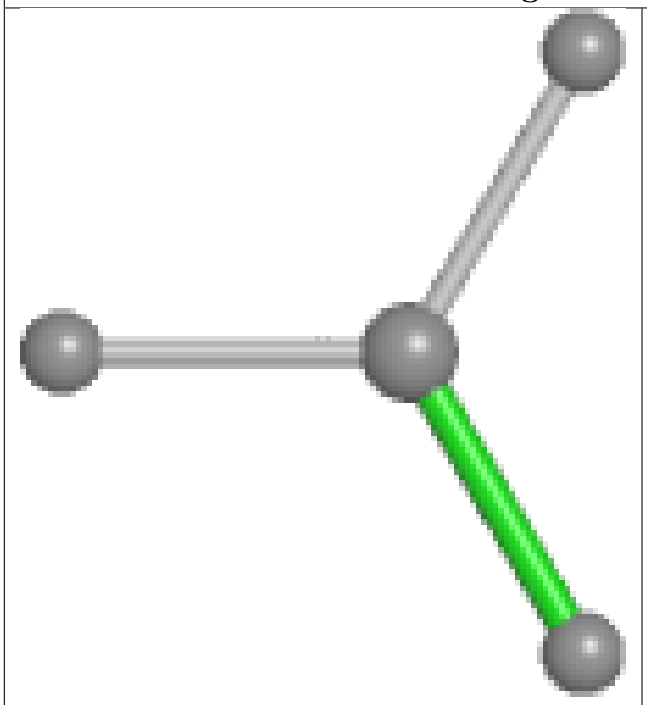
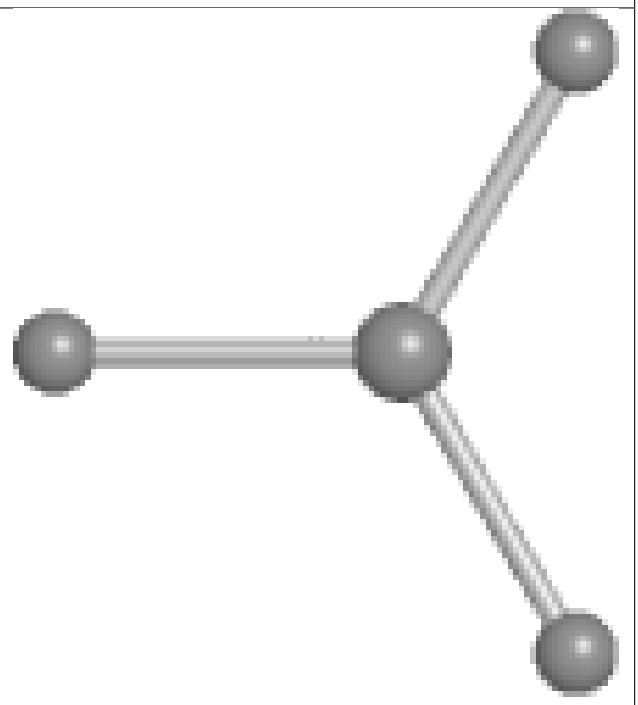
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1125	GOL	1	0
5	C	1108	SRM	4	0
3	C	1107	FAD	1	0
3	D	1106	FAD	1	0
2	A	1102	SF4	1	0
2	C	1102	SF4	1	0
7	D	1113	MPD	1	0
5	B	1008	SRM	3	0
4	A	1108	SO3	1	0
5	A	1109	SRM	6	0

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.

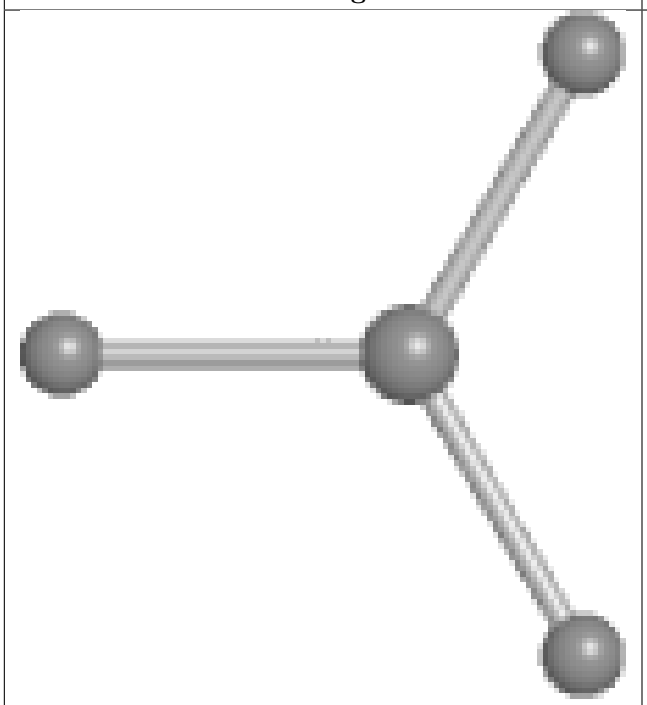
Ligand SO3 B 1013



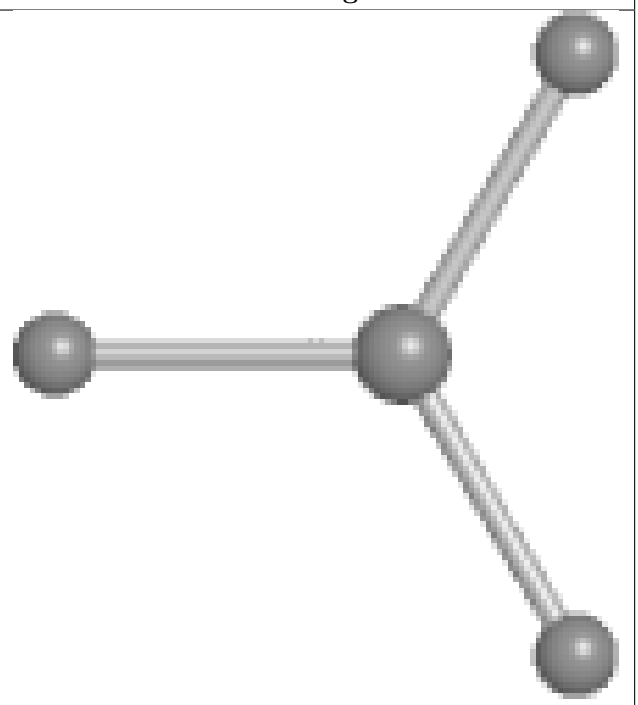
Bond lengths



Bond angles

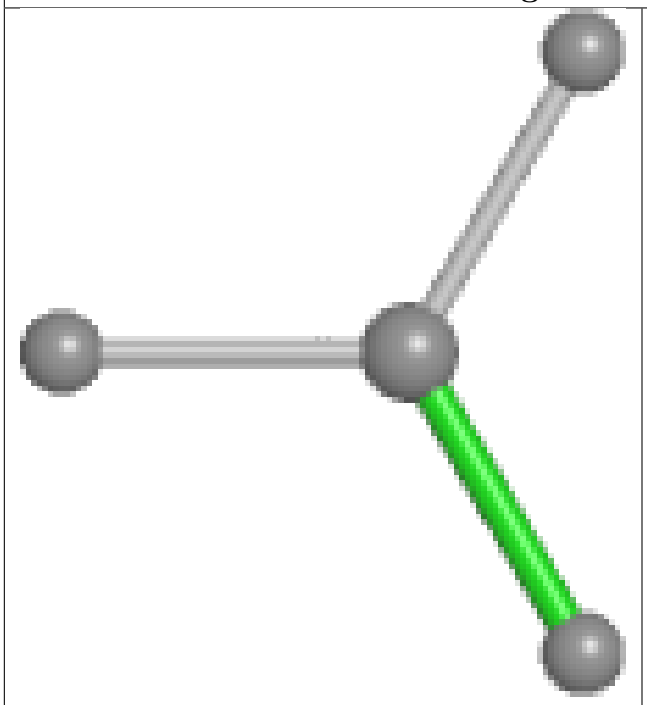


Torsions

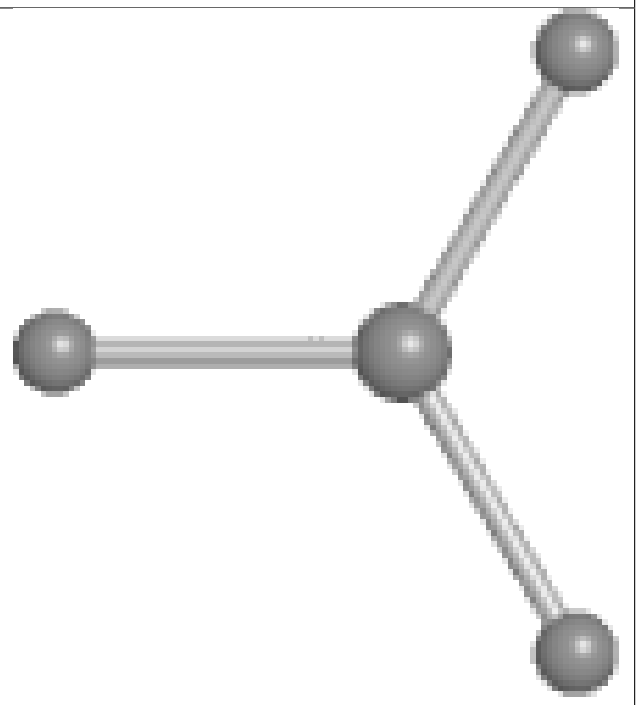


Rings

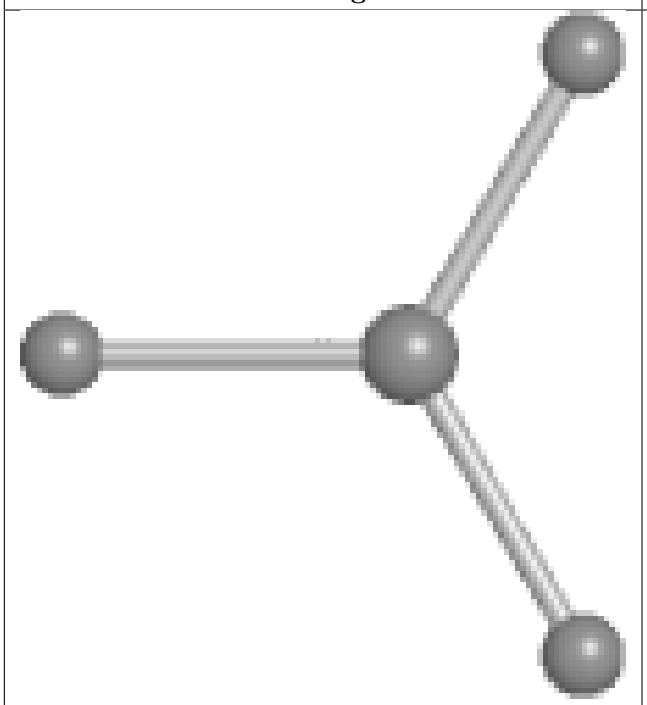
Ligand SO3 C 1117



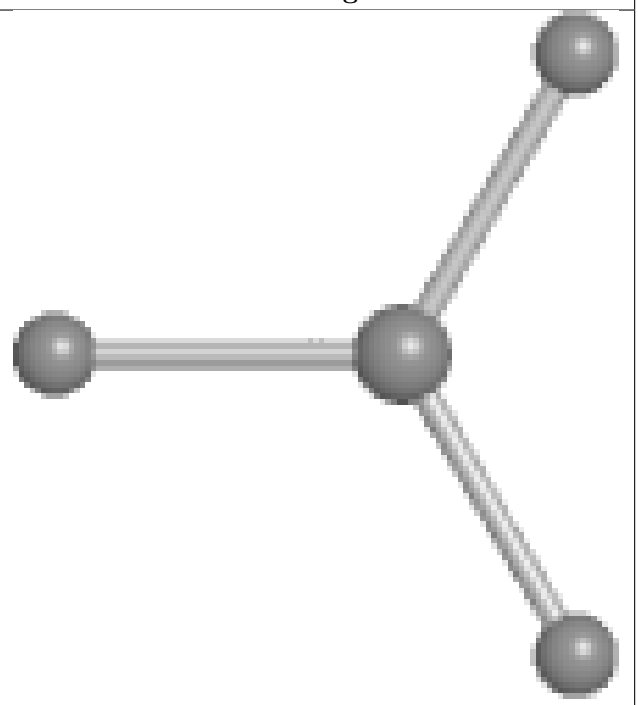
Bond lengths



Bond angles

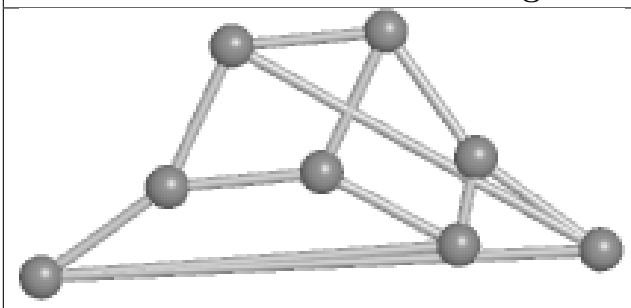


Torsions

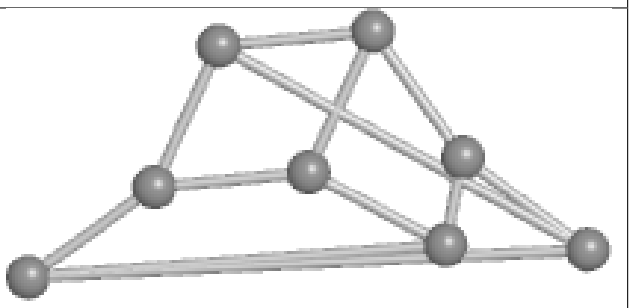


Rings

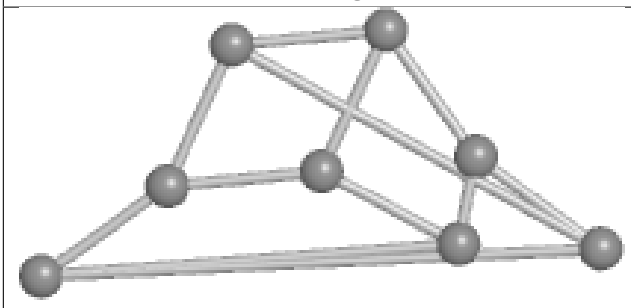
Ligand SF4 B 1004



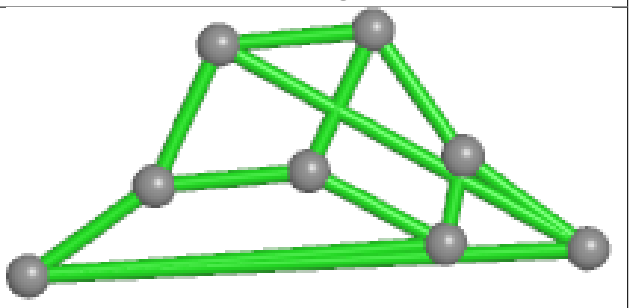
Bond lengths



Bond angles

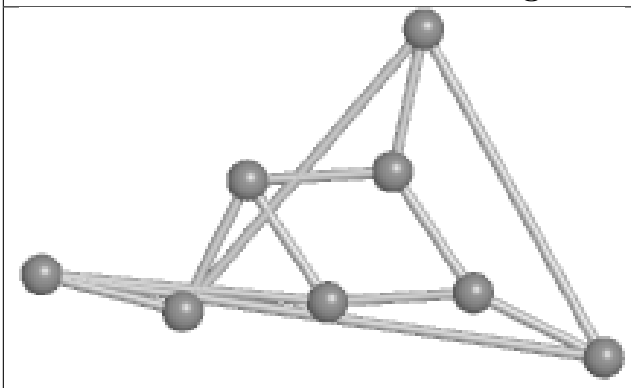


Torsions



Rings

Ligand SF4 B 1007



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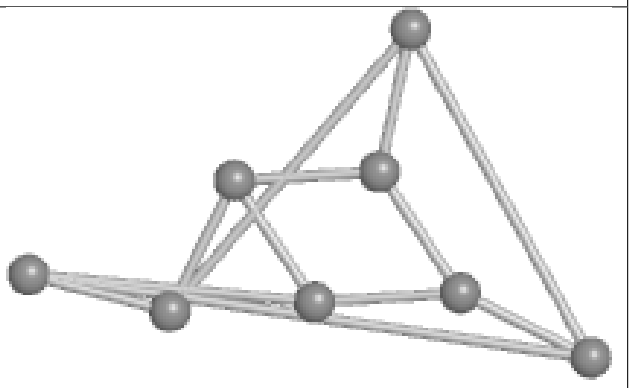
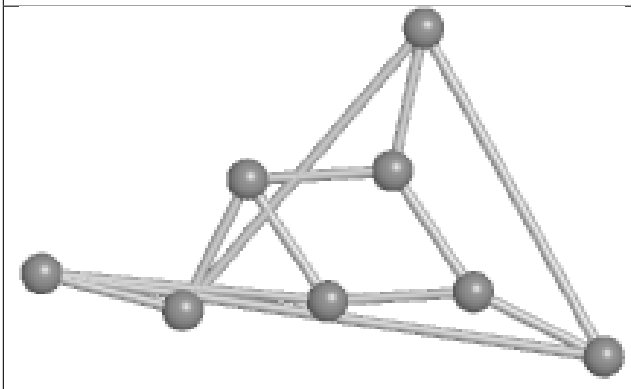
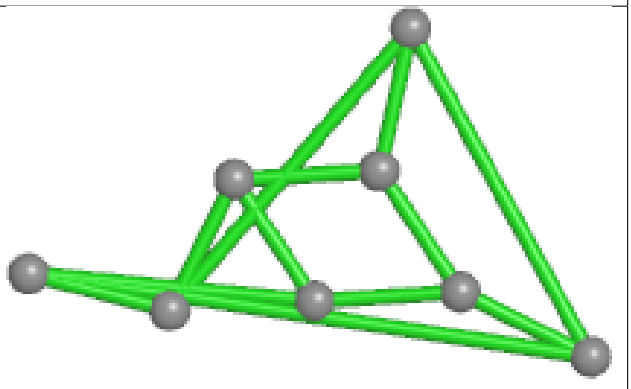


Bond angles

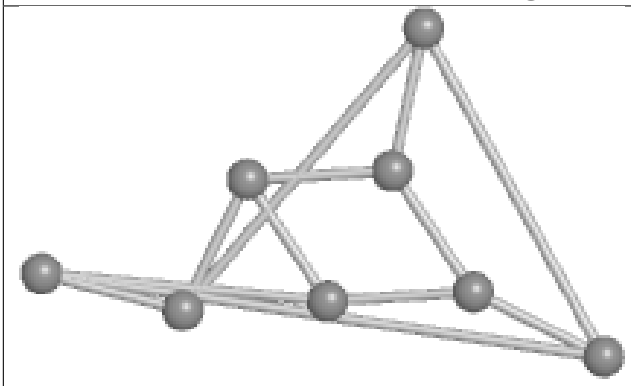


Torsions

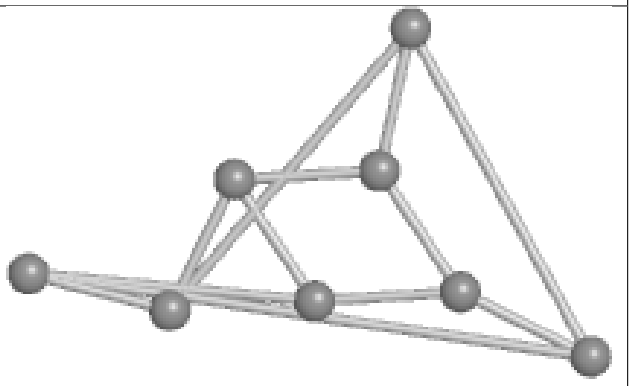


Rings

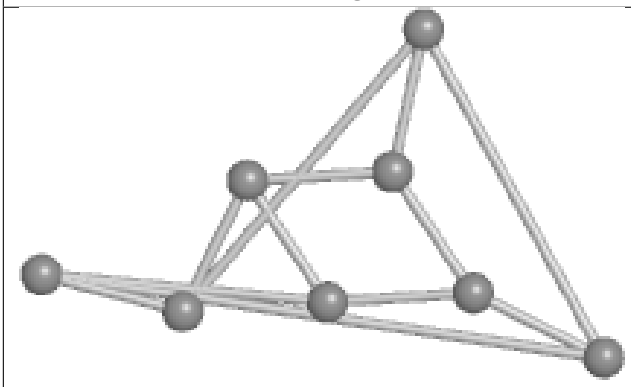
Ligand SF4 C 1103



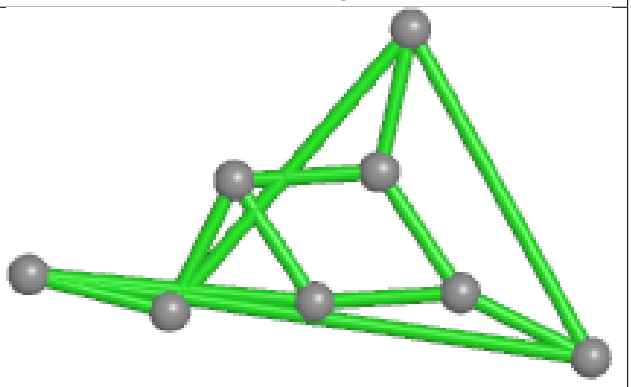
Bond lengths



Bond angles

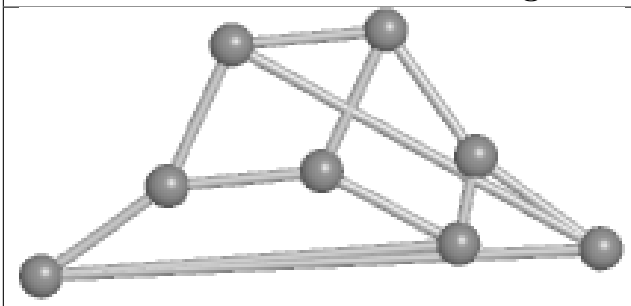


Torsions



Rings

Ligand SF4 C 1104



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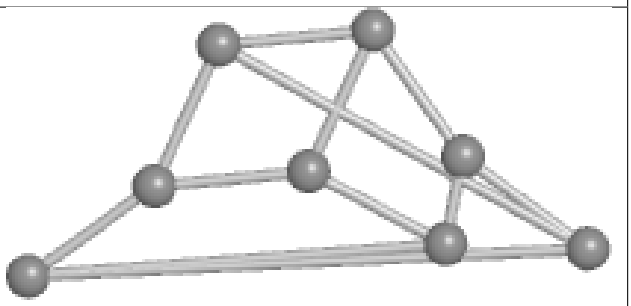
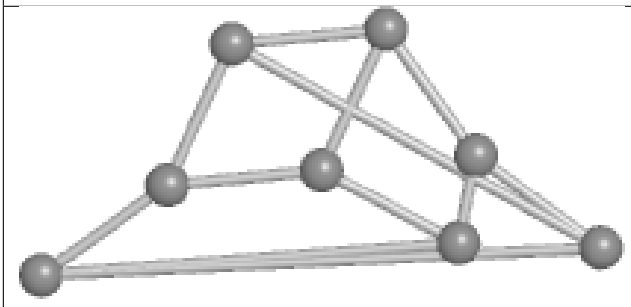


Bond angles



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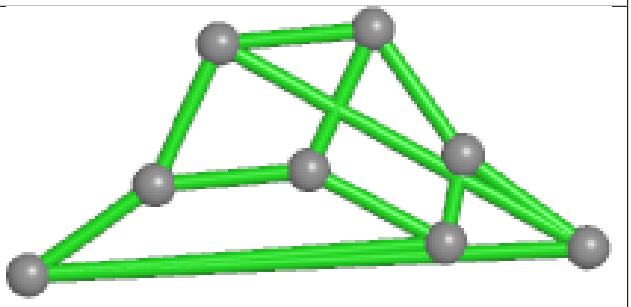
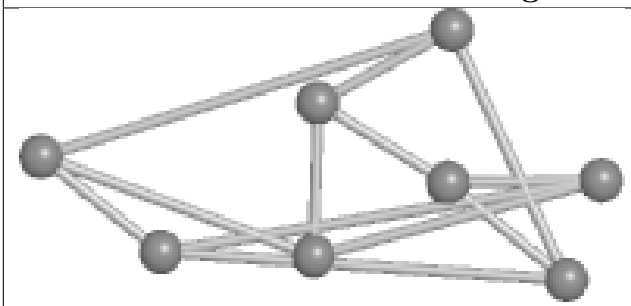


Rings

Ligand SF4 A 1107



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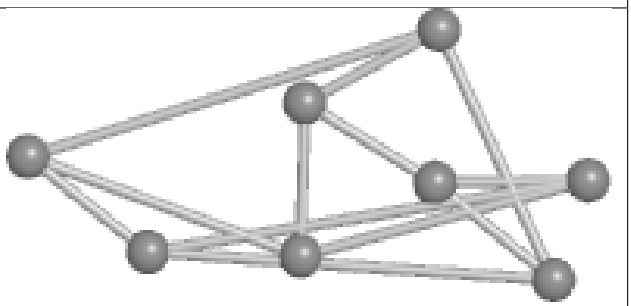
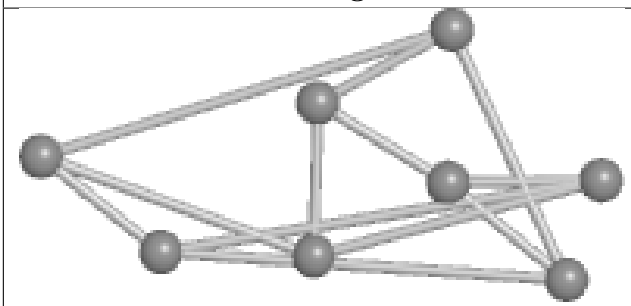


Bond angles



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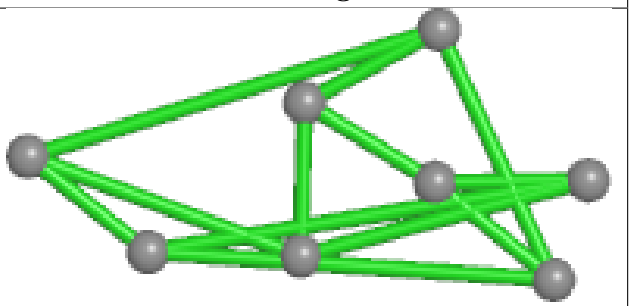
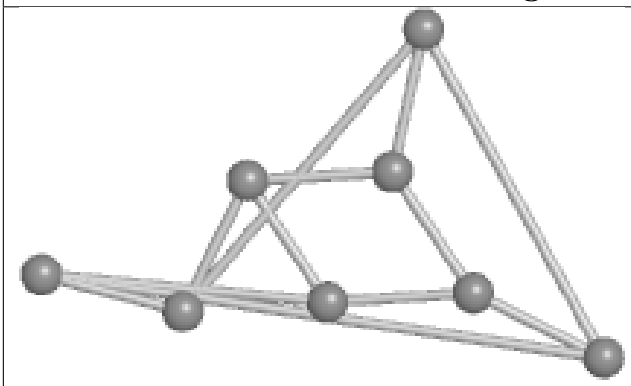


Rings

Ligand SF4 B 1005



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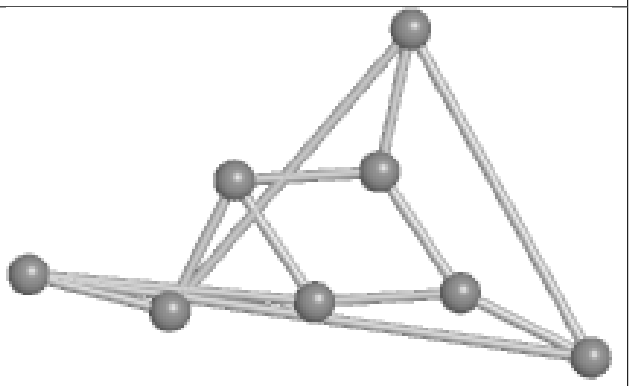
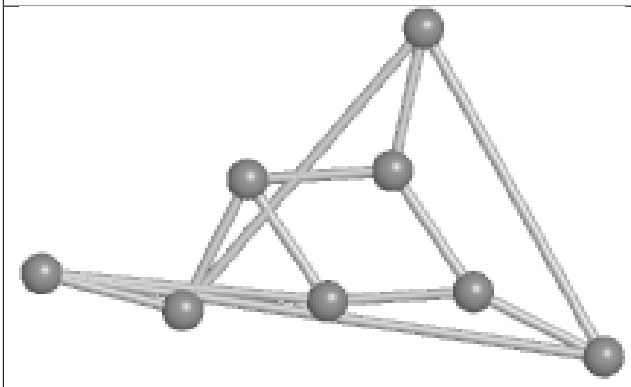


Bond angles



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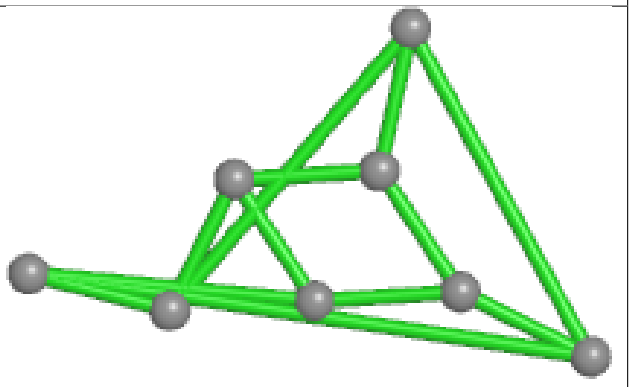
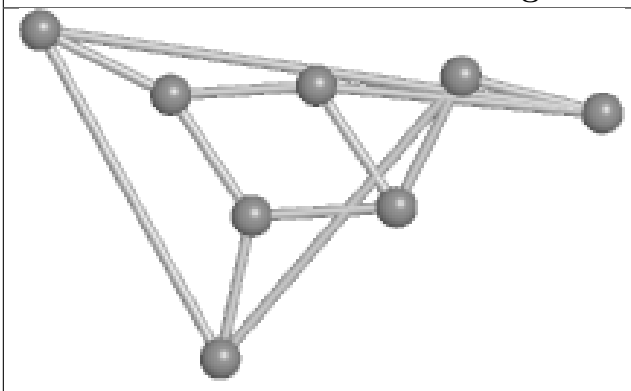


Rings

Ligand SF4 A 1103



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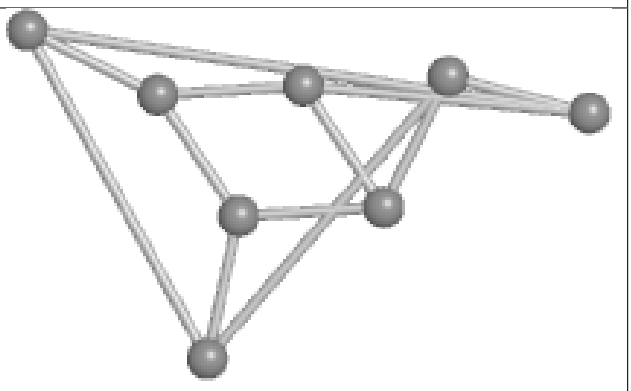
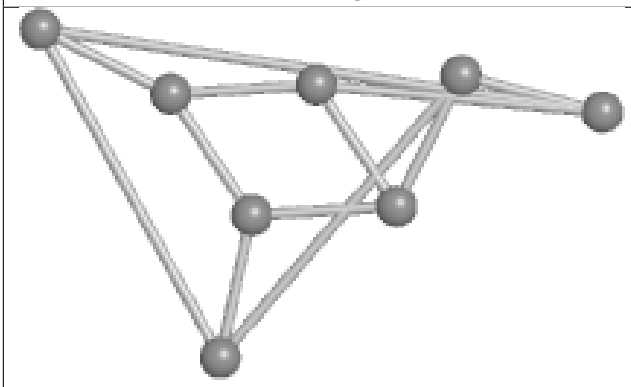


Bond angles



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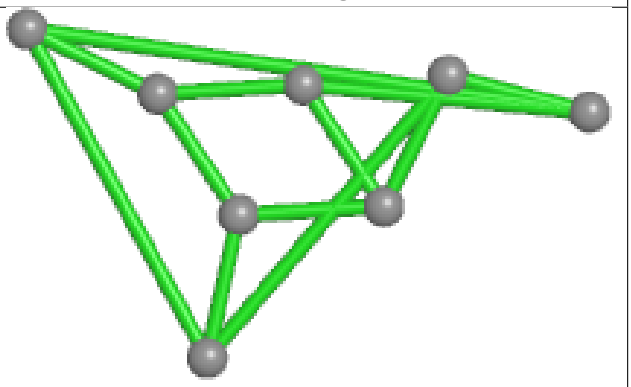
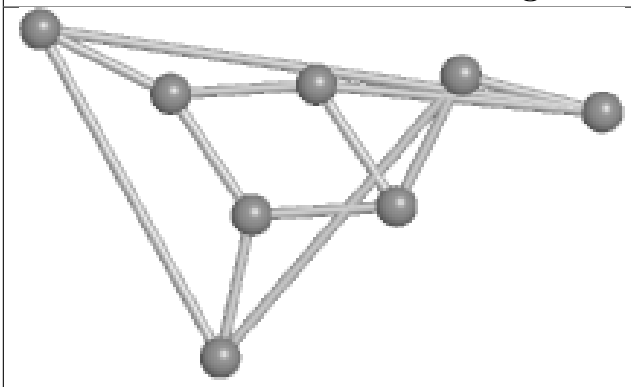


Rings

Ligand SF4 A 1104



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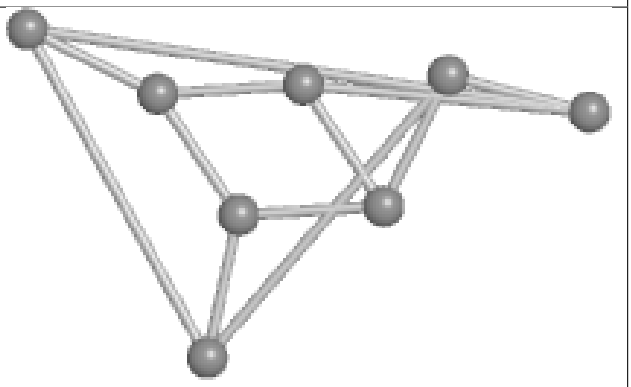
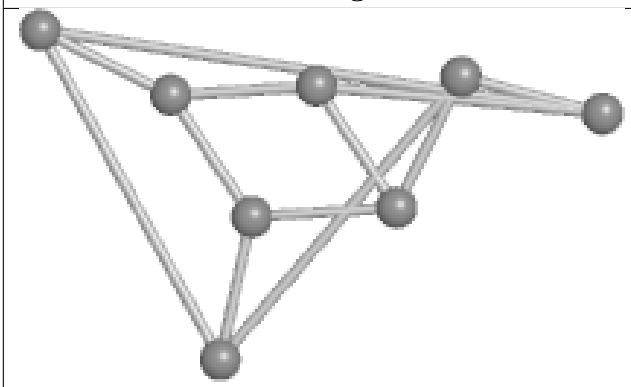
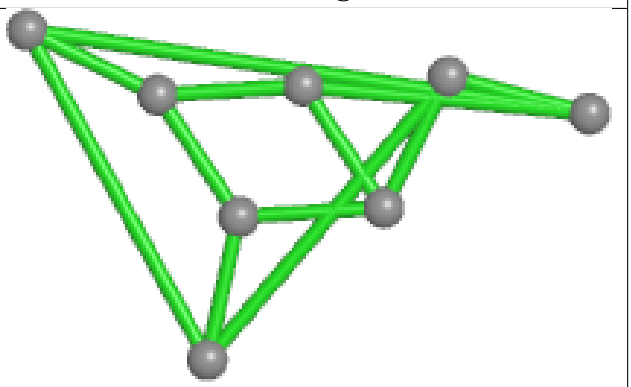


Bond angles

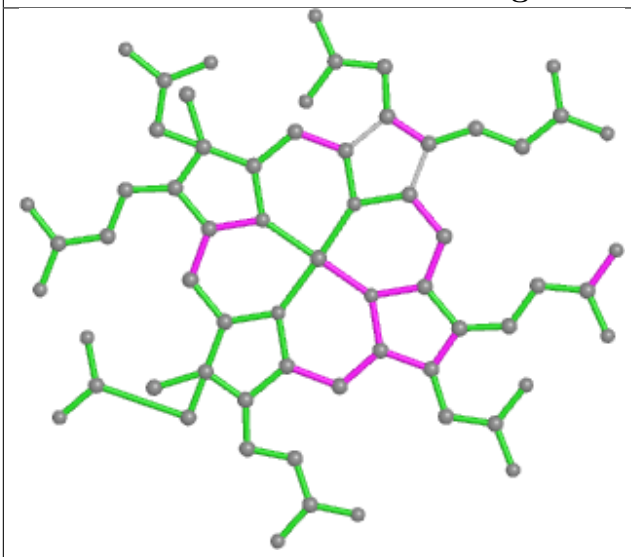


Torsions



Rings

Ligand SRM D 1109



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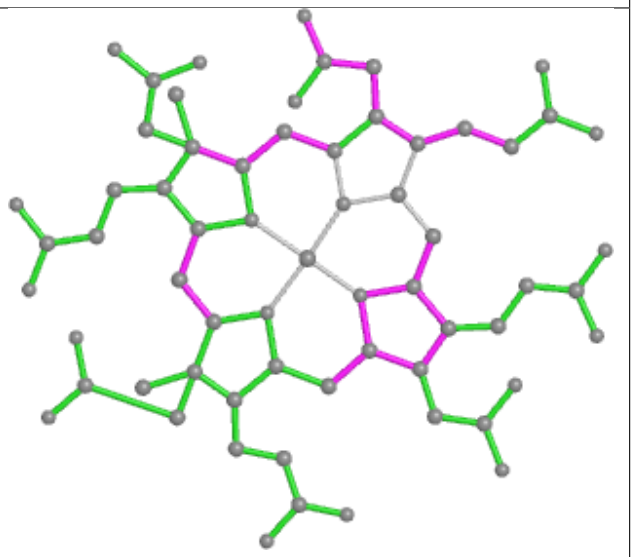
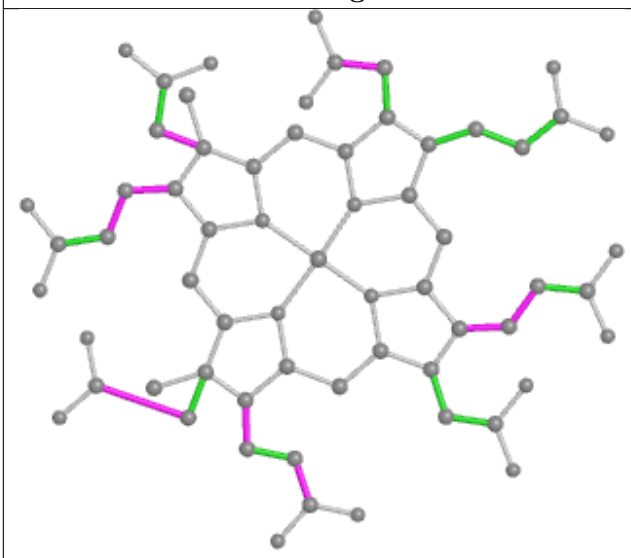
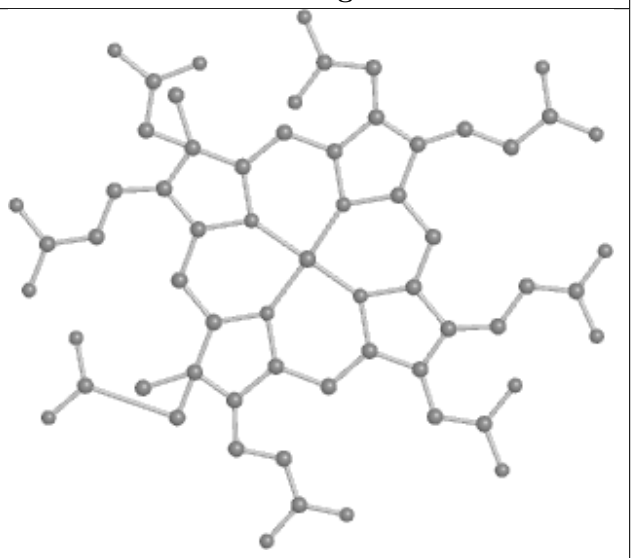


Bond angles

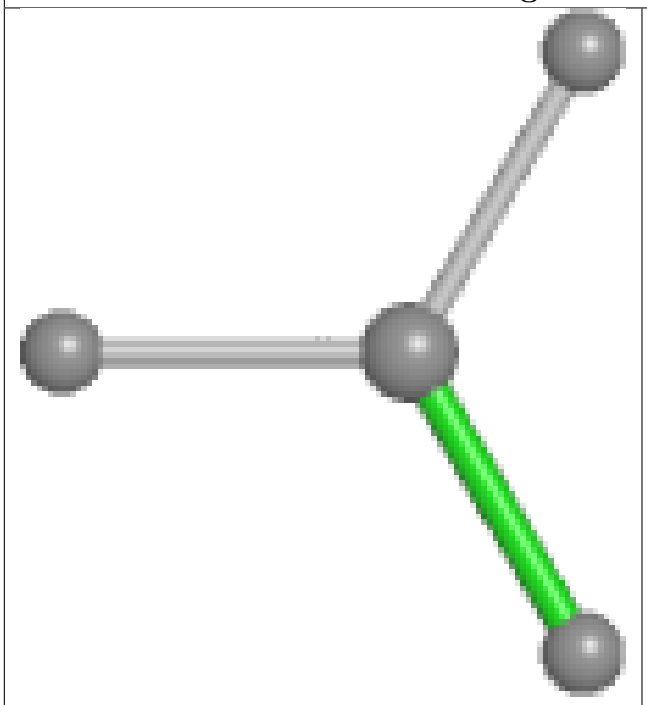


Torsions



Rings

Ligand SO3 D 1108



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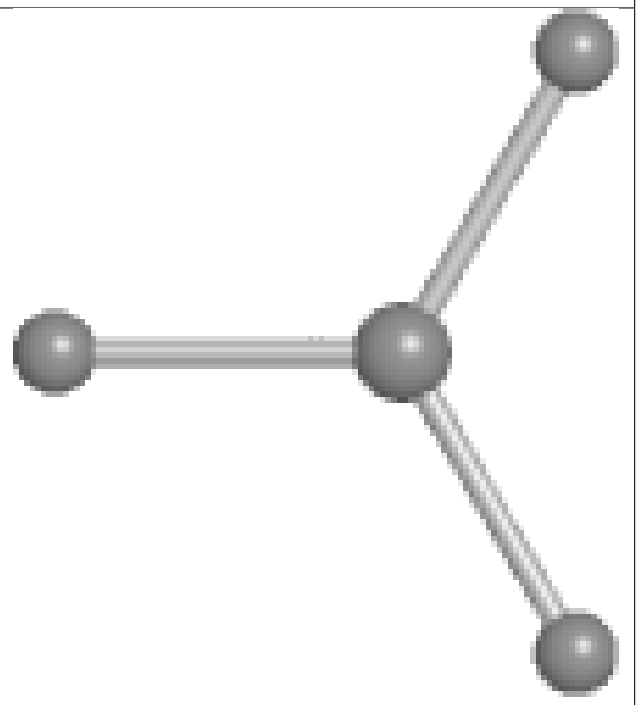
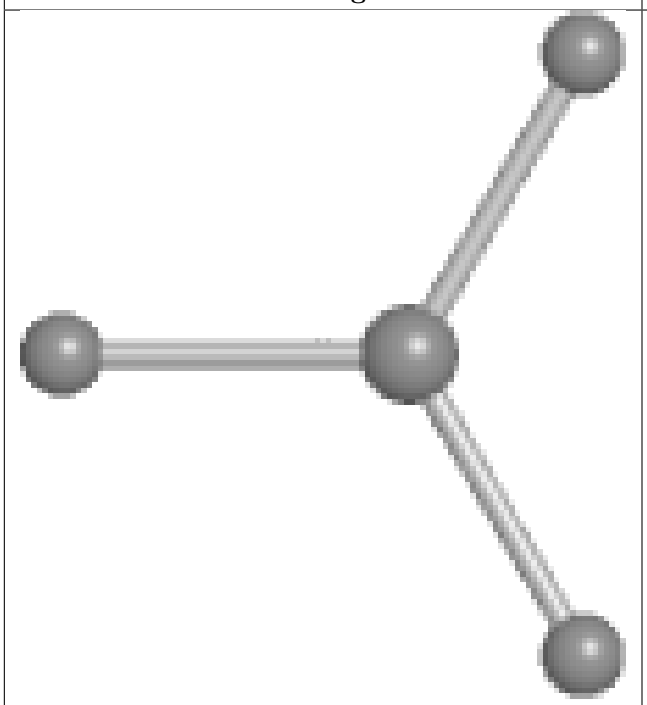
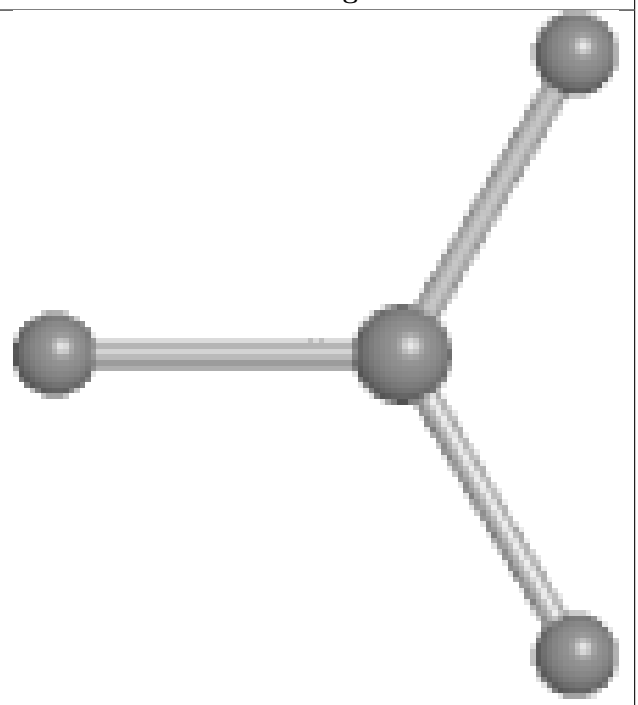


Bond angles

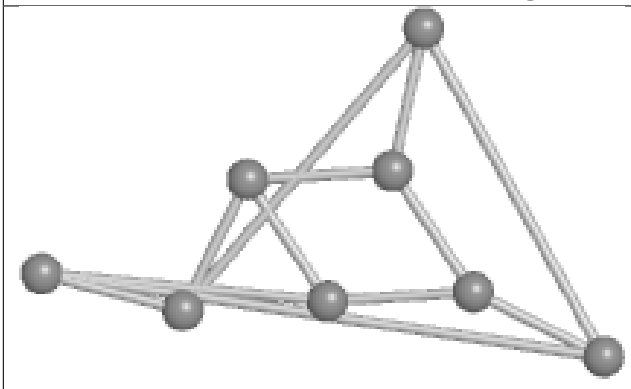


Torsions



Rings

Ligand SF4 D 1105



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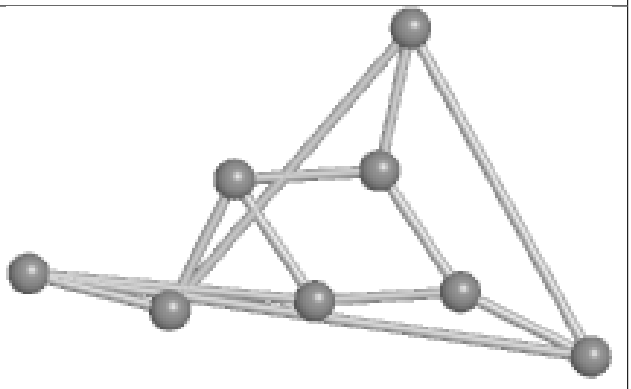
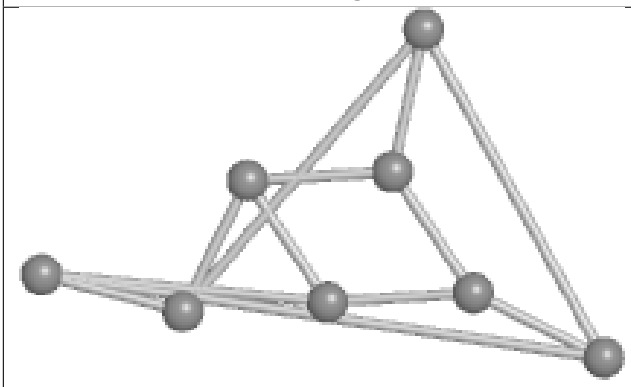
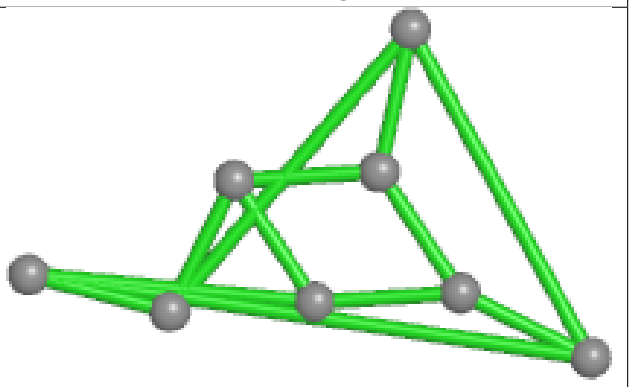


Bond angles

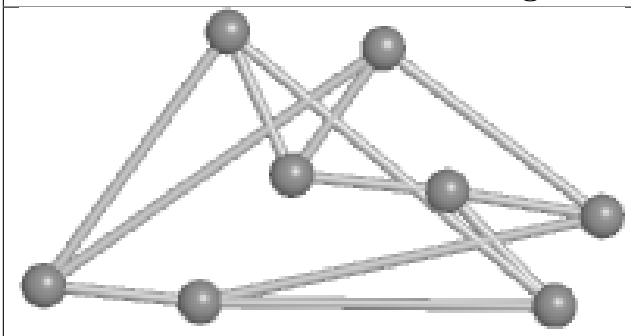


Torsions

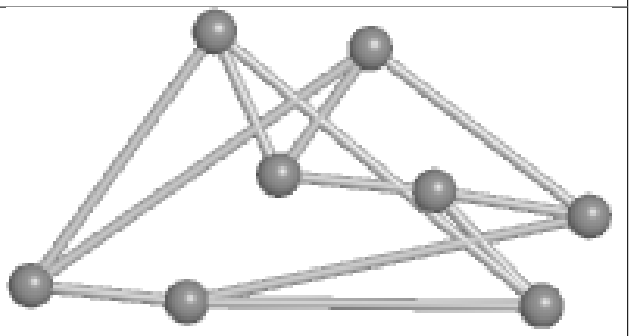


Rings

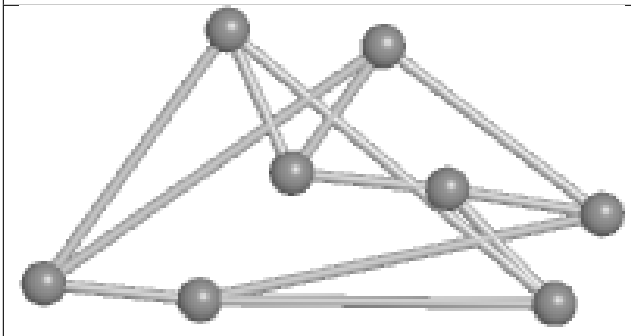
Ligand SF4 D 1101



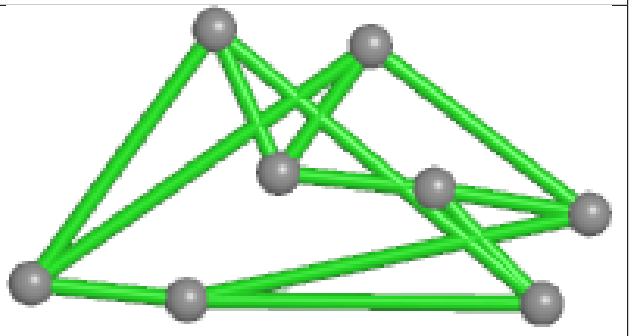
Bond lengths



Bond angles

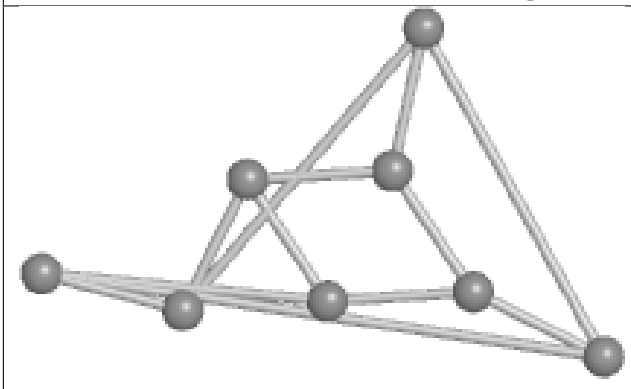


Torsions

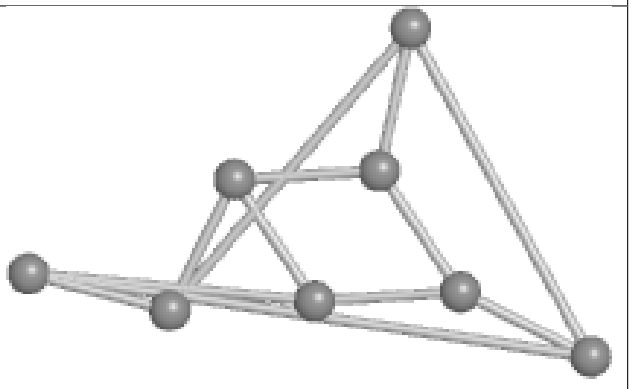


Rings

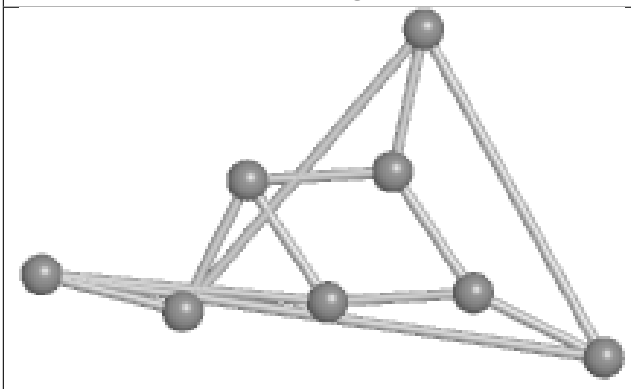
Ligand SF4 A 1105



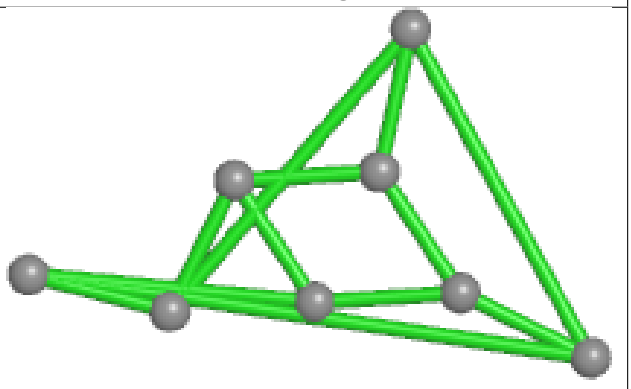
Bond lengths



Bond angles

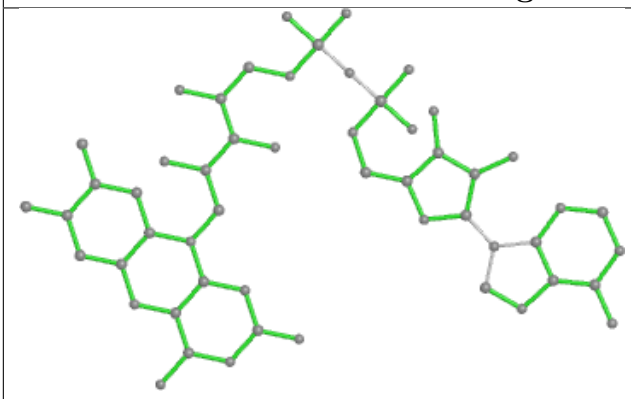


Torsions

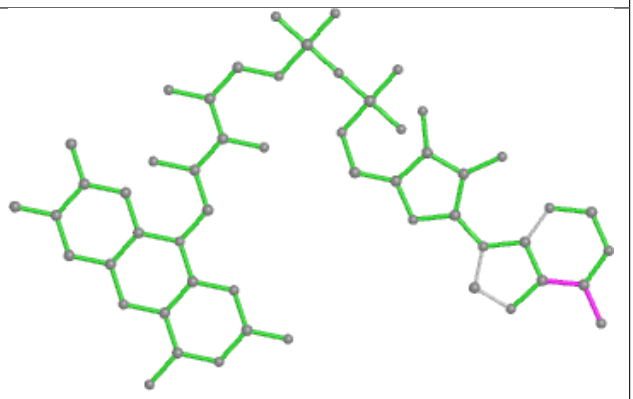


Rings

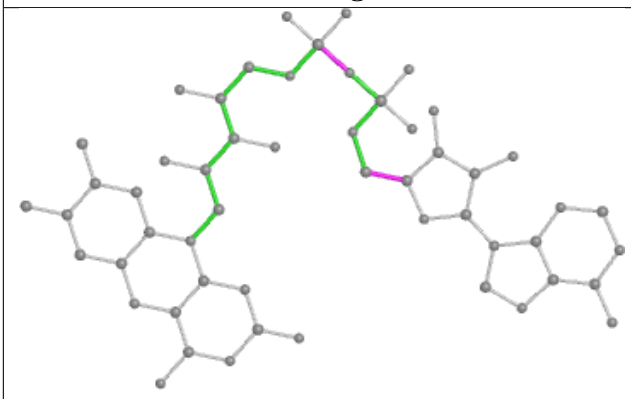
Ligand FAD B 1006



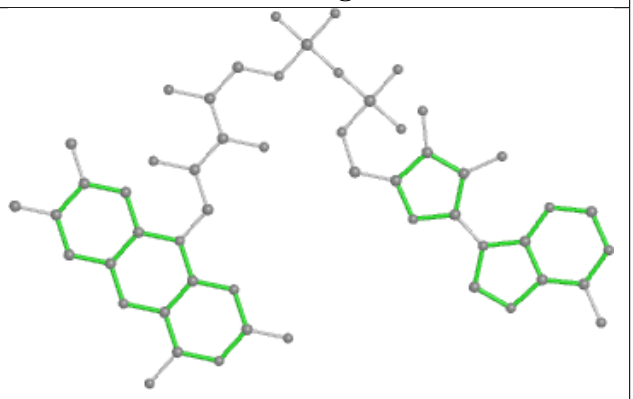
Bond lengths



Bond angles

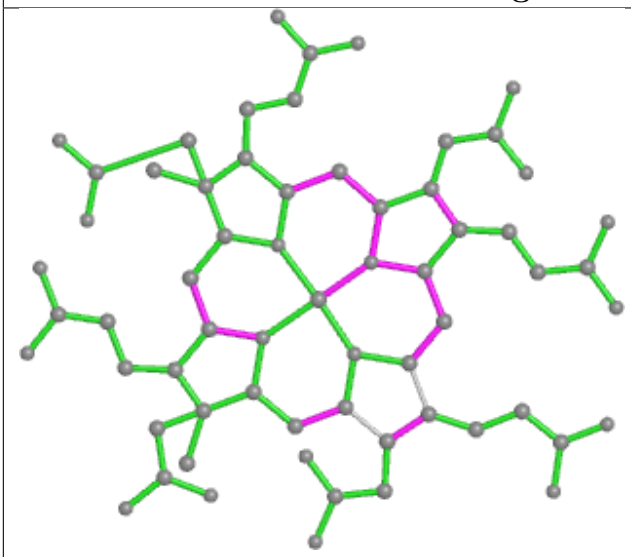


Torsions

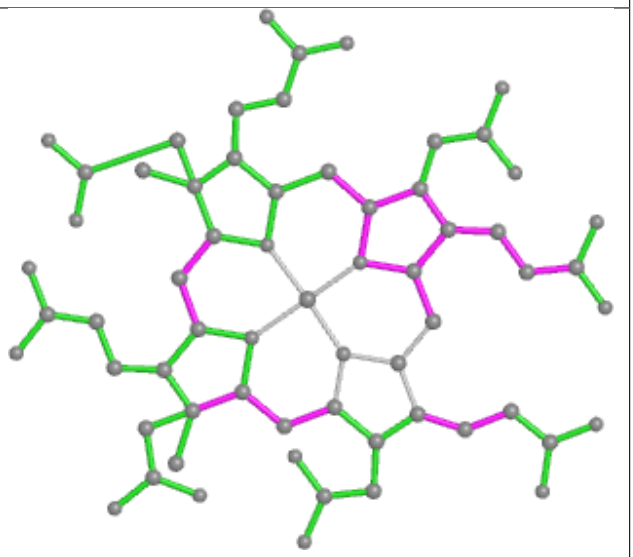


Rings

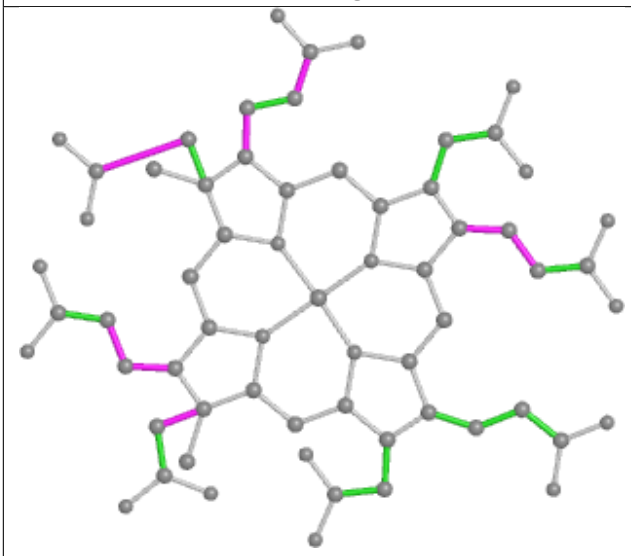
Ligand SRM C 1108



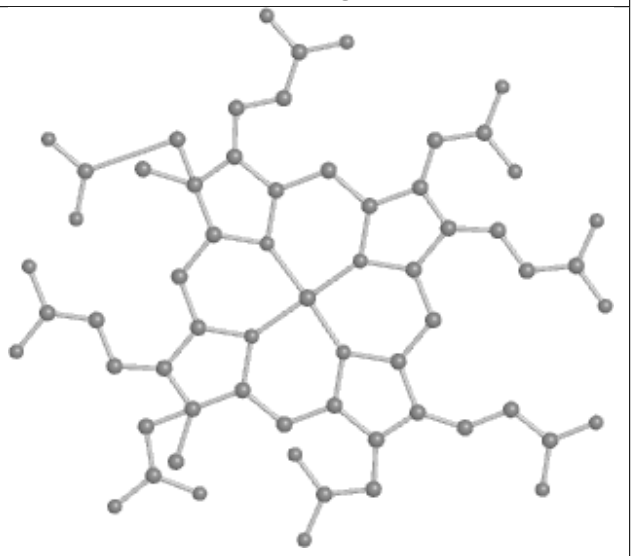
Bond lengths



Bond angles

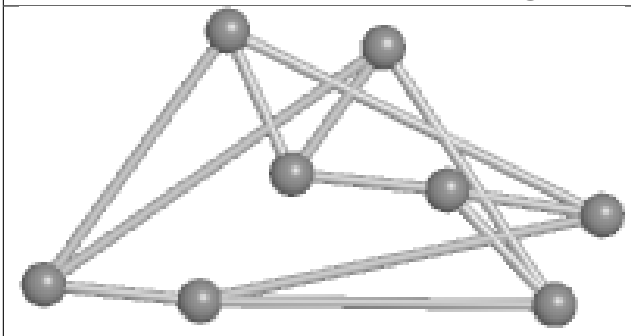


Torsions

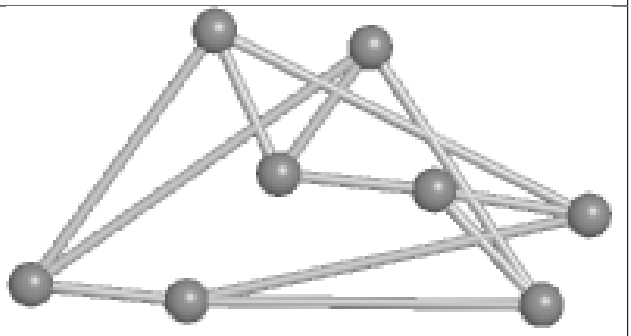


Rings

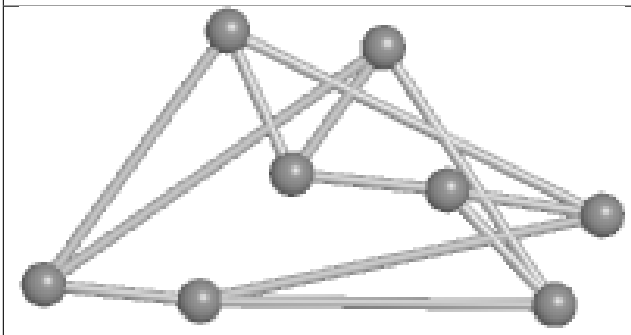
Ligand SF4 A 1101



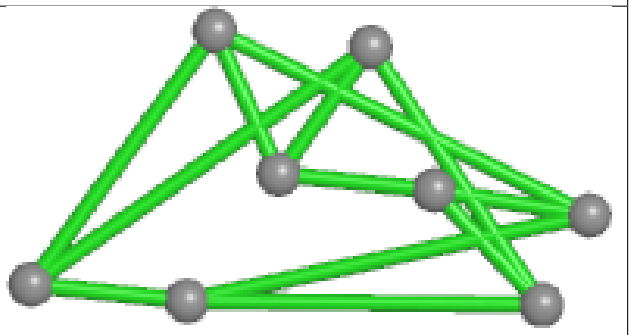
Bond lengths



Bond angles

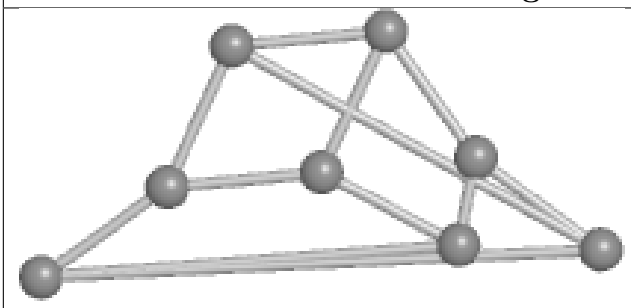


Torsions



Rings

Ligand SF4 C 1105



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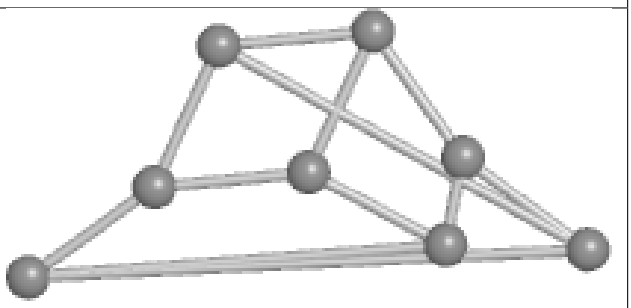
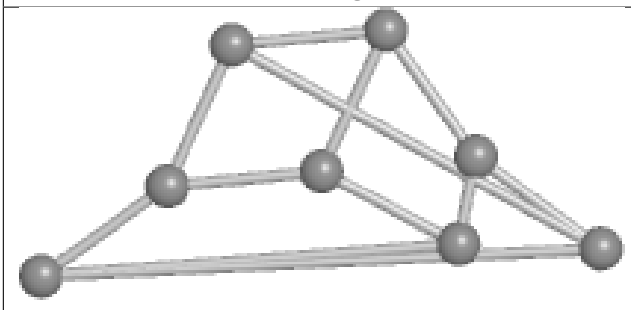
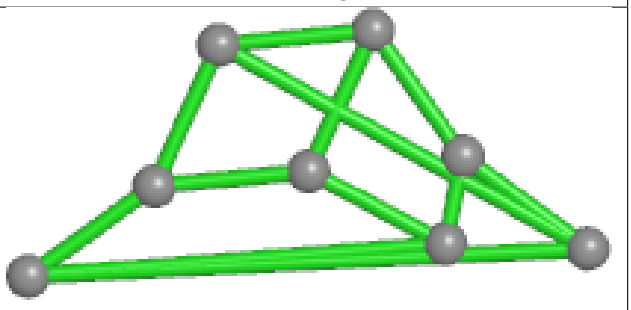


Bond angles

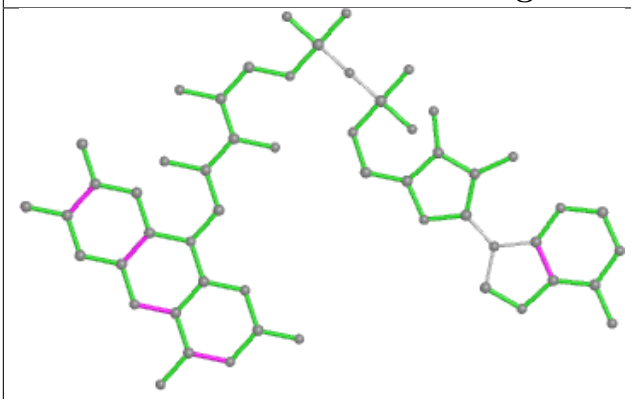


Torsions

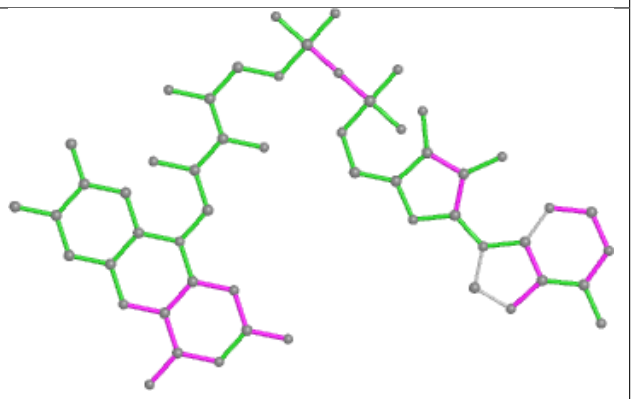


Rings

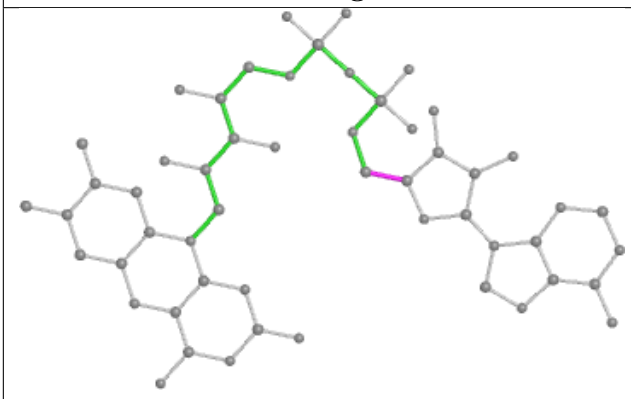
Ligand FAD C 1107



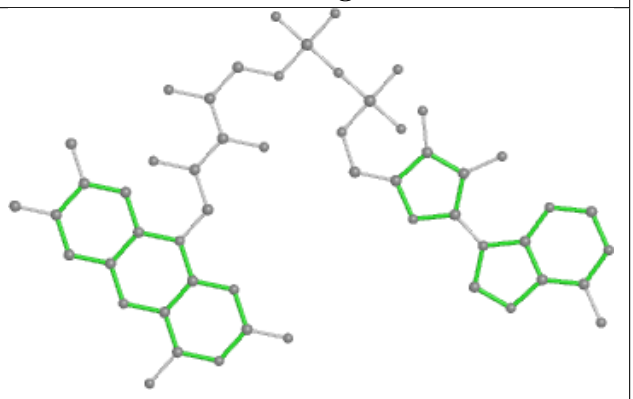
Bond lengths



Bond angles

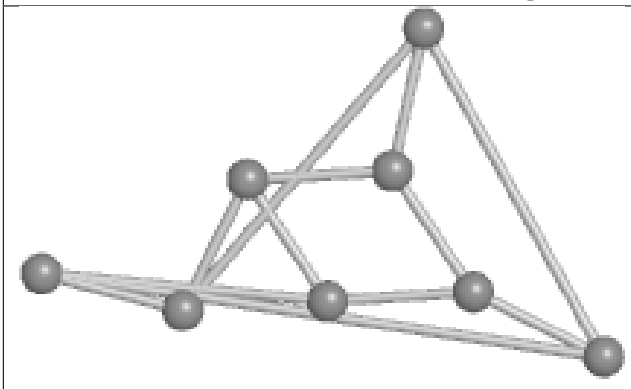


Torsions



Rings

Ligand SF4 D 1107



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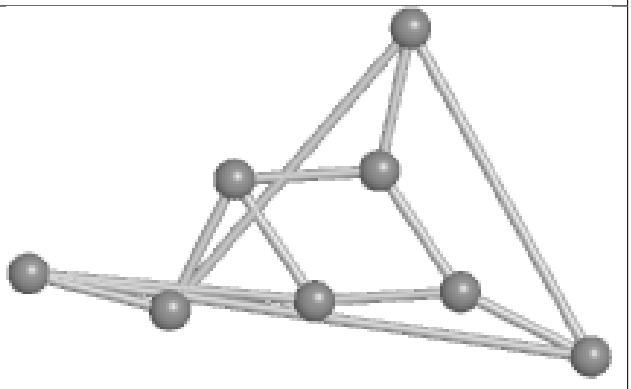
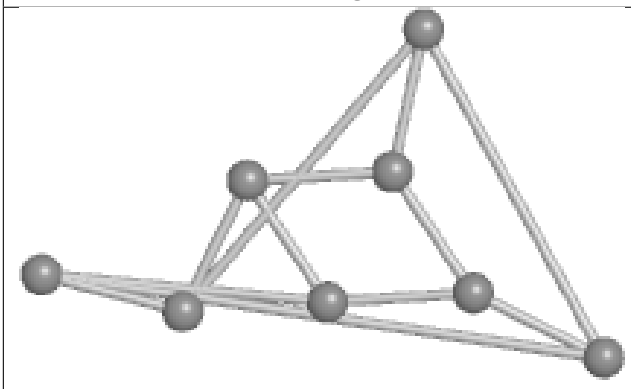
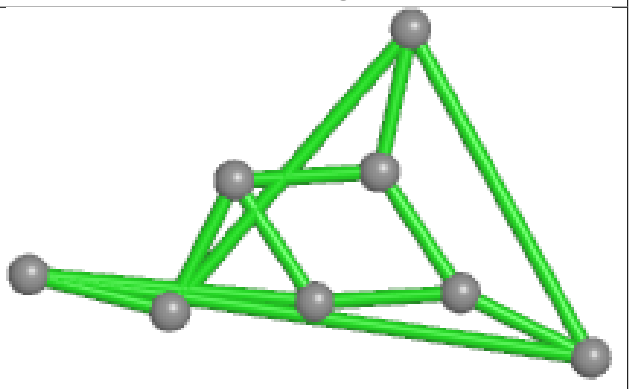


Bond angles

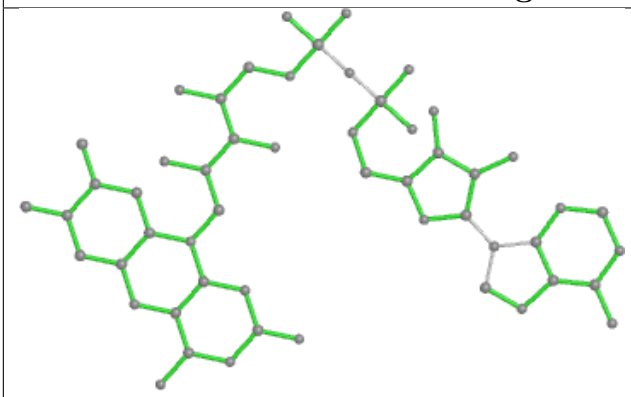


Torsions



Rings

Ligand FAD D 1106



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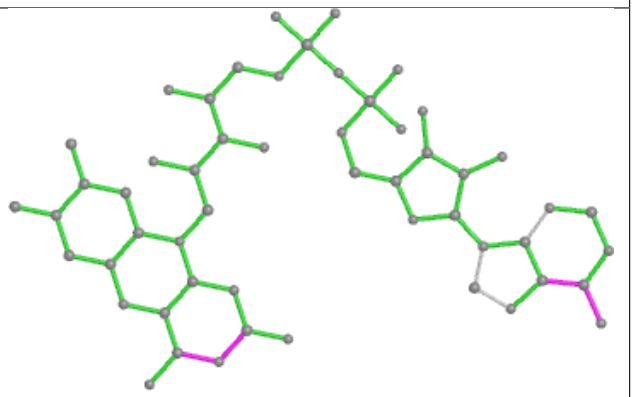
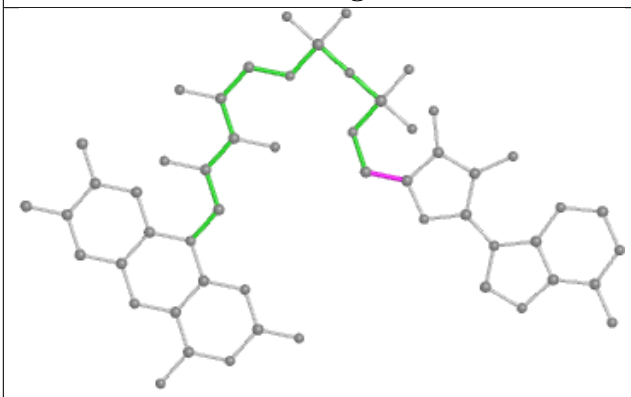


Bond angles



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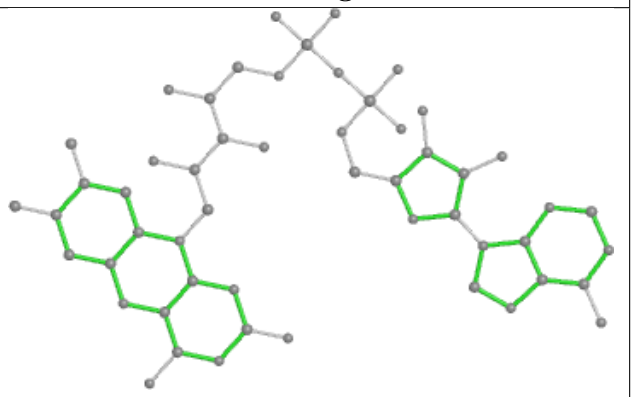
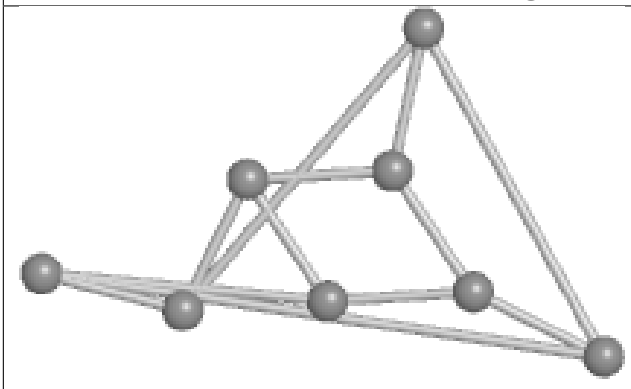
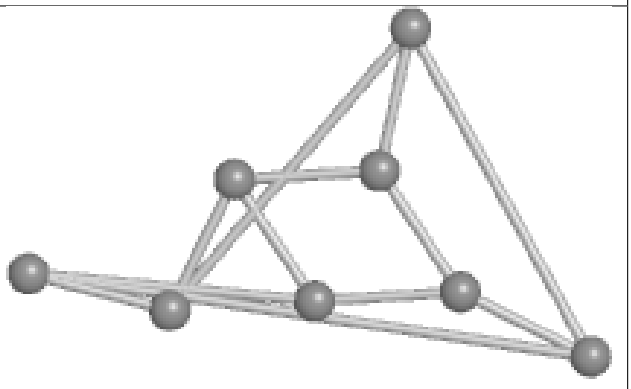


Rings

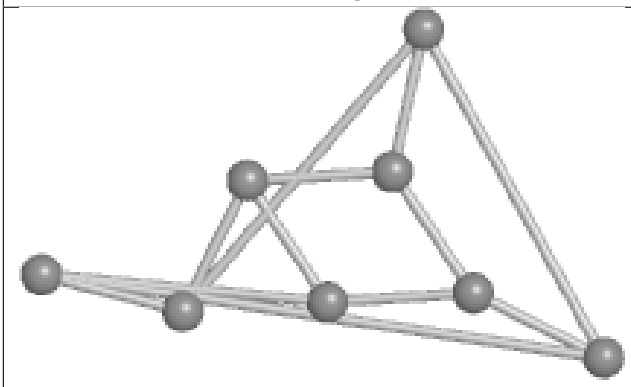
Ligand SF4 C 1106



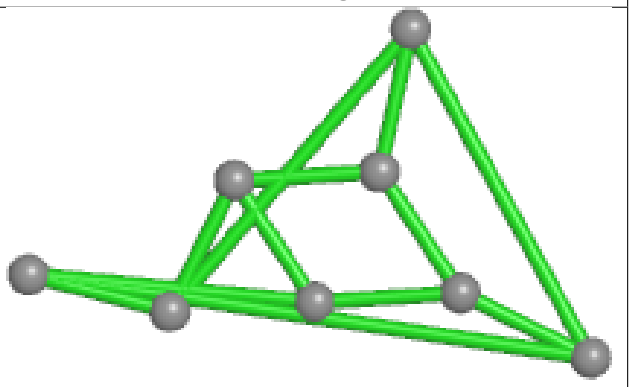
Bond lengths



Bond angles

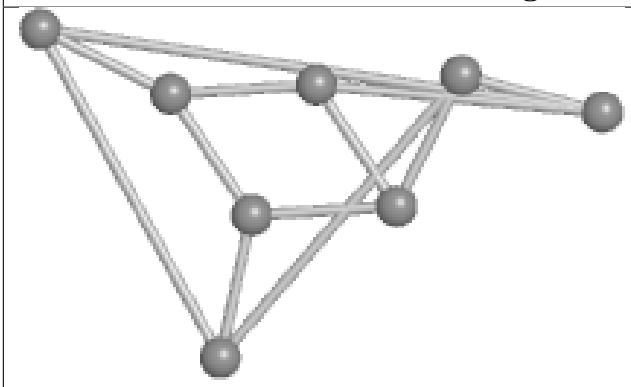


Torsions



Rings

Ligand SF4 D 1104



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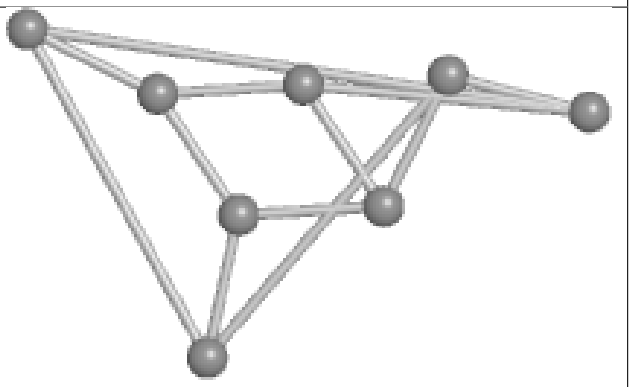
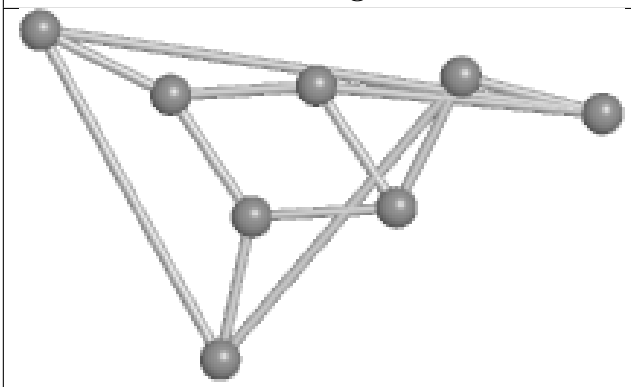
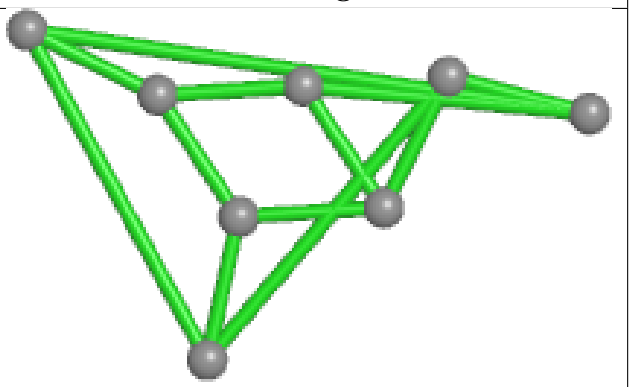


Bond angles

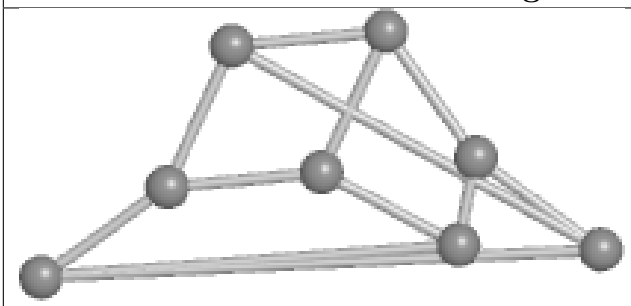


Torsions

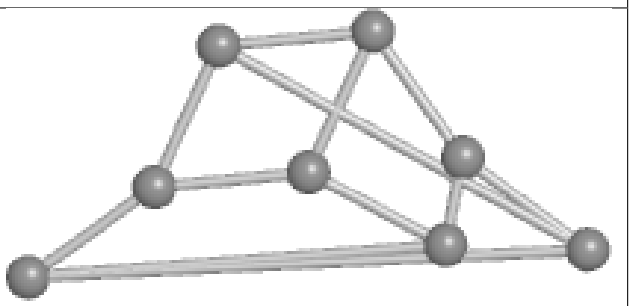


Rings

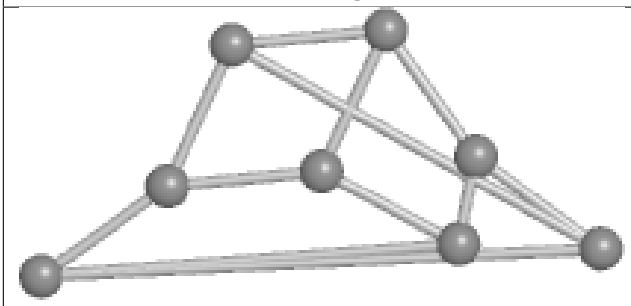
Ligand SF4 B 1001



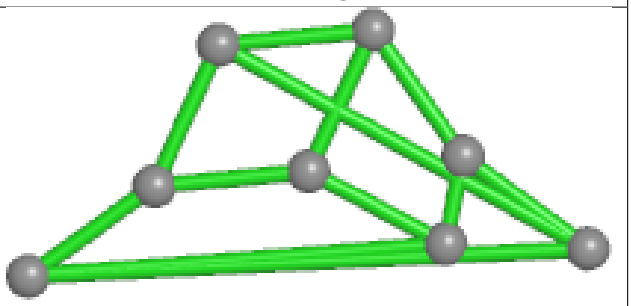
Bond lengths



Bond angles

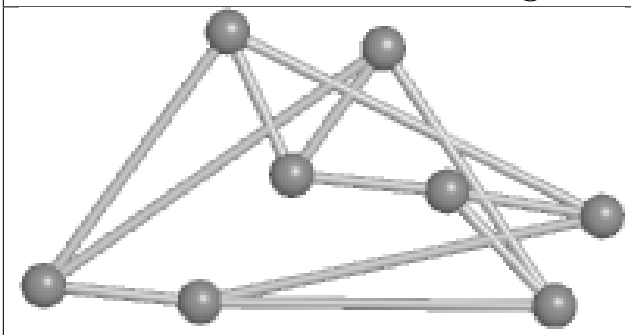


Torsions

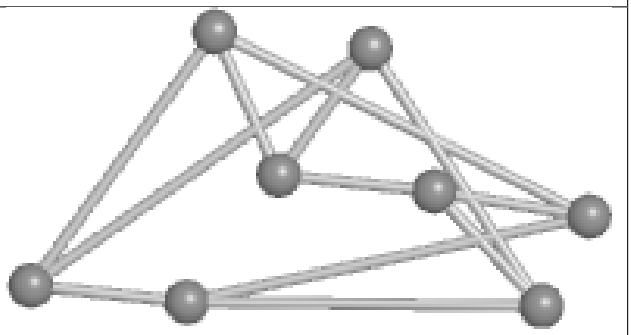


Rings

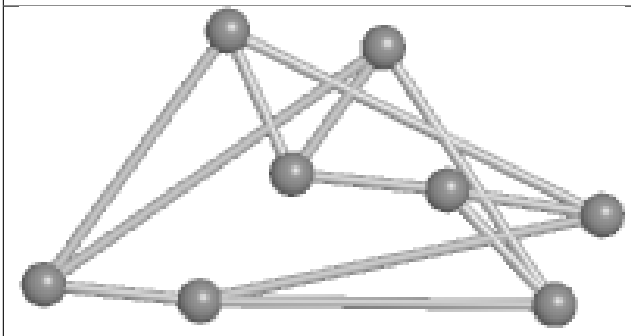
Ligand SF4 D 1103



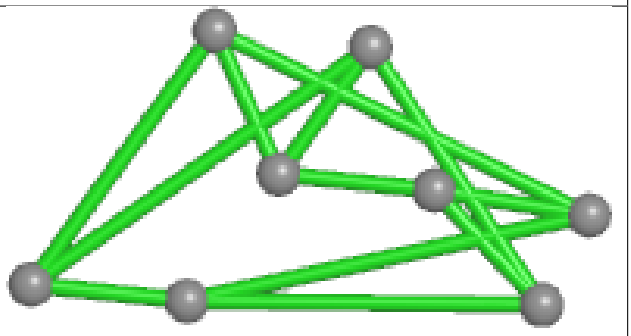
Bond lengths



Bond angles

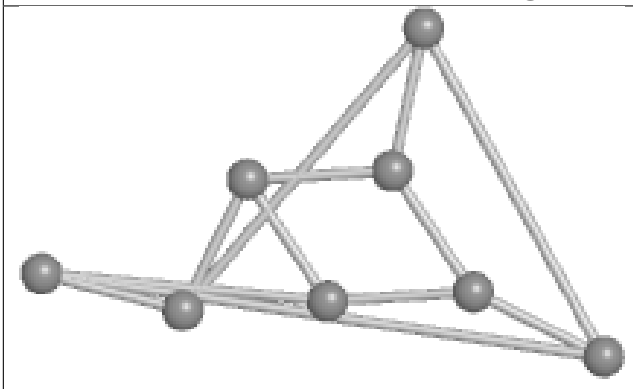


Torsions

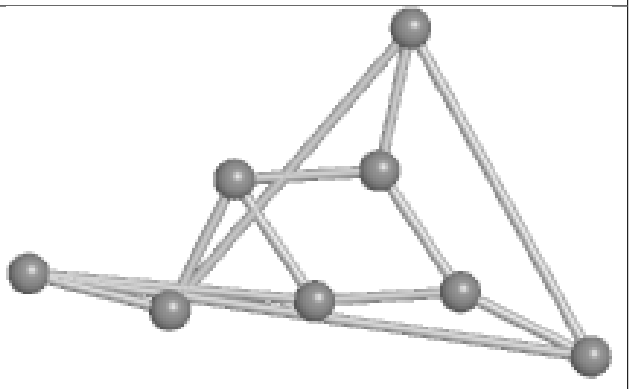


Rings

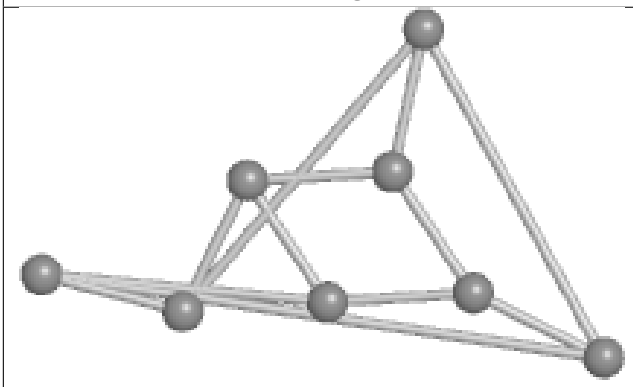
Ligand SF4 A 1102



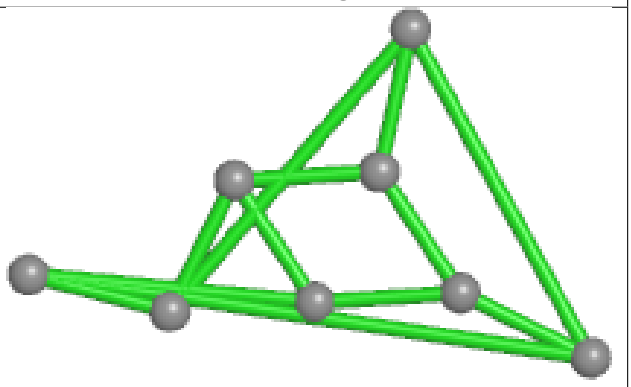
Bond lengths



Bond angles

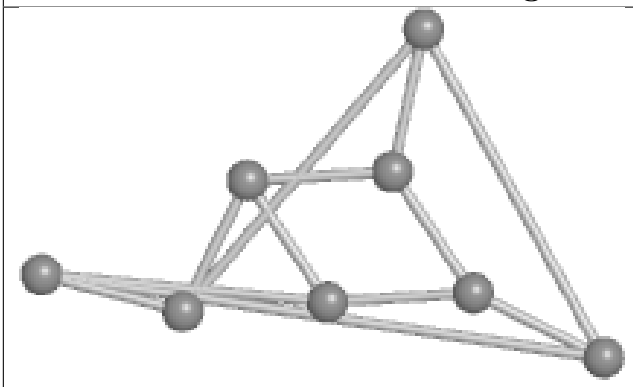


Torsions

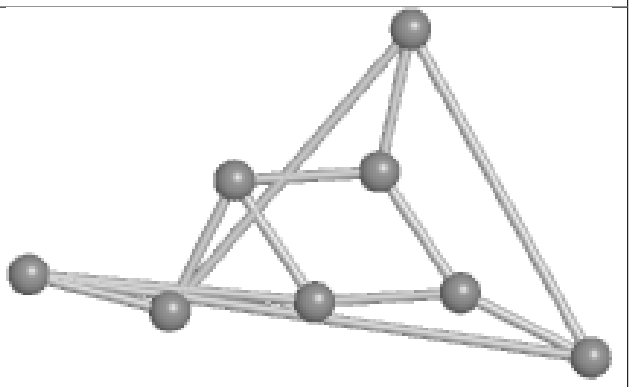


Rings

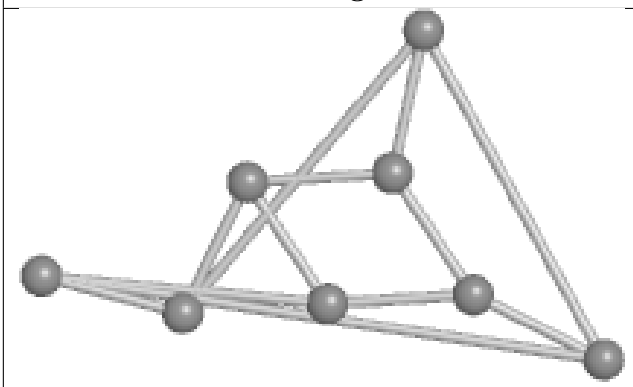
Ligand SF4 B 1003



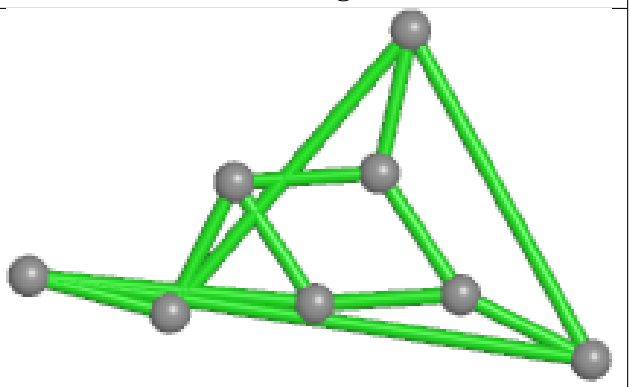
Bond lengths



Bond angles

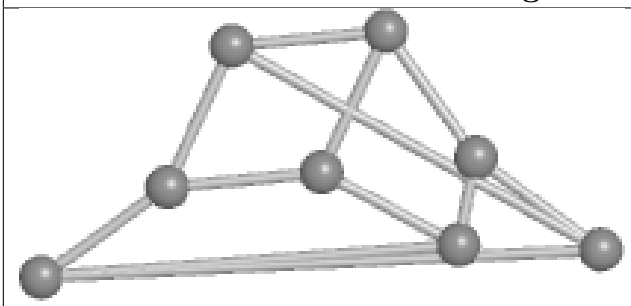


Torsions

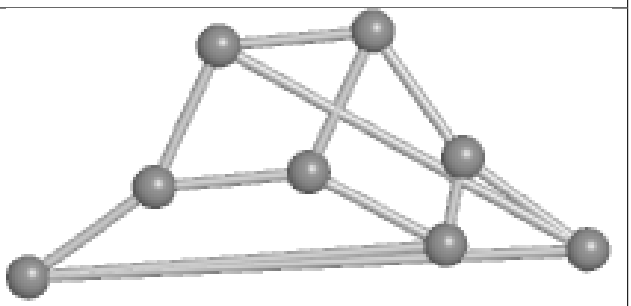


Rings

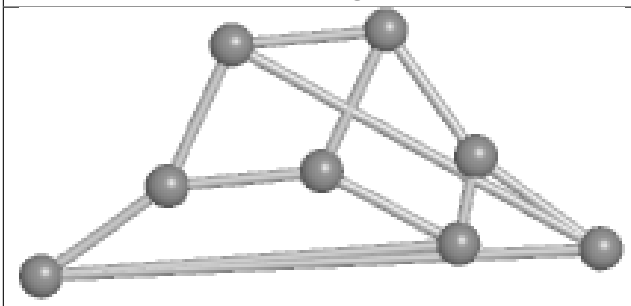
Ligand SF4 C 1102



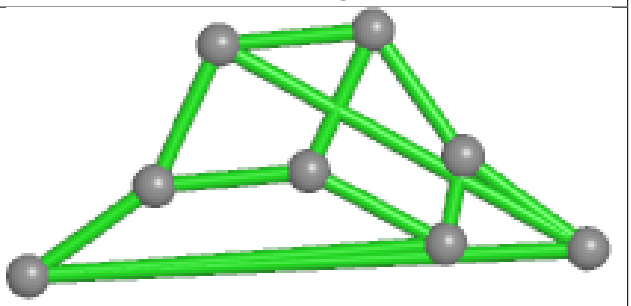
Bond lengths



Bond angles

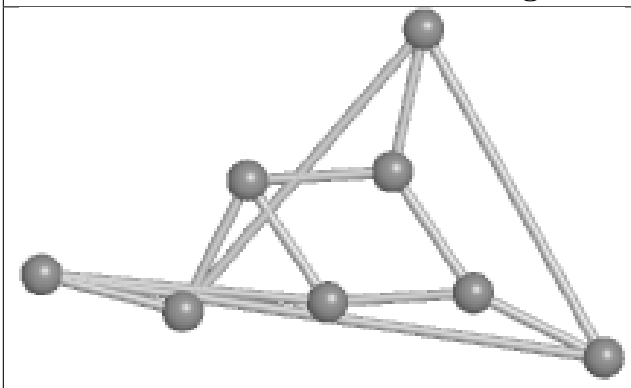


Torsions

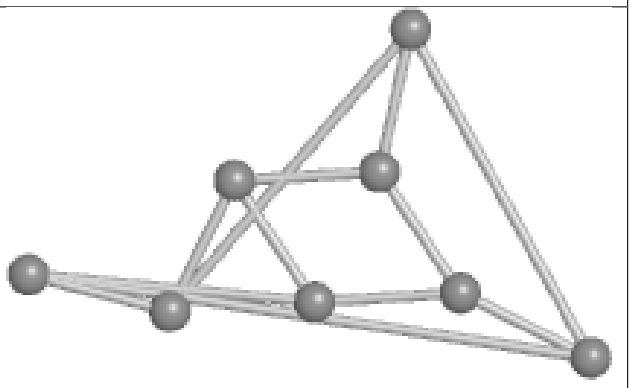


Rings

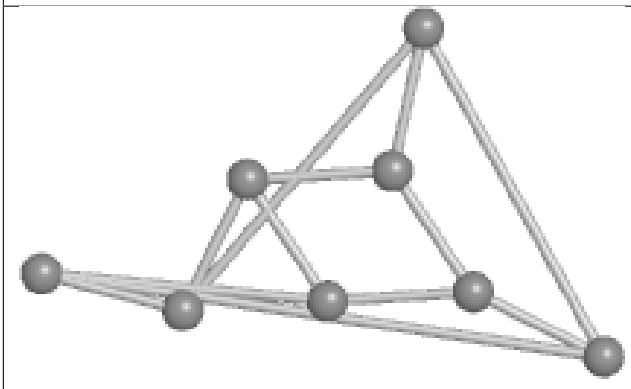
Ligand SF4 D 1102



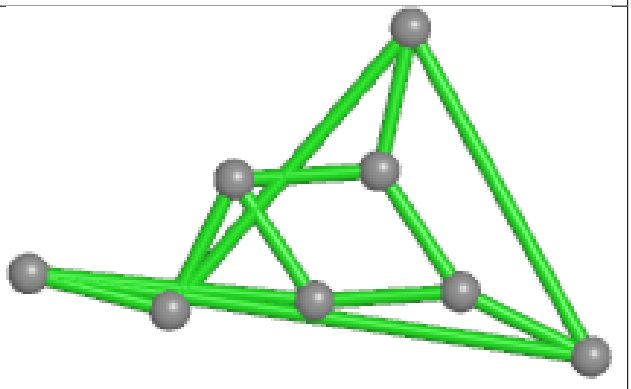
Bond lengths



Bond angles

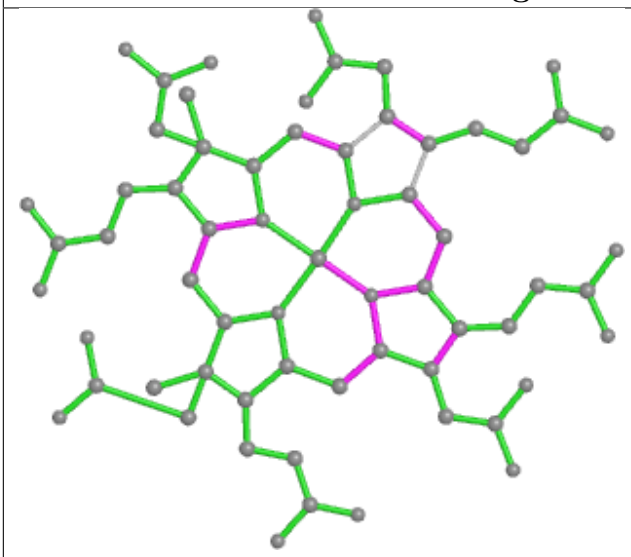


Torsions

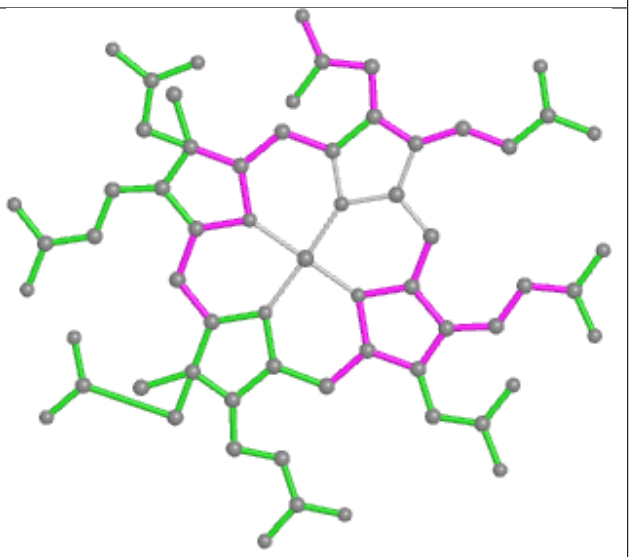


Rings

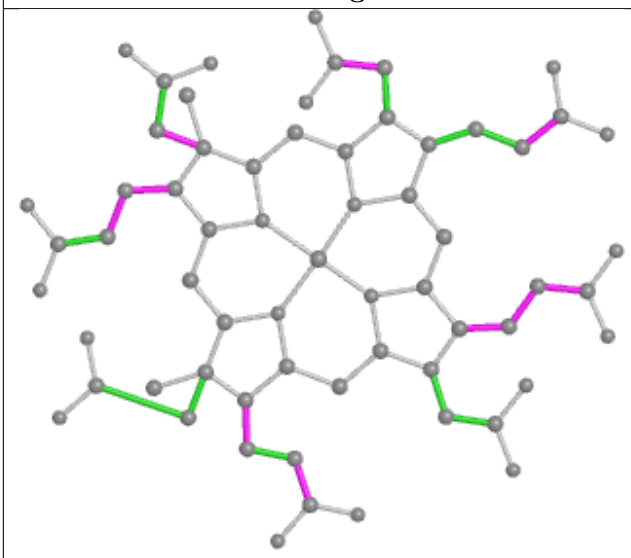
Ligand SRM B 1008



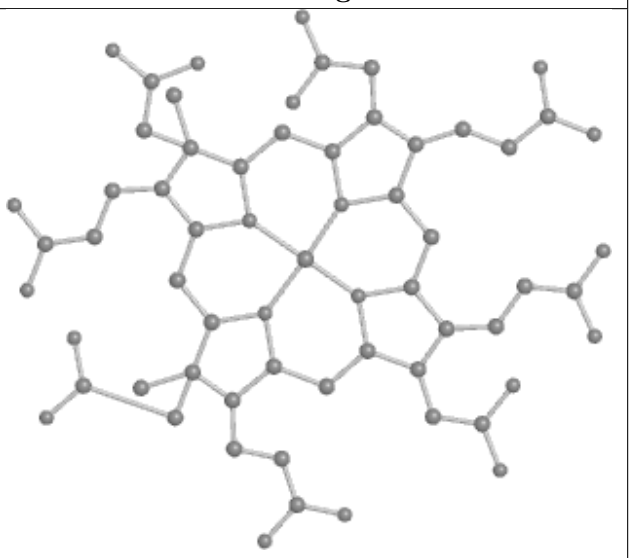
Bond lengths



Bond angles

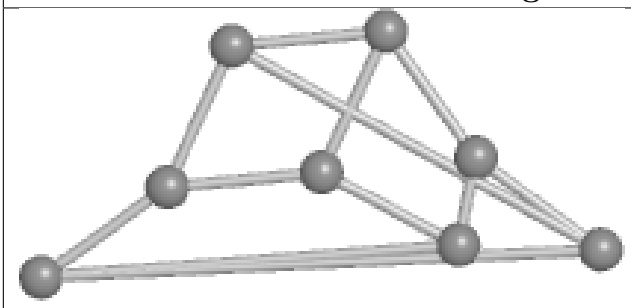


Torsions

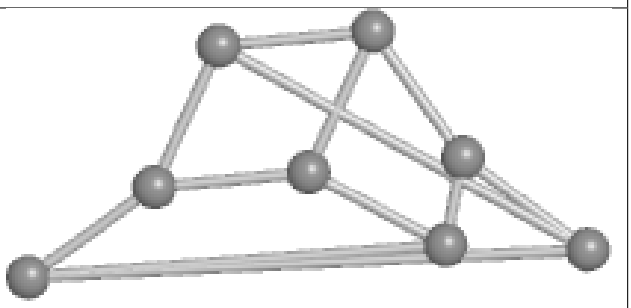


Rings

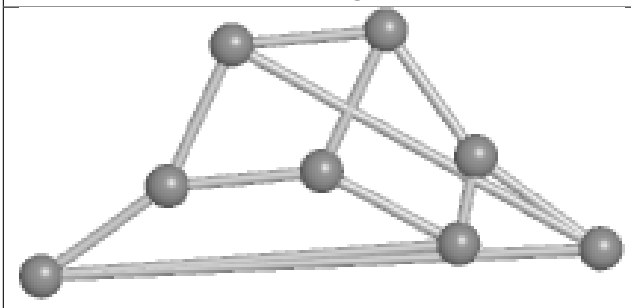
Ligand SF4 C 1101



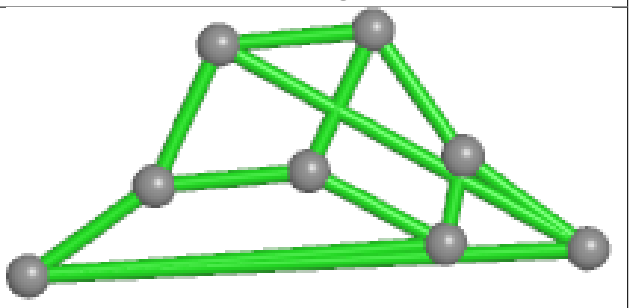
Bond lengths



Bond angles

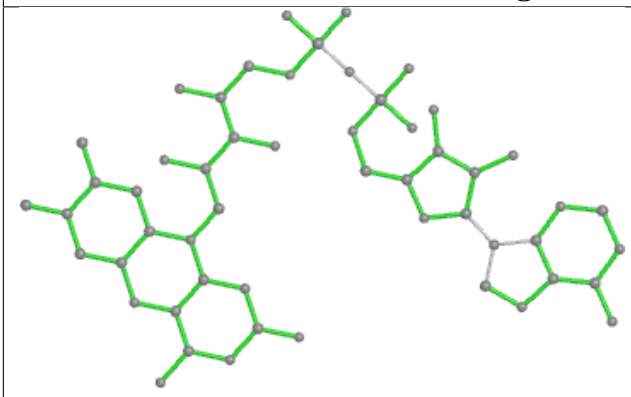


Torsions

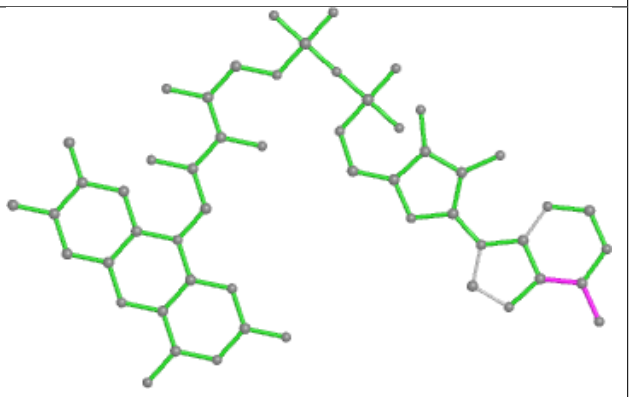


Rings

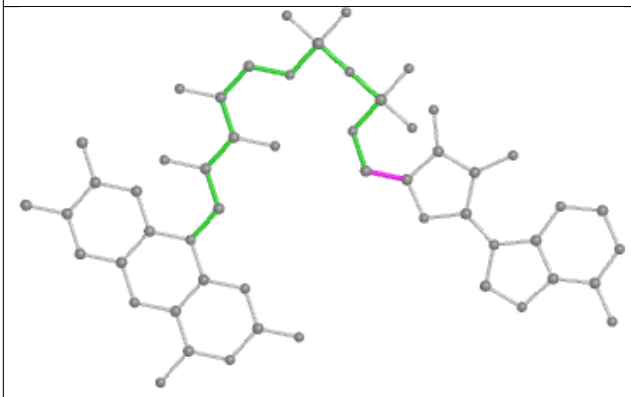
Ligand FAD A 1106



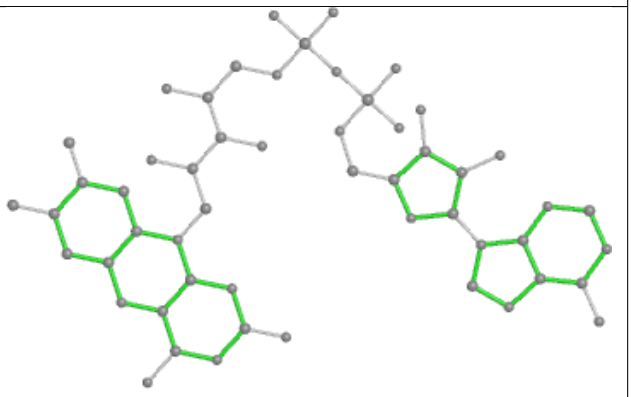
Bond lengths



Bond angles

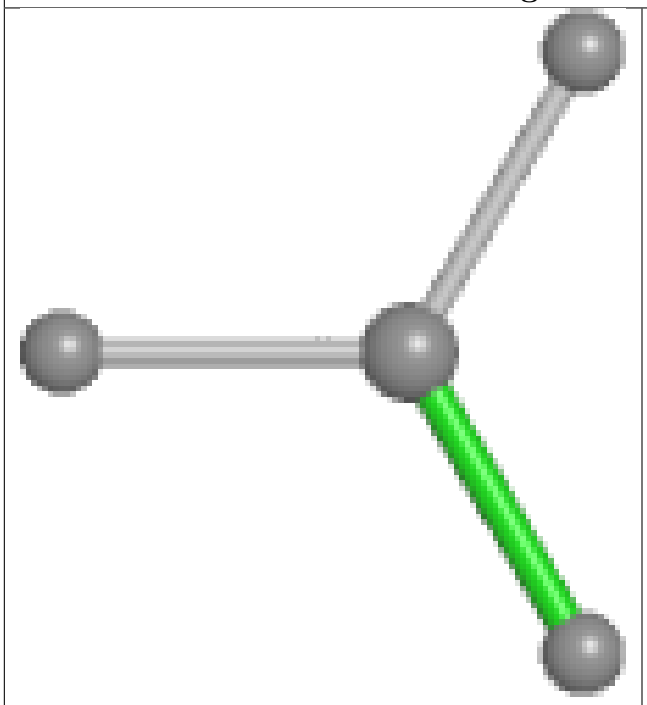


Torsions

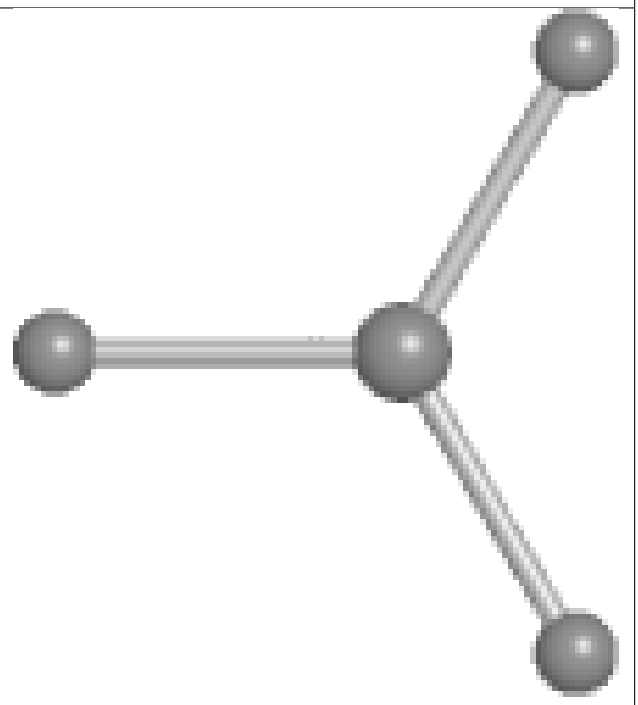


Rings

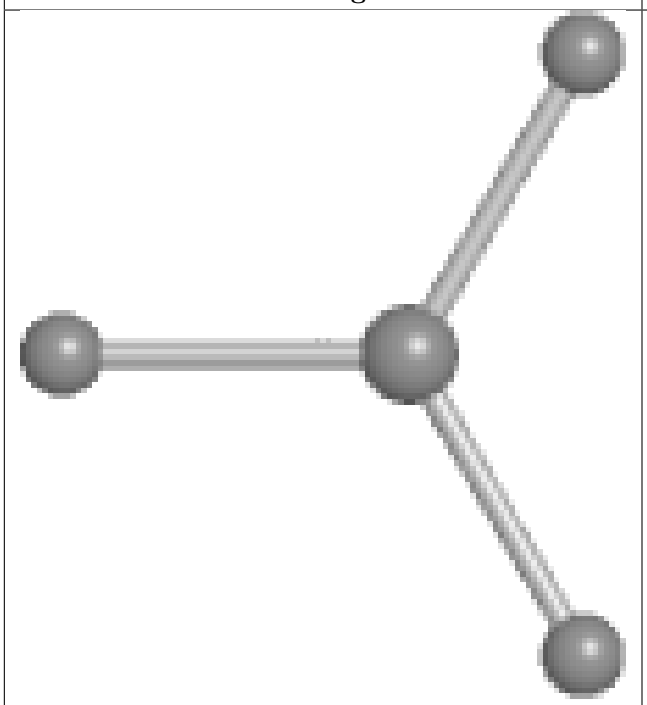
Ligand SO3 A 1108



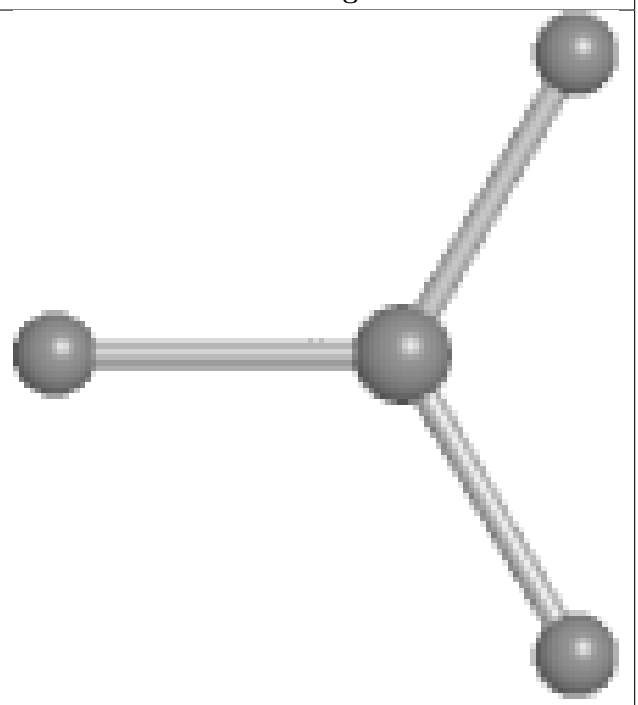
Bond lengths



Bond angles

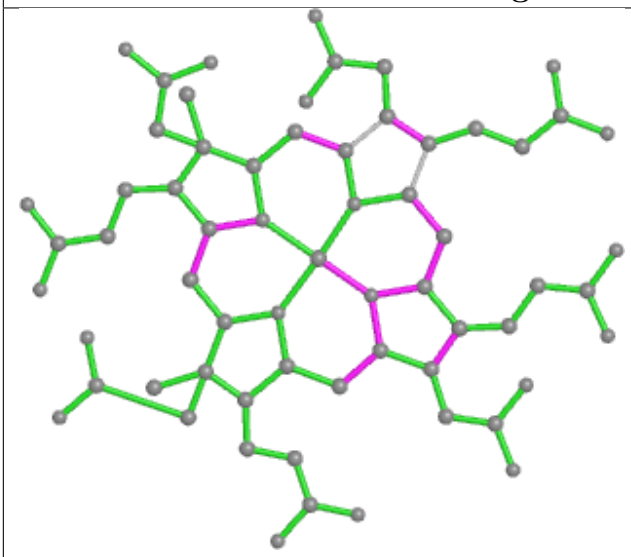


Torsions

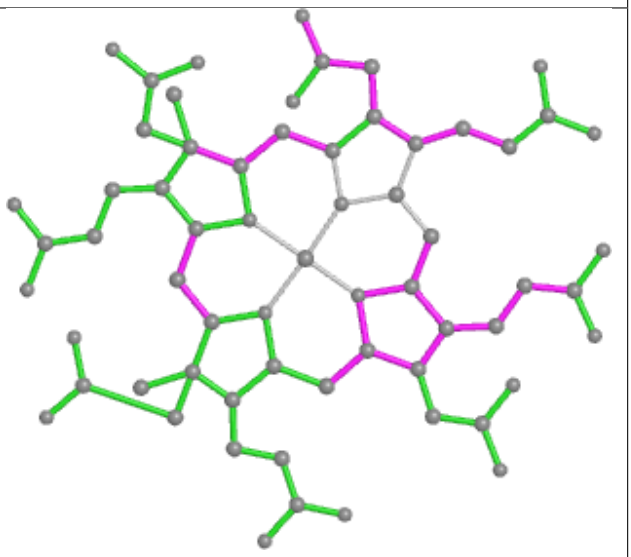


Rings

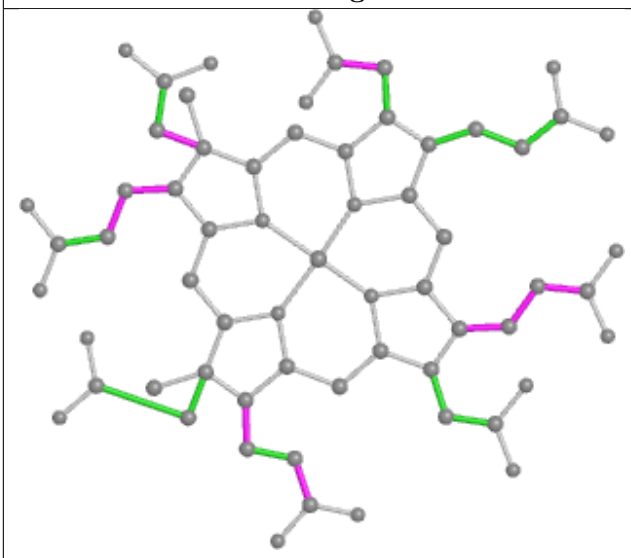
Ligand SRM A 1109



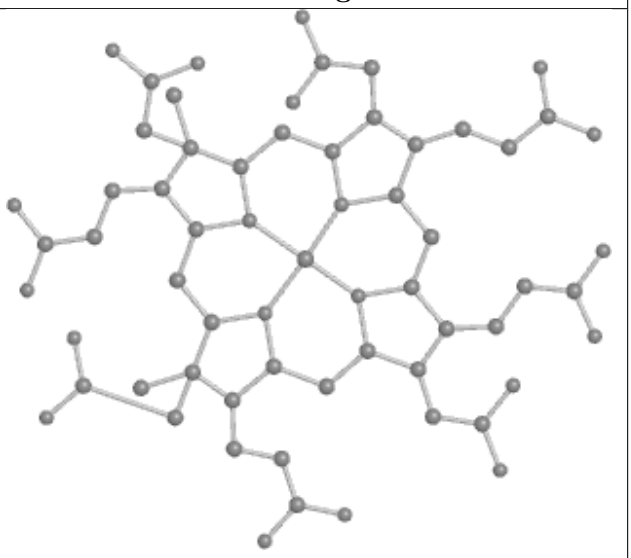
Bond lengths



Bond angles

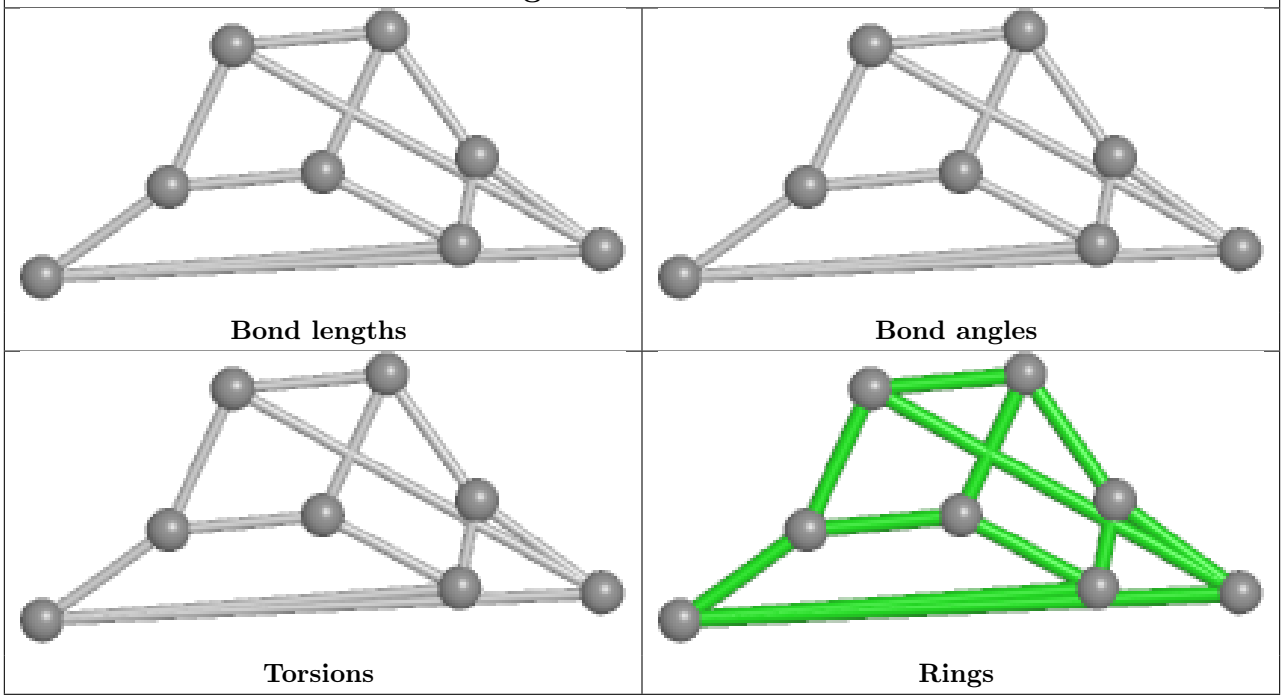


Torsions



Rings

Ligand SF4 B 1002



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	619/620 (99%)	-0.42	2 (0%)	94	96	25, 39, 66, 116	0
1	B	620/620 (100%)	-0.33	5 (0%)	86	89	24, 39, 65, 104	0
1	C	619/620 (99%)	-0.33	2 (0%)	94	96	24, 38, 68, 125	0
1	D	620/620 (100%)	-0.34	1 (0%)	95	96	23, 37, 67, 91	0
All	All	2478/2480 (99%)	-0.35	10 (0%)	92	95	23, 38, 67, 125	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	5.3
1	B	124	GLU	4.7
1	C	1	MET	4.6
1	B	2	TYR	3.5
1	A	619	ILE	3.1
1	B	1	MET	3.0
1	C	80	ASP	2.8
1	B	80	ASP	2.2
1	D	80	ASP	2.2
1	B	223	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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
6	GOL	D	1112	6/6	0.59	0.34	67,70,71,72	0
6	GOL	B	1017	6/6	0.60	0.36	68,73,79,82	0
8	CA	C	1116	1/1	0.60	0.13	94,94,94,94	0
6	GOL	A	1116	6/6	0.62	0.22	65,70,73,74	0
6	GOL	D	1120	6/6	0.64	0.26	72,73,76,78	0
6	GOL	A	1110	6/6	0.65	0.16	71,74,75,76	0
6	GOL	B	1016	6/6	0.66	0.21	76,79,80,81	0
6	GOL	D	1126	6/6	0.67	0.22	57,66,69,70	0
6	GOL	D	1117	6/6	0.67	0.50	79,81,81,82	0
6	GOL	D	1125	6/6	0.68	0.23	73,75,76,77	0
6	GOL	C	1119	6/6	0.68	0.20	68,69,71,72	0
6	GOL	B	1019	6/6	0.68	0.24	74,78,83,85	0
6	GOL	A	1114	6/6	0.69	0.48	84,90,93,93	0
8	CA	A	1113	1/1	0.70	0.10	77,77,77,77	0
7	MPD	C	1112	8/8	0.71	0.17	61,65,69,69	0
8	CA	C	1115	1/1	0.73	0.09	99,99,99,99	0
6	GOL	C	1118	6/6	0.73	0.20	61,70,72,73	0
7	MPD	C	1113	8/8	0.74	0.36	102,105,108,108	0
6	GOL	A	1115	6/6	0.74	0.15	60,63,66,68	0
8	CA	D	1114	1/1	0.76	0.09	73,73,73,73	0
6	GOL	B	1015	6/6	0.77	0.16	59,65,68,70	0
6	GOL	A	1117	6/6	0.78	0.16	67,69,70,70	0
6	GOL	C	1111	6/6	0.79	0.27	54,57,64,66	0
6	GOL	D	1124	6/6	0.79	0.15	65,71,73,75	0
8	CA	D	1116	1/1	0.79	0.15	84,84,84,84	0
7	MPD	B	1010	8/8	0.80	0.29	67,69,72,76	0
6	GOL	B	1018	6/6	0.81	0.13	63,64,65,66	0
6	GOL	B	1014	6/6	0.81	0.37	68,69,71,71	0
6	GOL	D	1119	6/6	0.81	0.19	57,61,65,69	0
7	MPD	A	1112	8/8	0.81	0.30	85,86,86,86	0
6	GOL	C	1110	6/6	0.81	0.24	68,69,70,71	0
6	GOL	D	1123	6/6	0.81	0.22	72,73,73,73	0
6	GOL	D	1118	6/6	0.82	0.27	104,108,114,117	0
6	GOL	C	1120	6/6	0.84	0.16	70,77,80,83	0
6	GOL	D	1111	6/6	0.84	0.17	50,50,53,54	0
7	MPD	D	1113	8/8	0.85	0.21	59,63,67,69	0
6	GOL	B	1009	6/6	0.85	0.21	49,53,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	CA	D	1115[A]	1/1	0.86	0.12	70,70,70,70	0
8	CA	B	1012	1/1	0.87	0.07	104,104,104,104	0
6	GOL	D	1121	6/6	0.87	0.20	39,50,53,56	0
9	CL	A	1118	1/1	0.87	0.19	78,78,78,78	0
6	GOL	D	1122	6/6	0.88	0.17	59,62,65,66	0
8	CA	B	1011	1/1	0.90	0.12	68,68,68,68	0
6	GOL	D	1110	6/6	0.90	0.10	59,62,65,66	0
6	GOL	A	1111	6/6	0.92	0.18	45,48,52,56	0
8	CA	C	1114	1/1	0.92	0.05	72,72,72,72	0
6	GOL	C	1109	6/6	0.93	0.18	47,50,50,55	0
4	SO3	B	1013	4/4	0.93	0.28	83,83,85,86	0
4	SO3	D	1108	4/4	0.94	0.26	76,77,77,81	0
5	SRM	D	1109	63/63	0.96	0.12	20,34,42,58	0
3	FAD	D	1106	53/53	0.96	0.11	18,37,48,51	0
3	FAD	A	1106	53/53	0.96	0.10	26,40,48,48	0
4	SO3	C	1117	4/4	0.96	0.26	60,64,64,66	0
3	FAD	C	1107	53/53	0.96	0.10	29,38,43,47	0
5	SRM	A	1109	63/63	0.96	0.10	28,37,45,54	0
5	SRM	B	1008	63/63	0.96	0.11	25,34,42,64	0
5	SRM	C	1108	63/63	0.96	0.12	27,35,43,67	0
9	CL	C	1121	1/1	0.96	0.12	54,54,54,54	0
10	FE	D	1127	1/1	0.96	0.06	47,47,47,47	0
3	FAD	B	1006	53/53	0.97	0.10	25,37,46,49	0
9	CL	C	1122	1/1	0.97	0.07	40,40,40,40	0
4	SO3	A	1108	4/4	0.97	0.17	58,58,59,63	0
9	CL	B	1020	1/1	0.98	0.08	40,40,40,40	0
2	SF4	B	1001	8/8	0.98	0.10	34,38,39,45	0
2	SF4	A	1104	8/8	0.98	0.10	35,37,43,45	0
9	CL	D	1128	1/1	0.98	0.07	36,36,36,36	0
9	CL	A	1119	1/1	0.98	0.12	39,39,39,39	0
2	SF4	D	1107	8/8	0.99	0.11	24,29,31,33	0
2	SF4	A	1103	8/8	0.99	0.10	31,34,39,42	0
2	SF4	A	1101	8/8	0.99	0.08	33,36,39,43	0
2	SF4	A	1105	8/8	0.99	0.10	28,33,34,37	0
2	SF4	A	1107	8/8	0.99	0.10	32,34,38,39	0
2	SF4	A	1102	8/8	0.99	0.13	30,36,38,41	0
2	SF4	B	1002	8/8	0.99	0.11	34,38,40,41	0
2	SF4	B	1003	8/8	0.99	0.09	31,34,38,40	0
2	SF4	B	1004	8/8	0.99	0.12	34,36,39,41	0
2	SF4	B	1005	8/8	0.99	0.09	33,37,38,40	0
2	SF4	B	1007	8/8	0.99	0.09	34,38,39,43	0
2	SF4	C	1101	8/8	0.99	0.09	33,35,37,38	0

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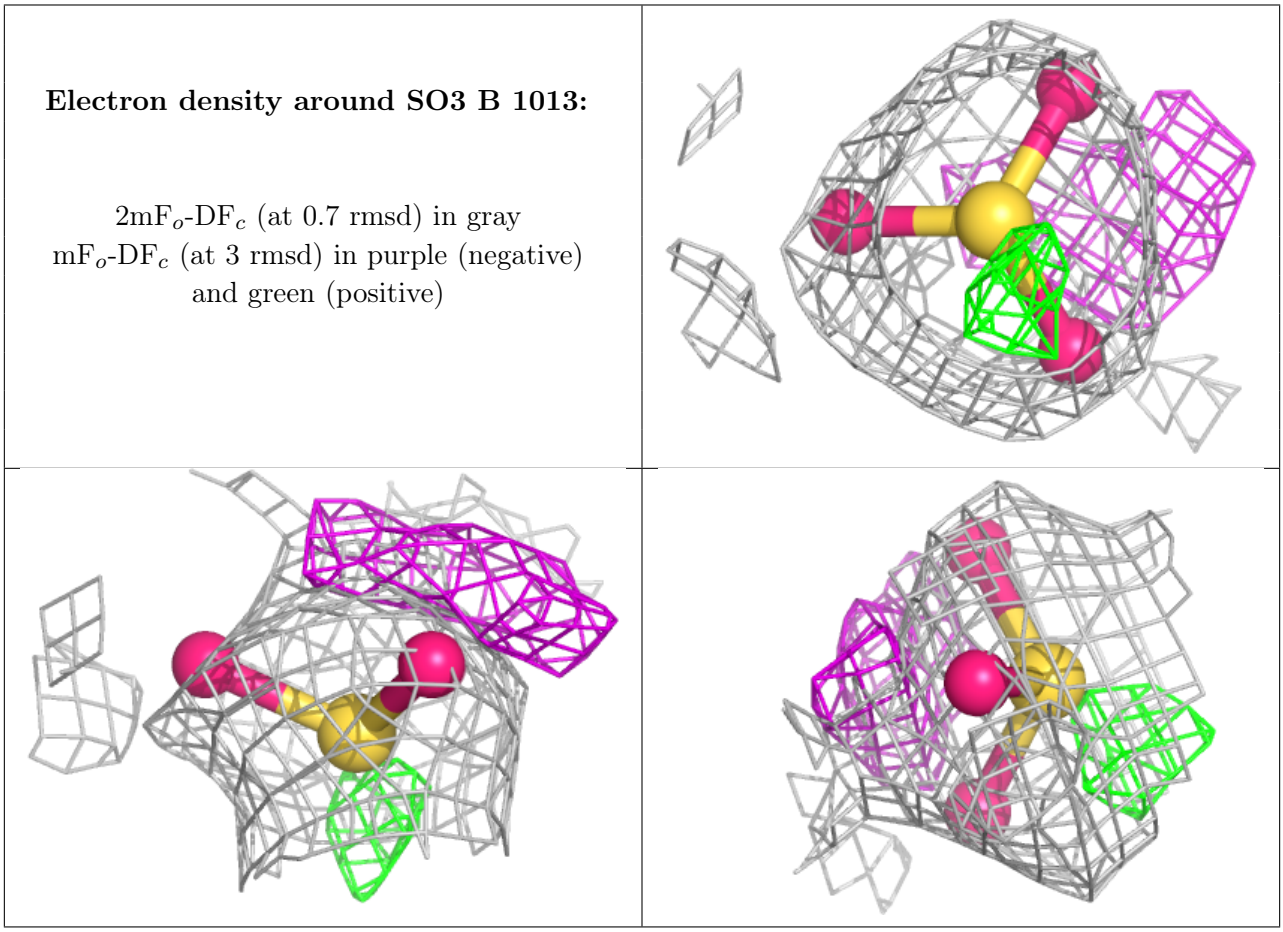
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SF4	C	1102	8/8	0.99	0.12	27,34,36,36	0
2	SF4	C	1103	8/8	0.99	0.11	26,30,32,37	0
2	SF4	C	1104	8/8	0.99	0.09	27,31,33,34	0
2	SF4	C	1105	8/8	0.99	0.12	23,28,31,32	0
2	SF4	C	1106	8/8	0.99	0.10	31,34,36,39	0
2	SF4	D	1101	8/8	0.99	0.10	29,31,34,38	0
2	SF4	D	1102	8/8	0.99	0.13	23,28,31,32	0
2	SF4	D	1103	8/8	0.99	0.10	25,28,32,35	0
2	SF4	D	1104	8/8	0.99	0.11	29,34,37,40	0
2	SF4	D	1105	8/8	0.99	0.12	27,31,35,35	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.

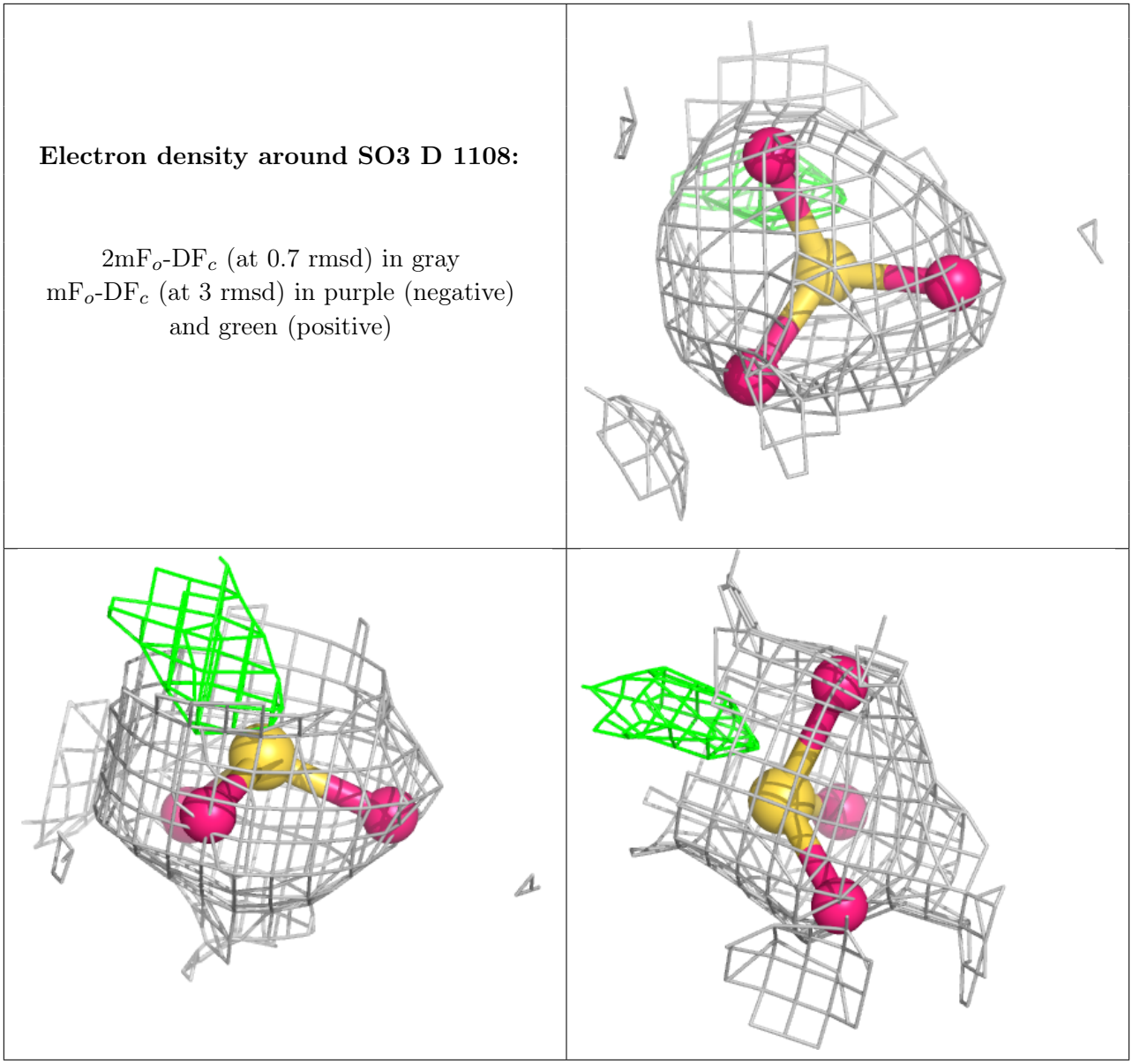
Electron density around SO3 B 1013:

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



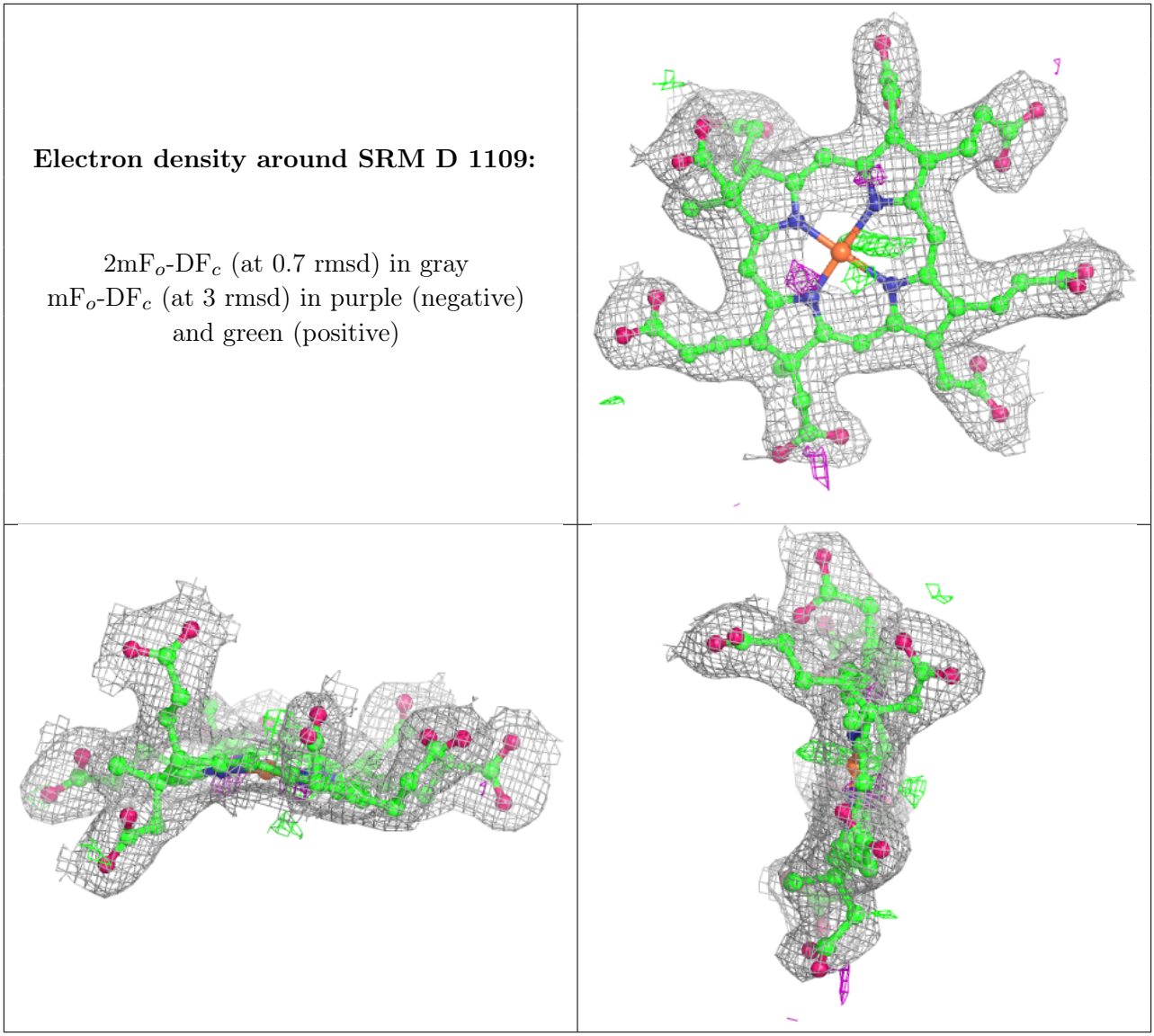
Electron density around SO3 D 1108:

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



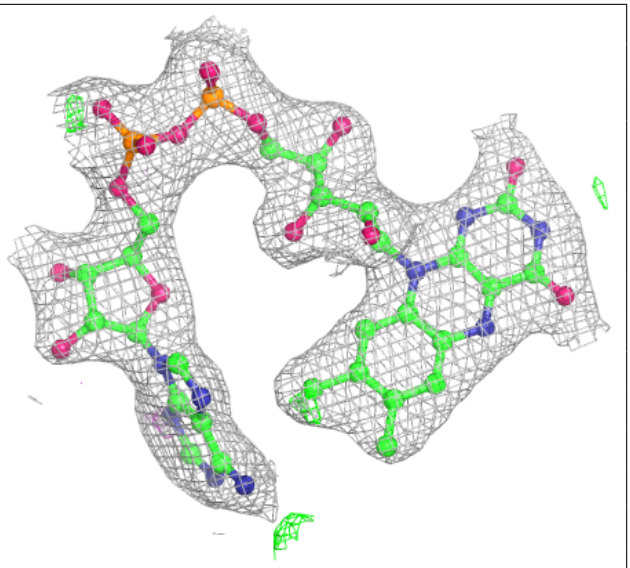
Electron density around SRM D 1109:

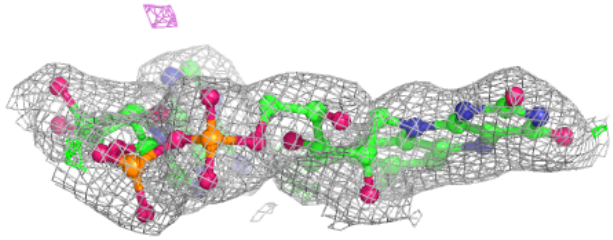
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

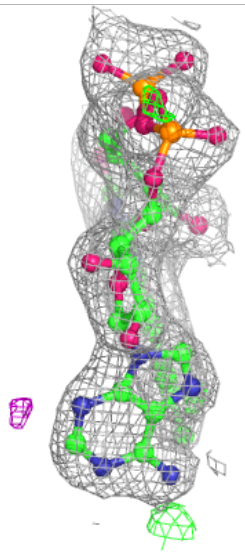


Electron density around FAD D 1106:

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

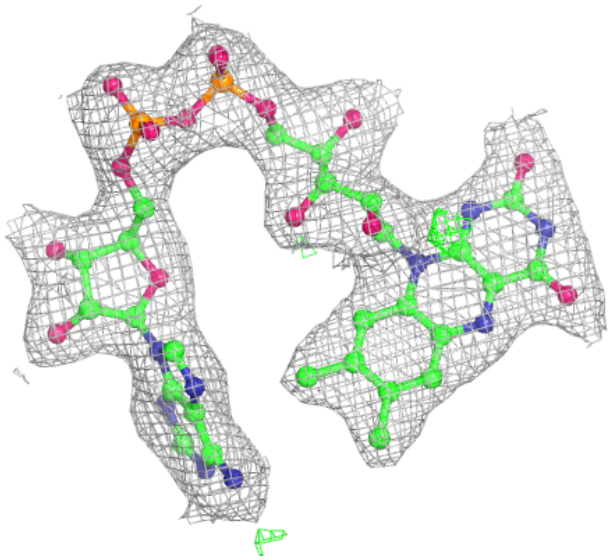


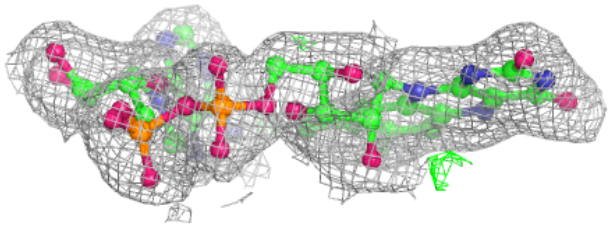


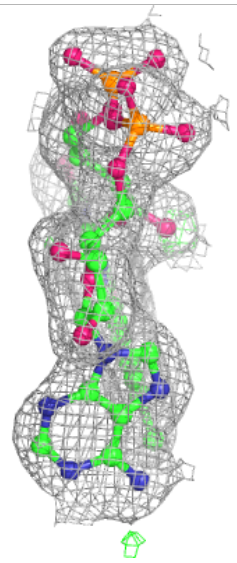


Electron density around FAD A 1106:

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

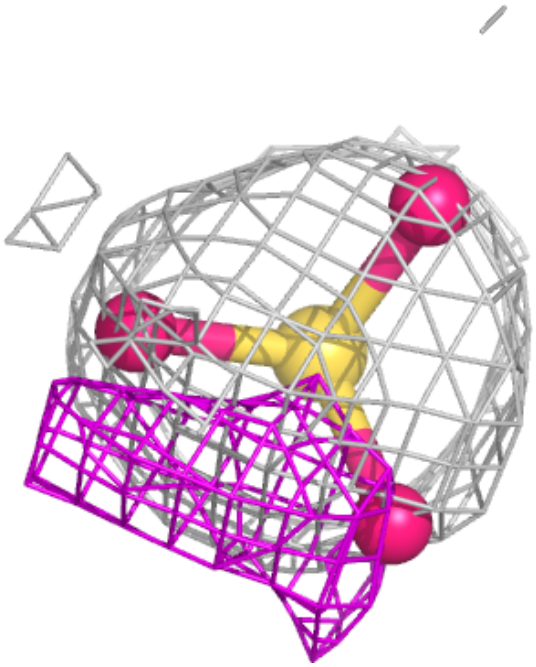


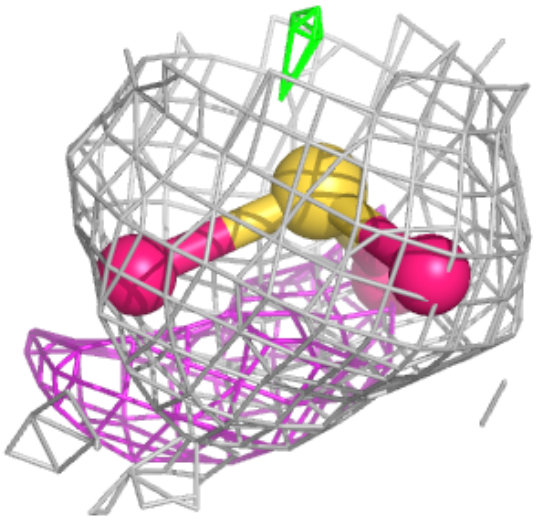


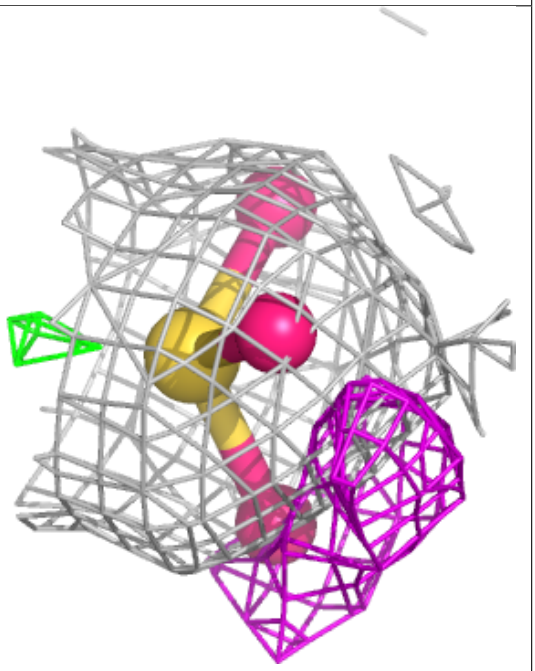


Electron density around SO3 C 1117:

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

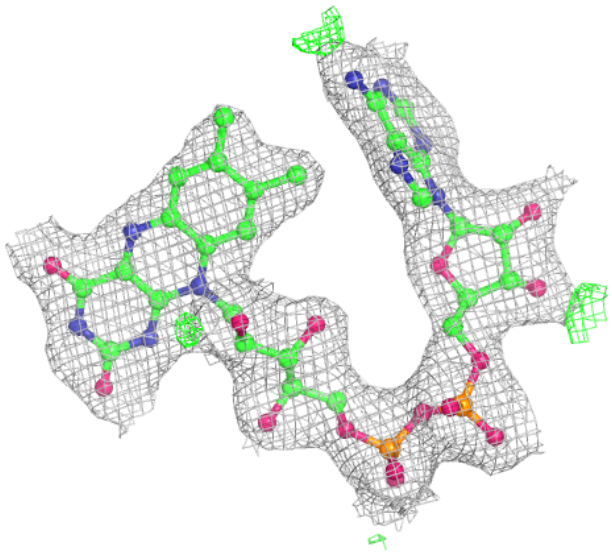


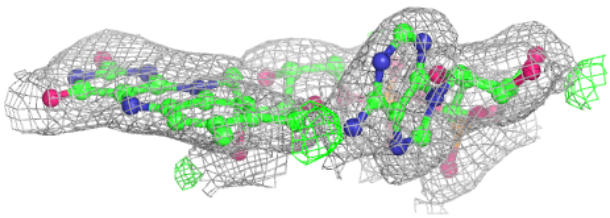


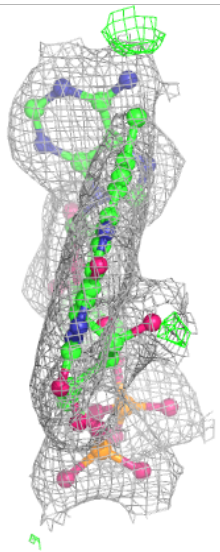


Electron density around FAD C 1107:

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

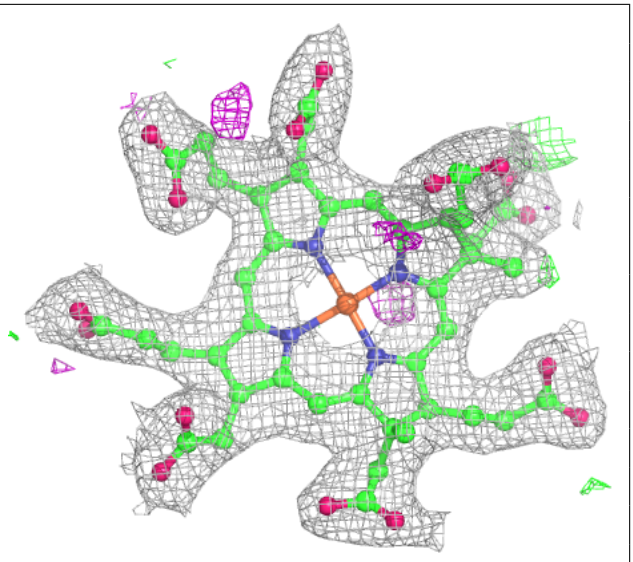


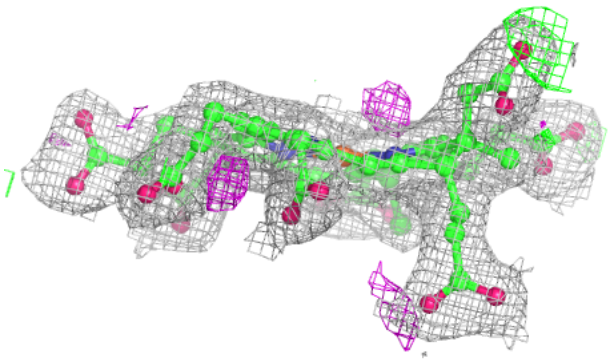


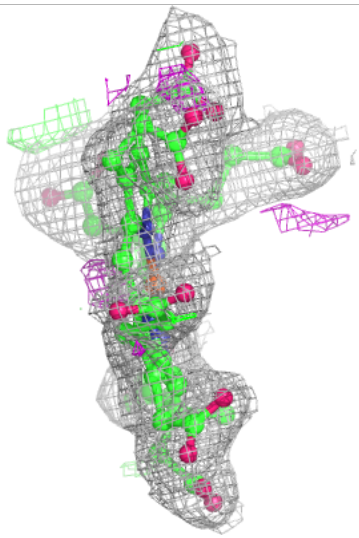


Electron density around SRM A 1109:

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

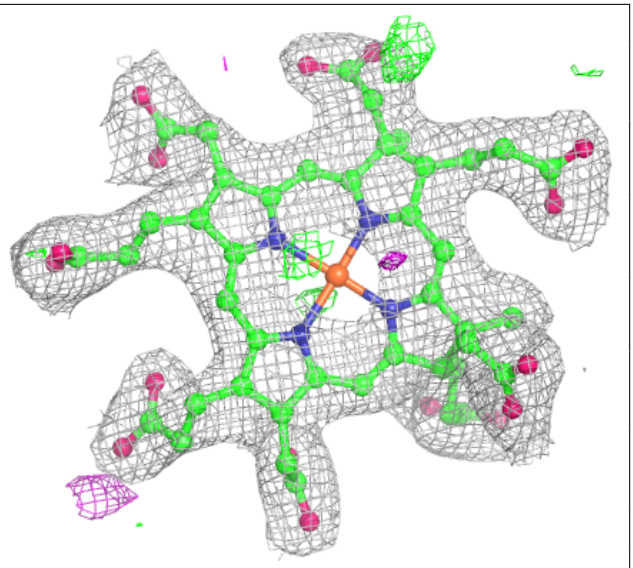


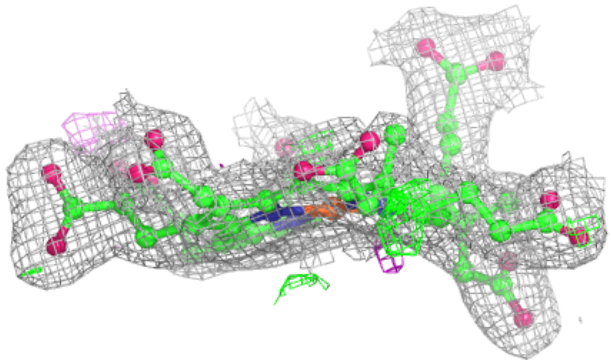


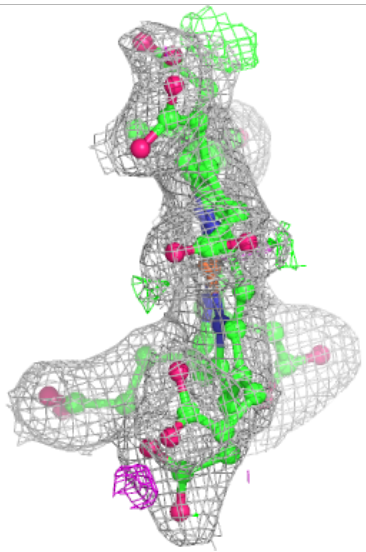


Electron density around SRM B 1008:

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

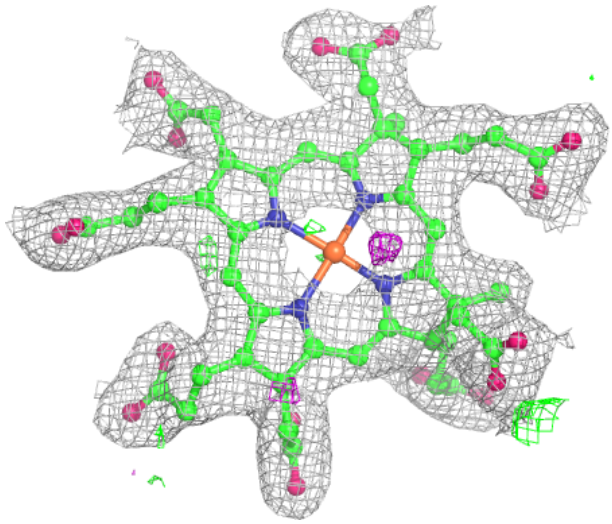


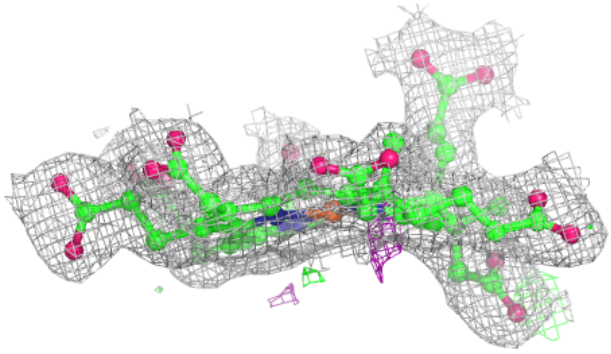


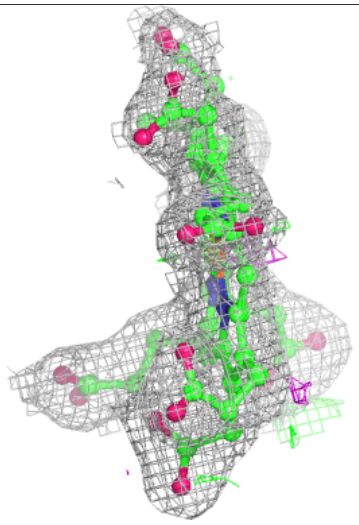


Electron density around SRM C 1108:

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

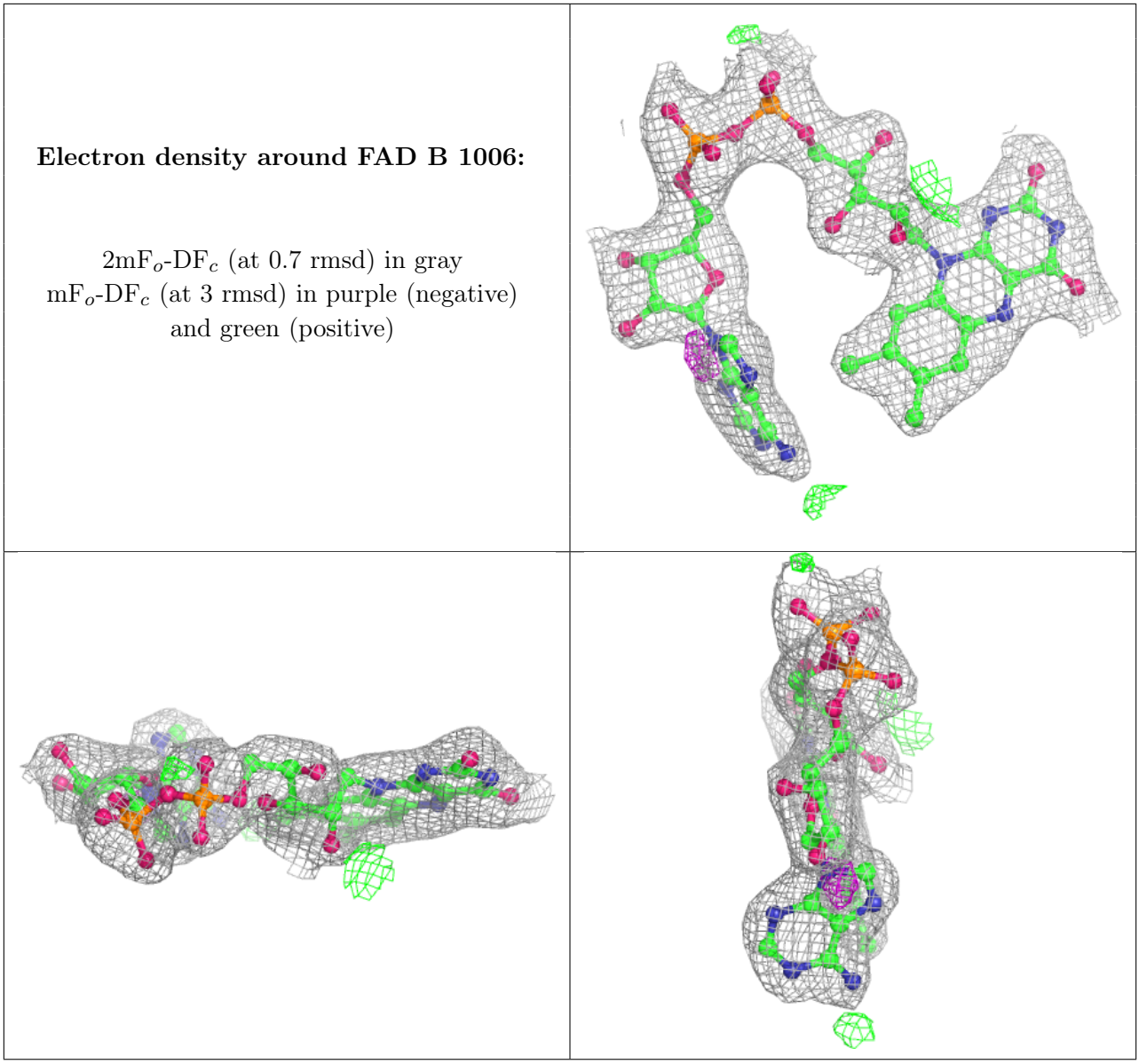






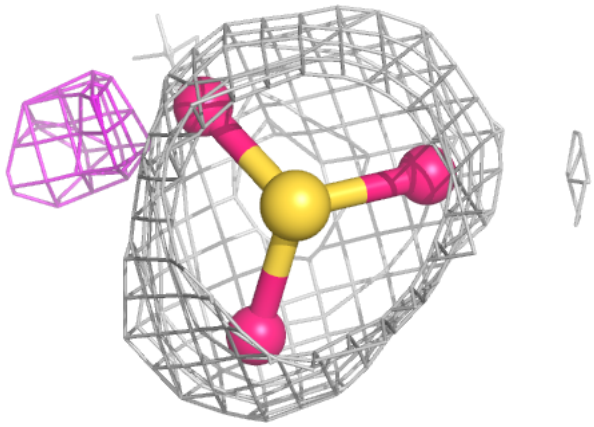
Electron density around FAD B 1006:

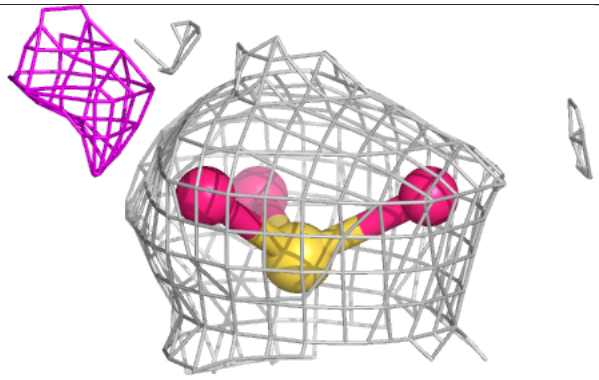
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

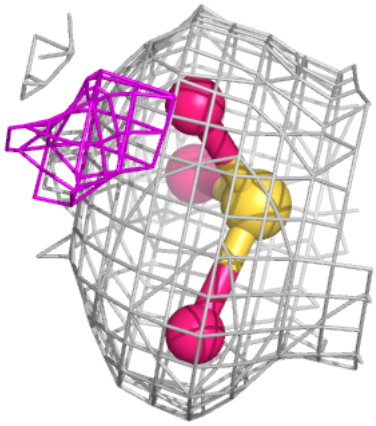


Electron density around SO3 A 1108:

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

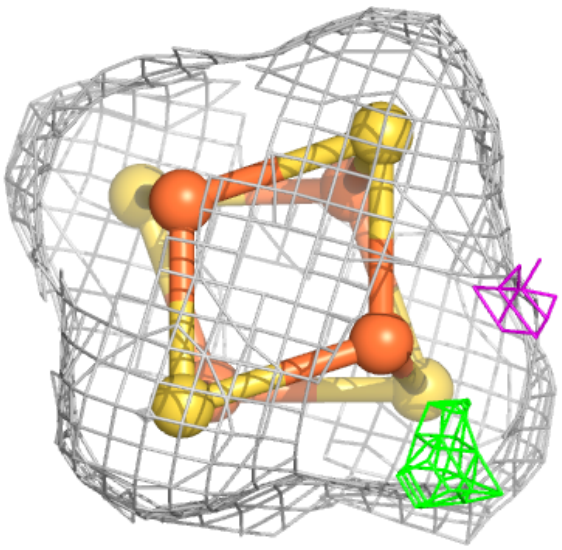


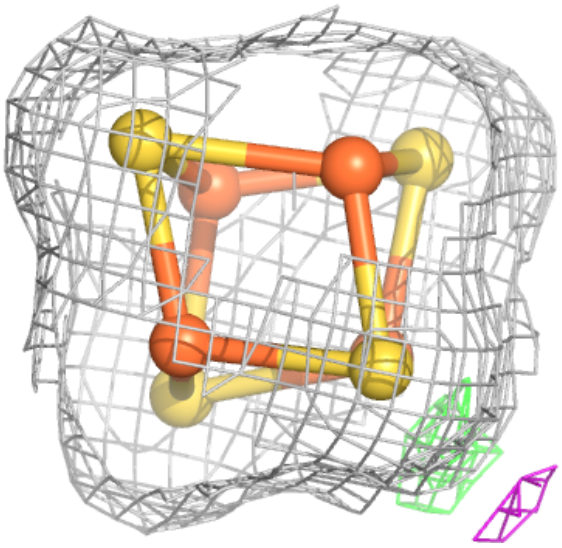


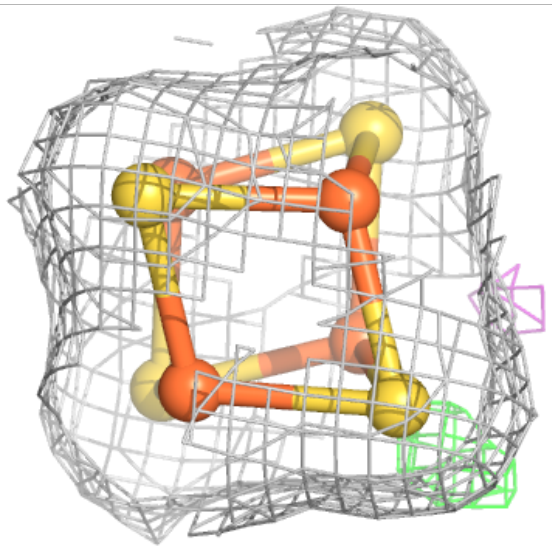


Electron density around SF4 B 1001:

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

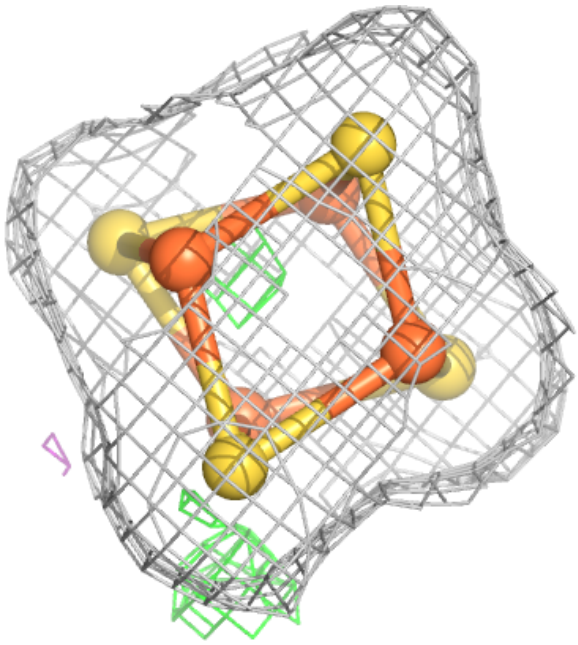


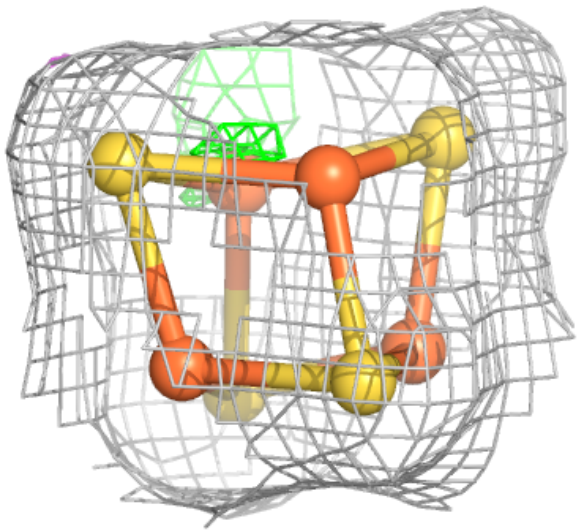


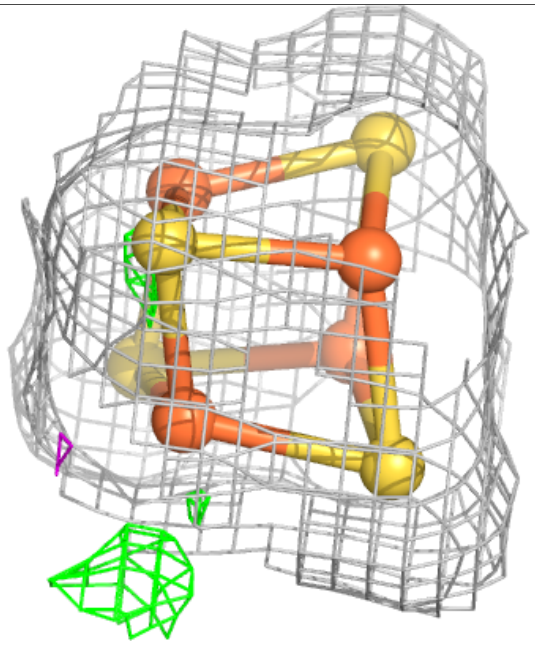


Electron density around SF4 A 1104:

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

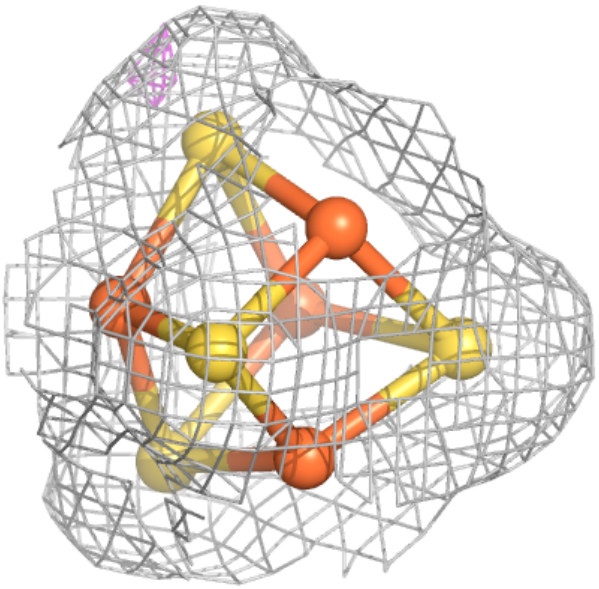


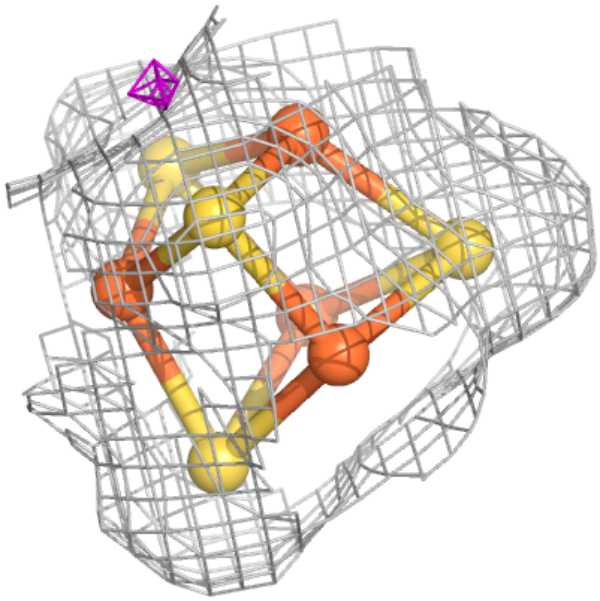


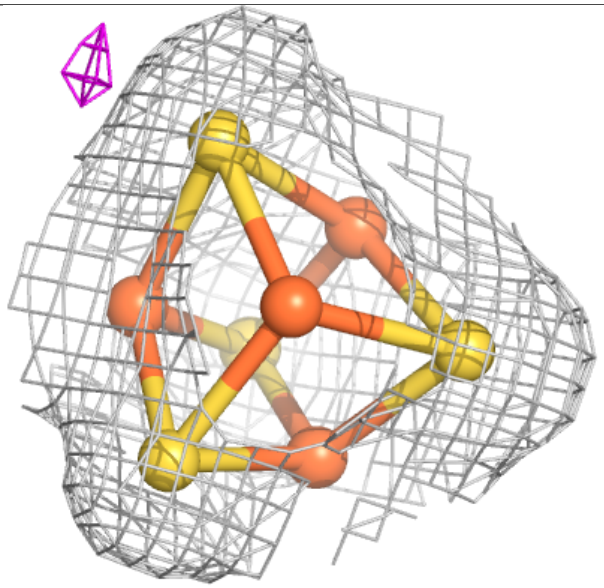


Electron density around SF4 D 1107:

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

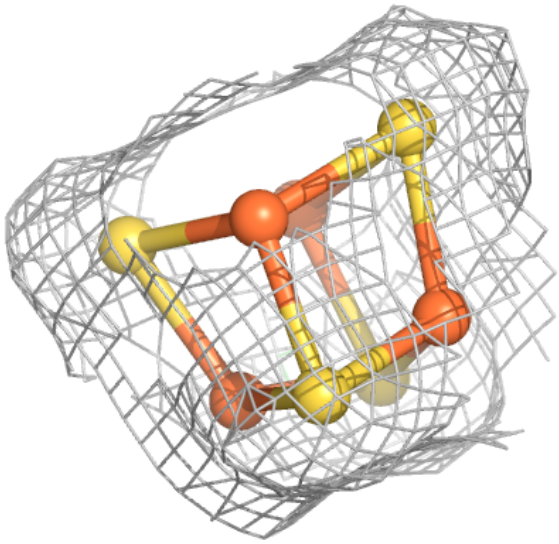


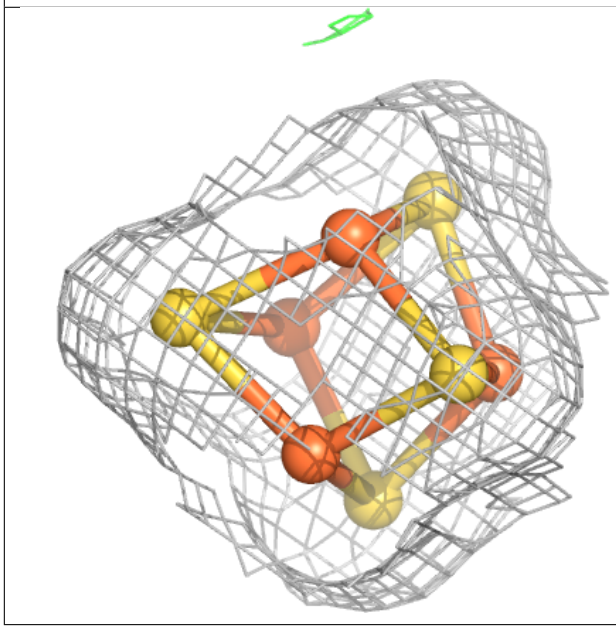


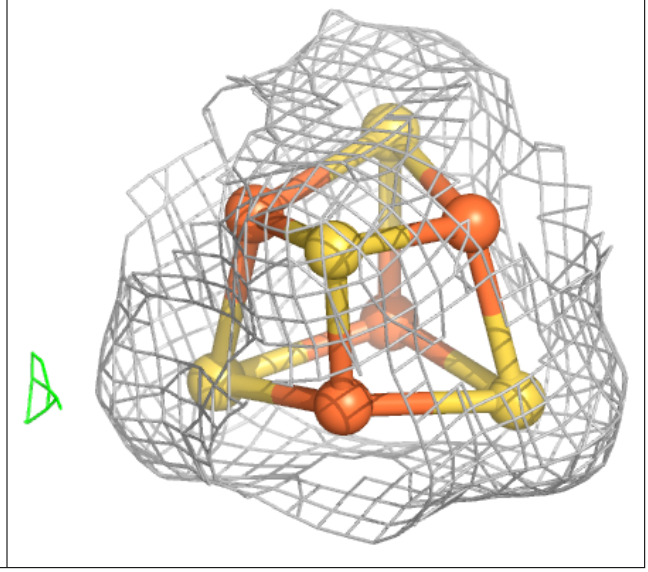


Electron density around SF4 A 1103:

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

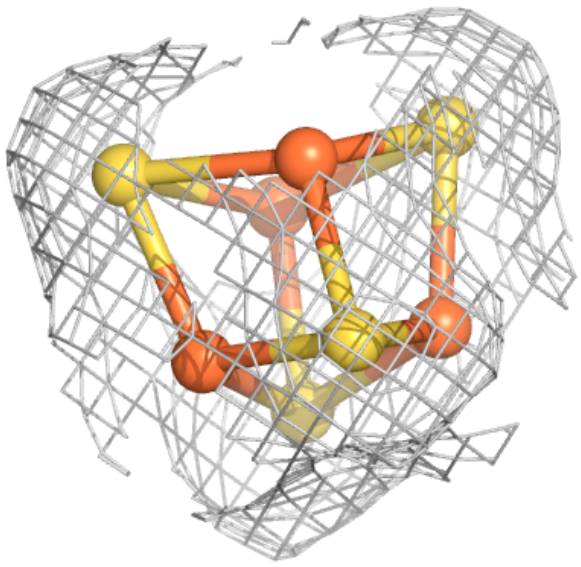


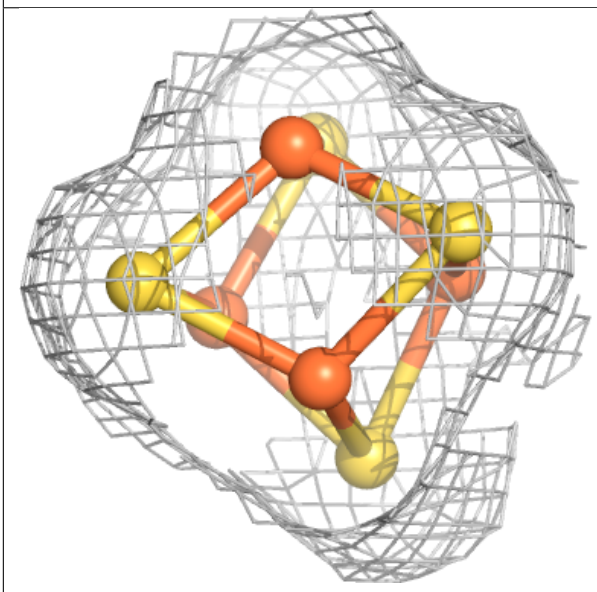


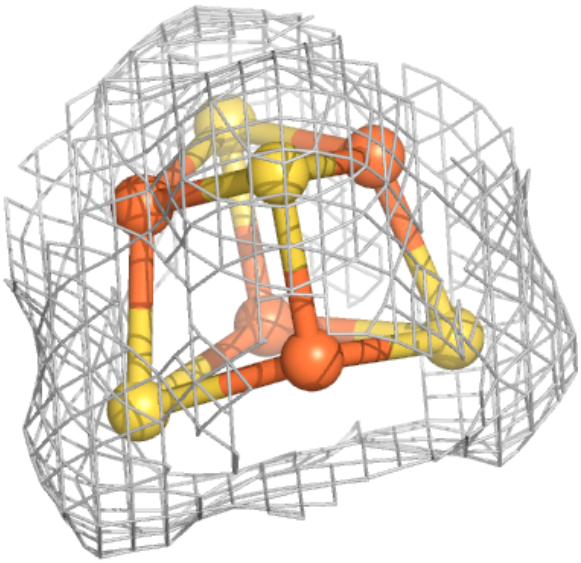


Electron density around SF4 A 1101:

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

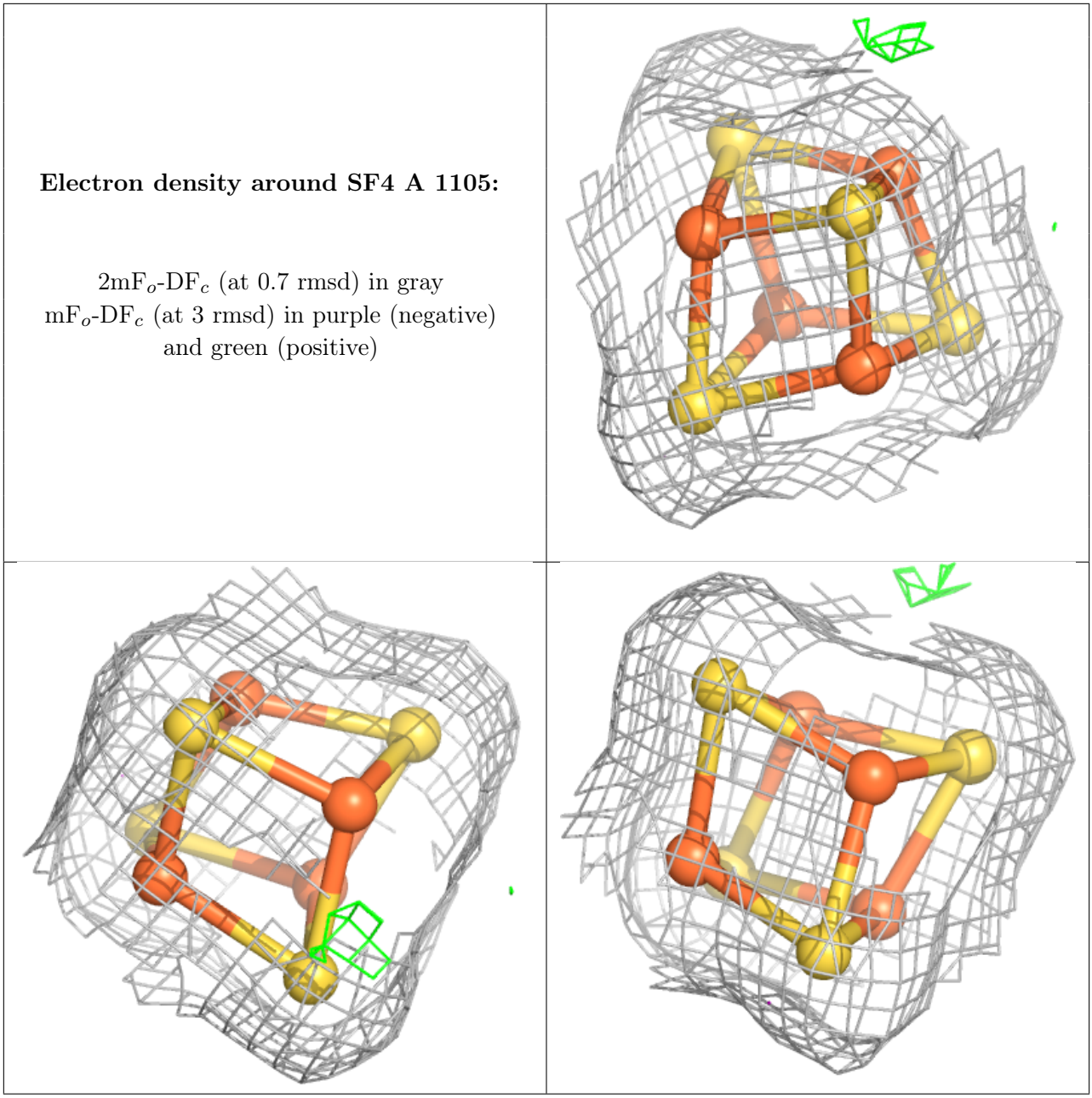






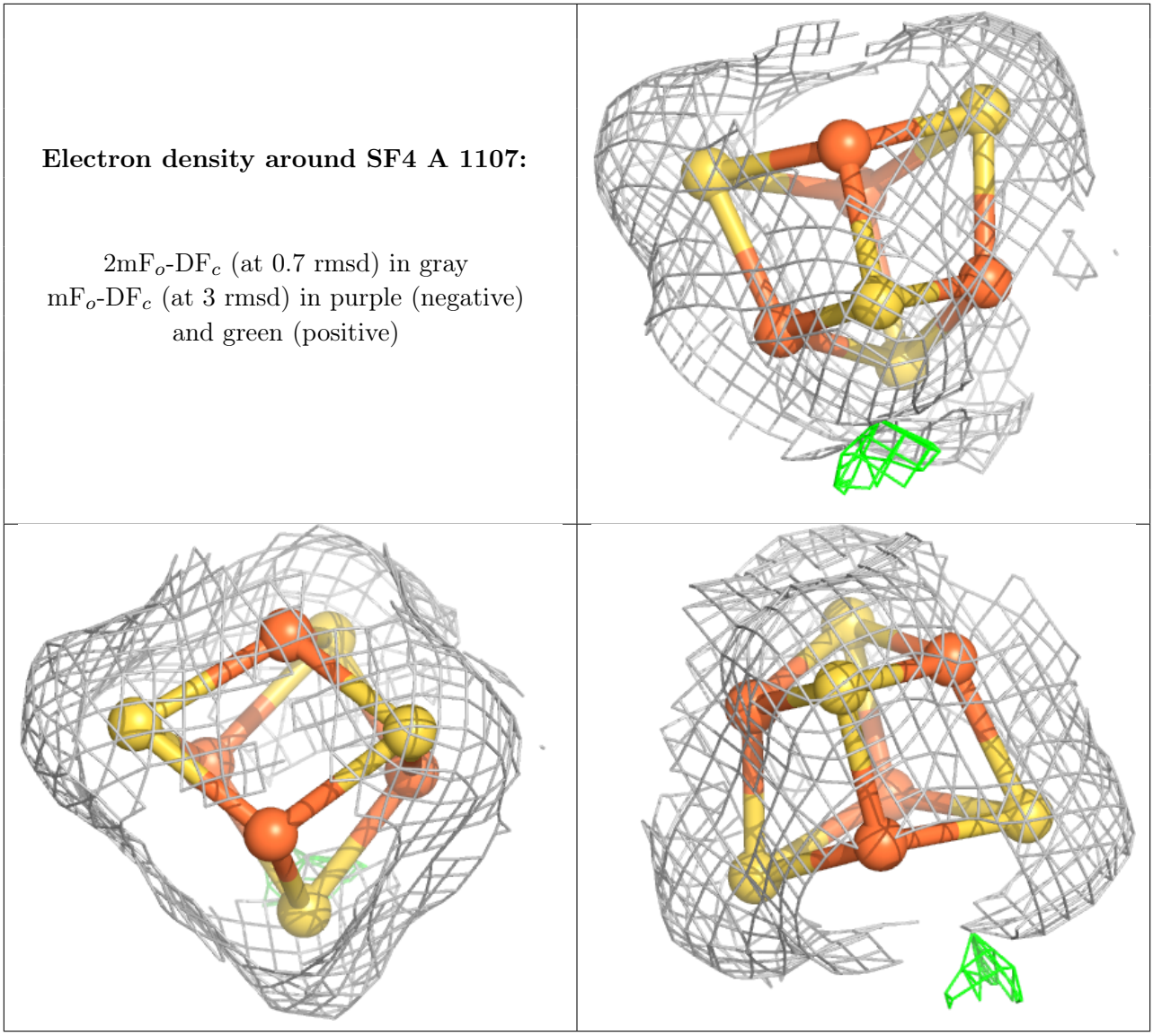
Electron density around SF4 A 1105:

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



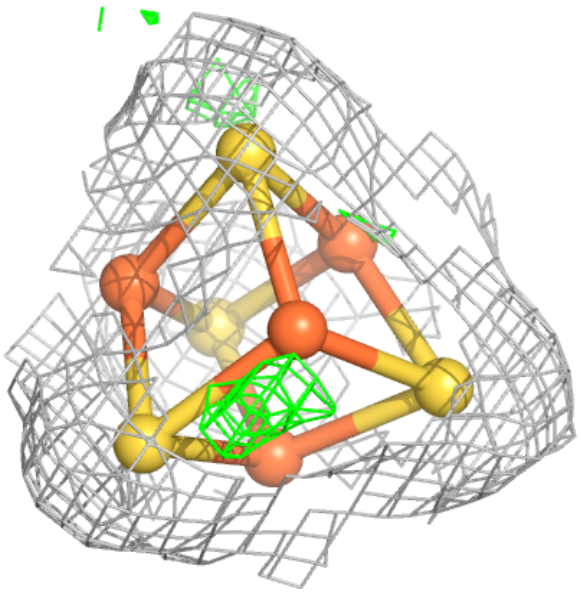
Electron density around SF4 A 1107:

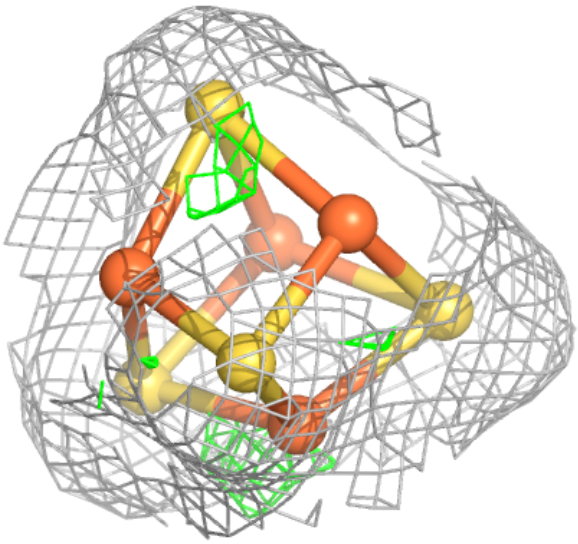
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

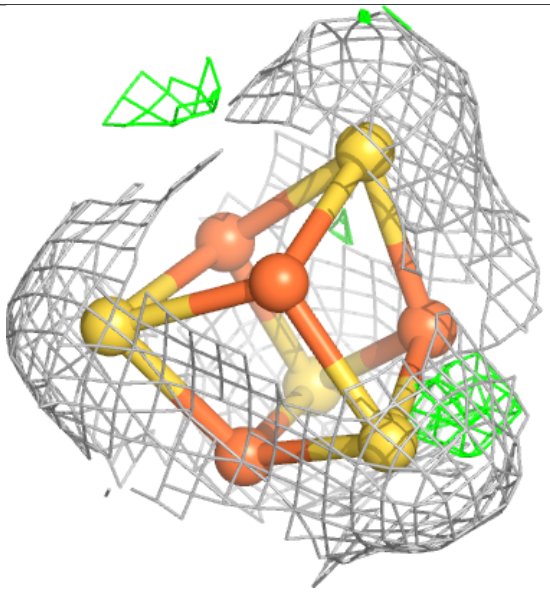


Electron density around SF4 A 1102:

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

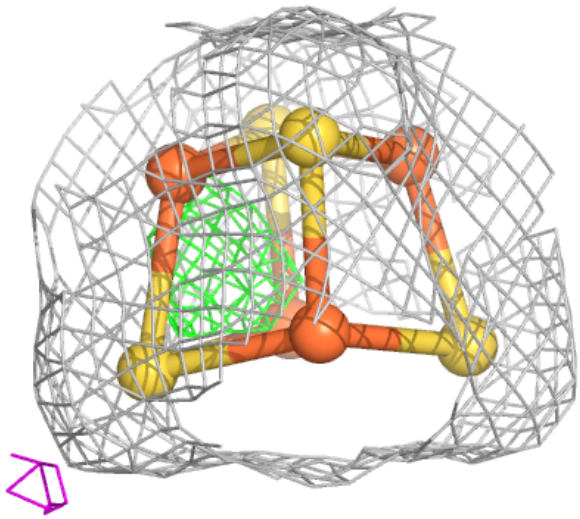


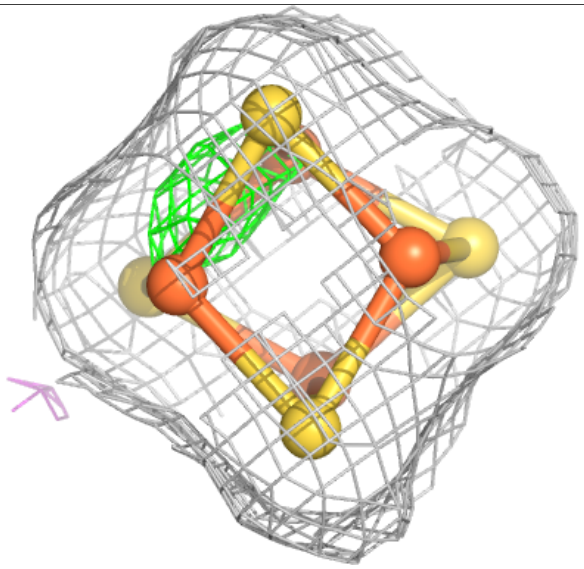


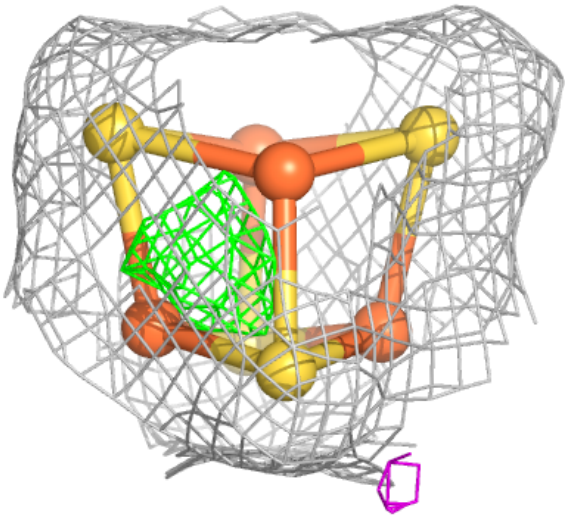


Electron density around SF4 B 1002:

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

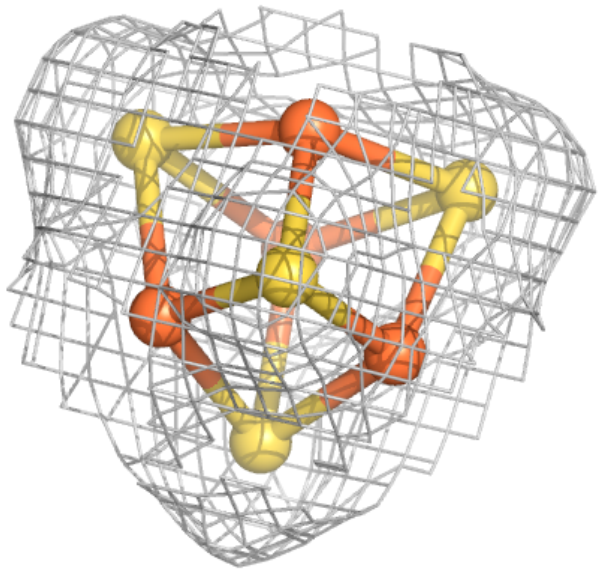


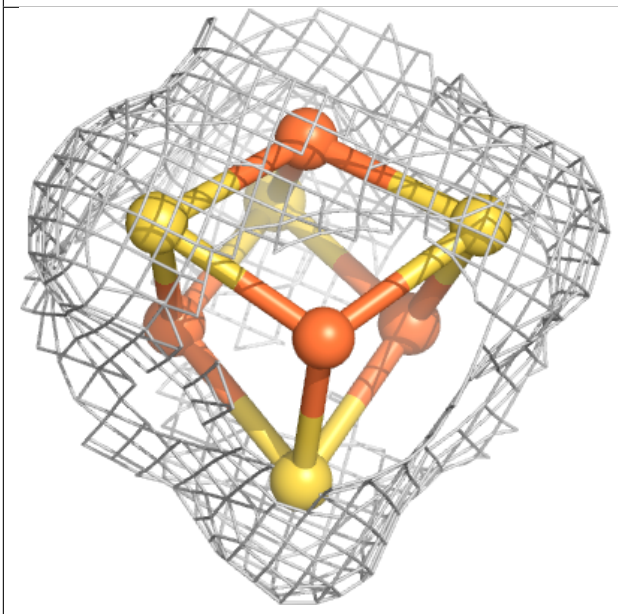


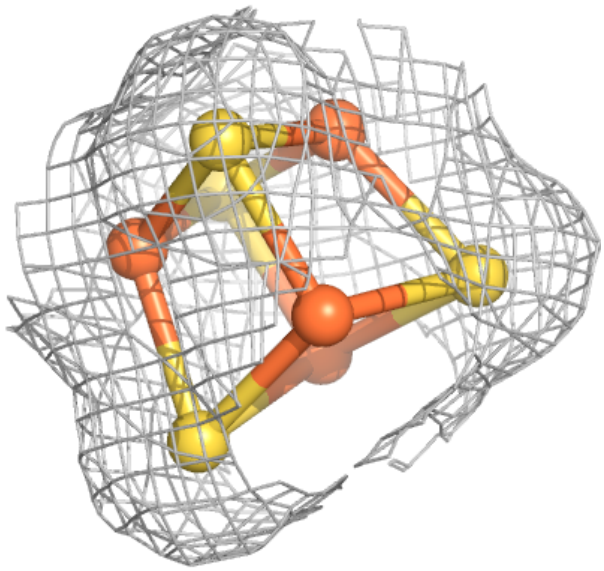


Electron density around SF4 B 1003:

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

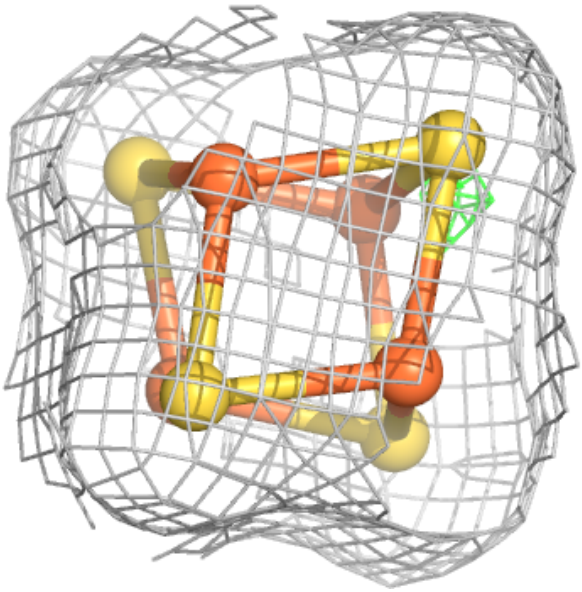


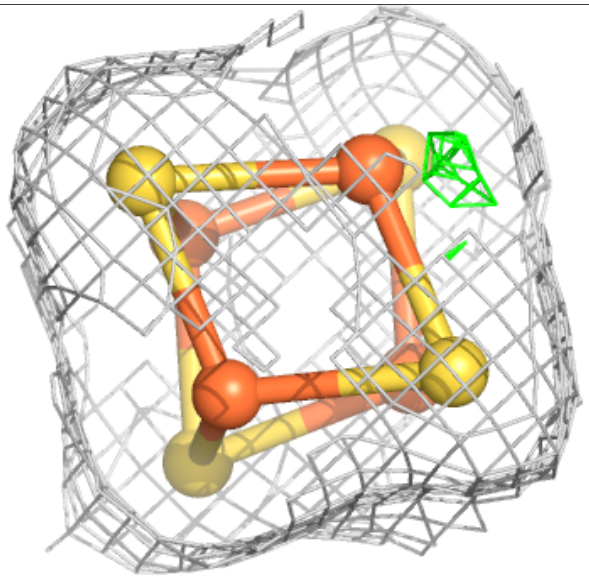


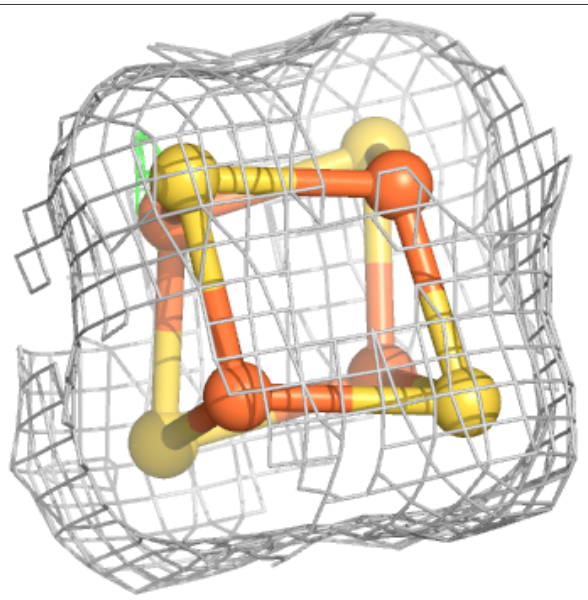


Electron density around SF4 B 1004:

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

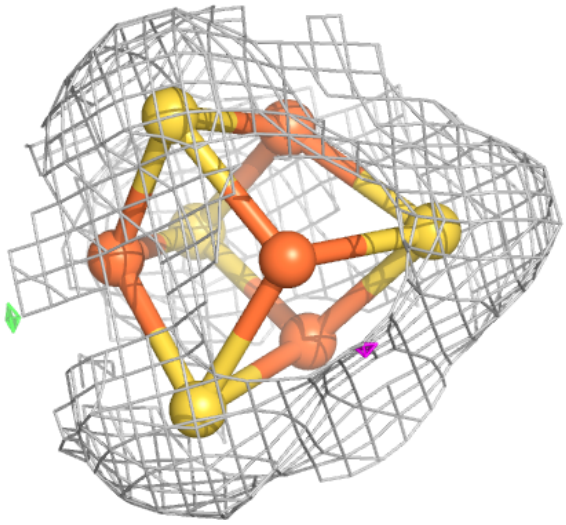


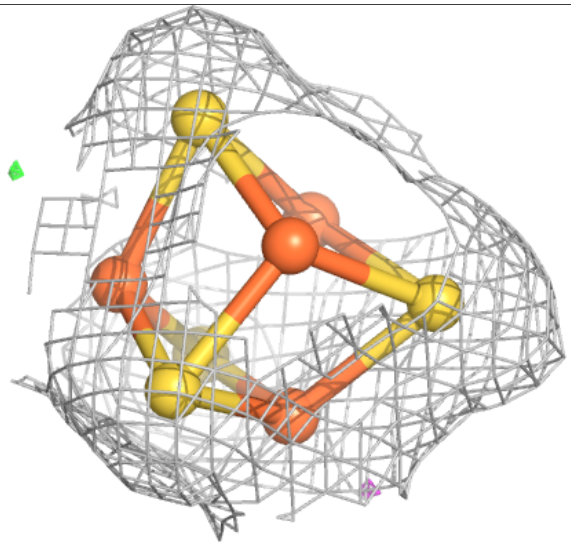


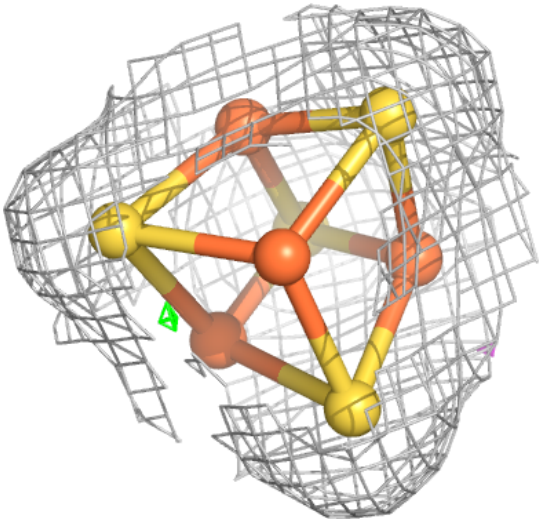


Electron density around SF4 B 1005:

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

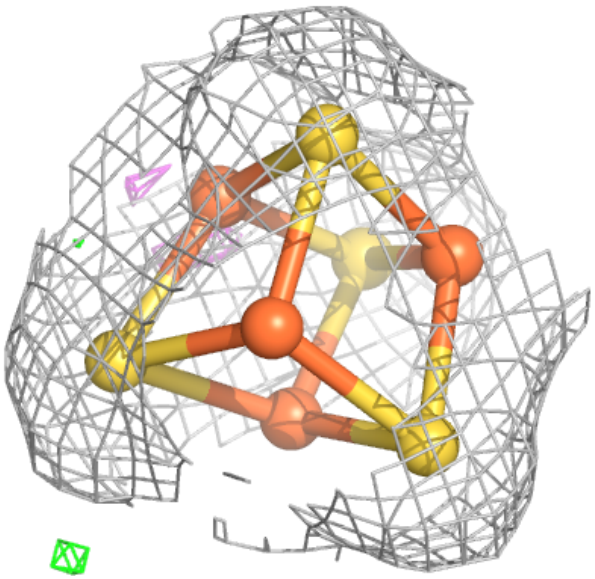


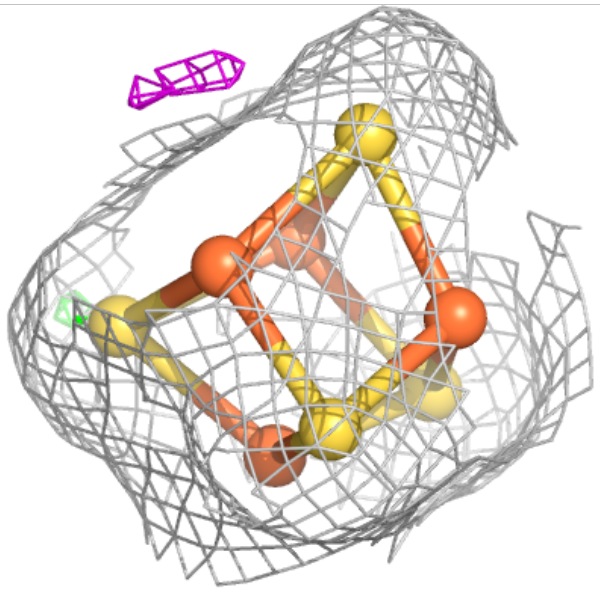


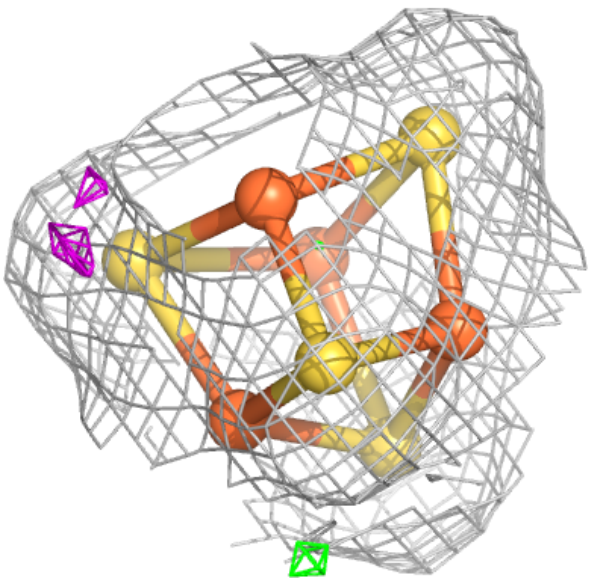


Electron density around SF4 B 1007:

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

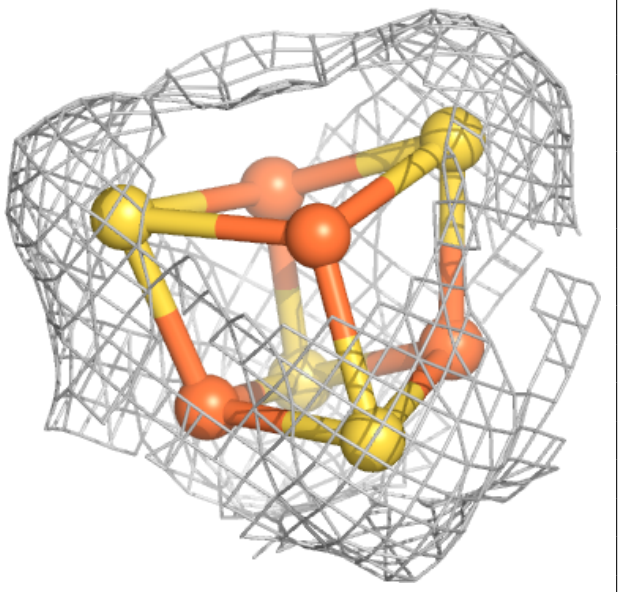


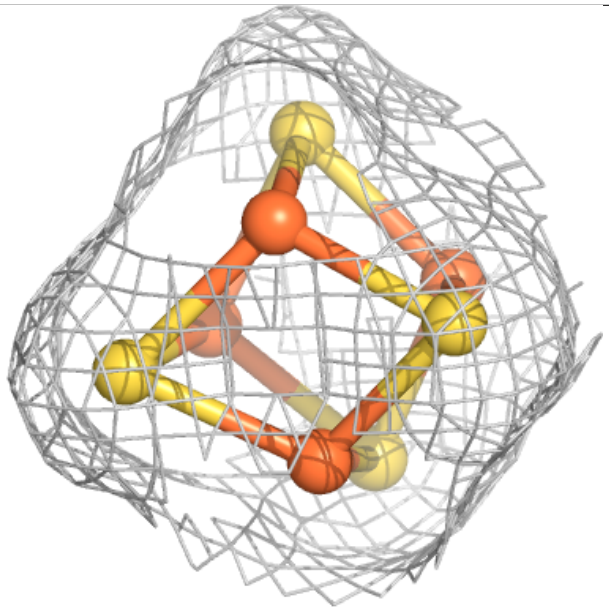


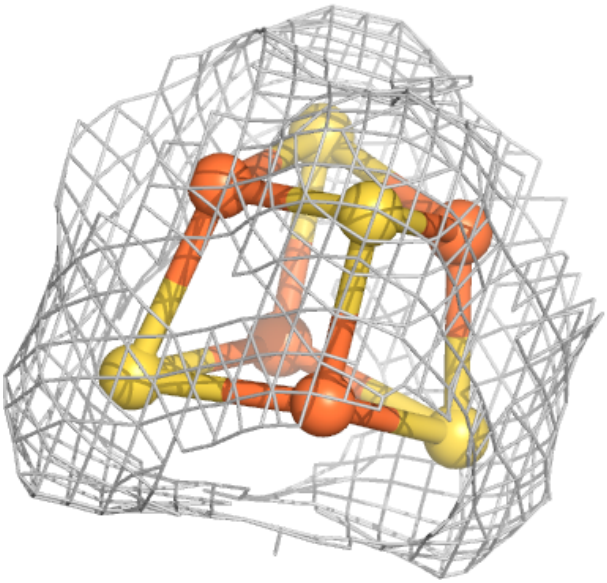


Electron density around SF4 C 1101:

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

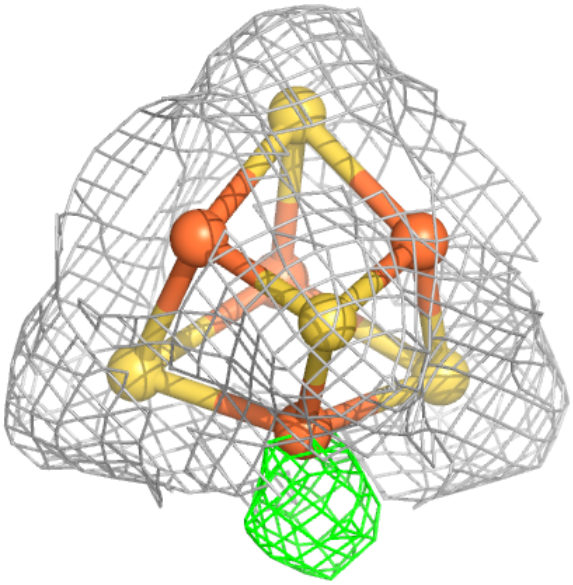


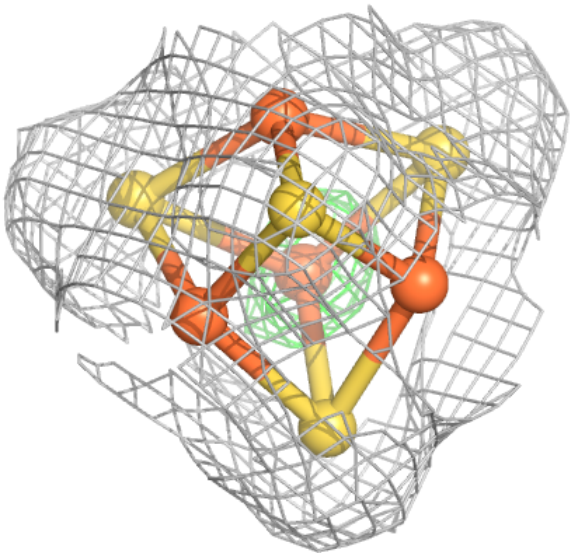


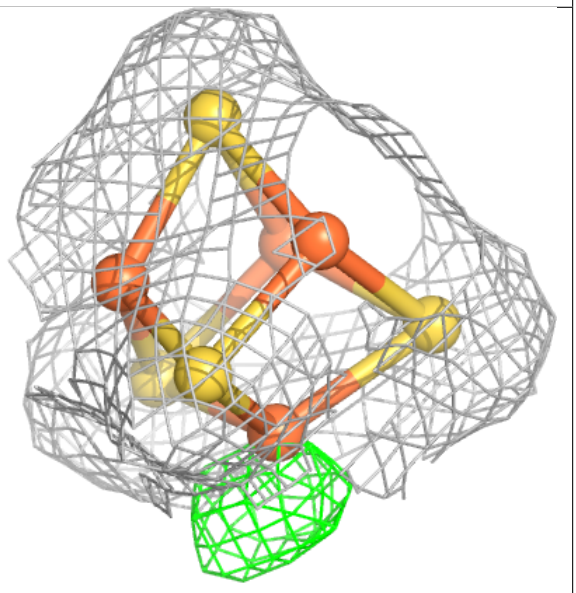


Electron density around SF4 C 1102:

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

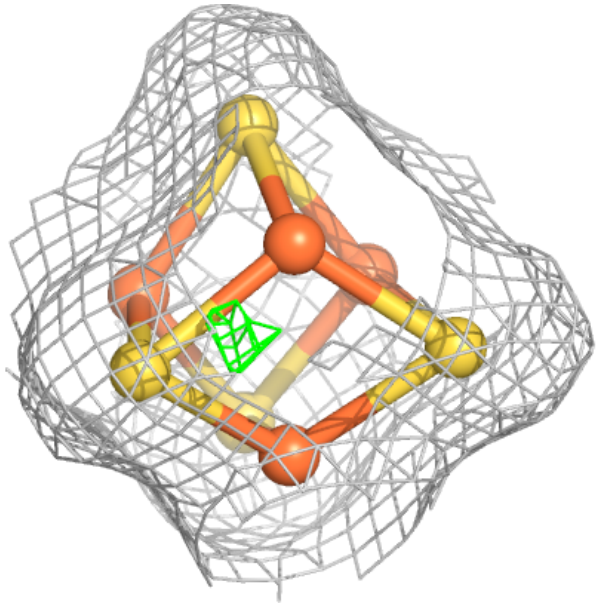


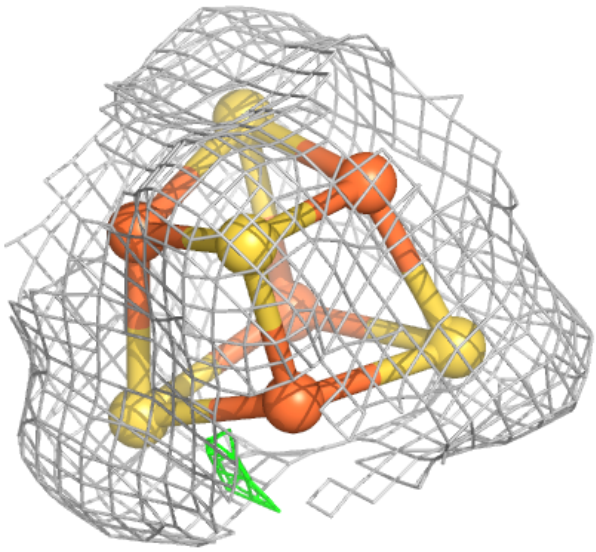


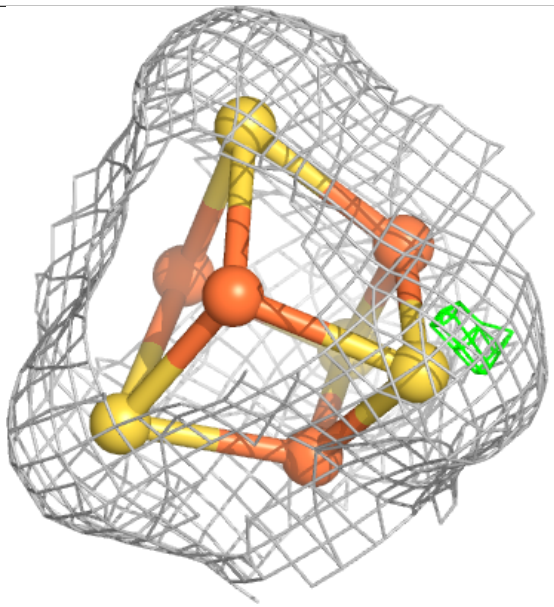


Electron density around SF4 C 1103:

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

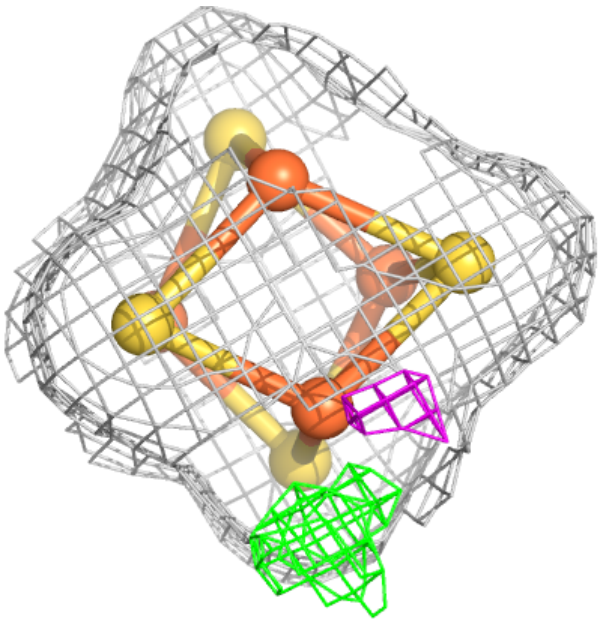


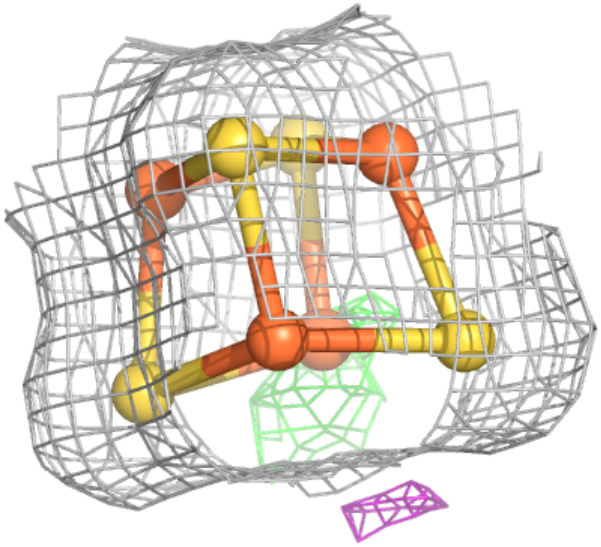


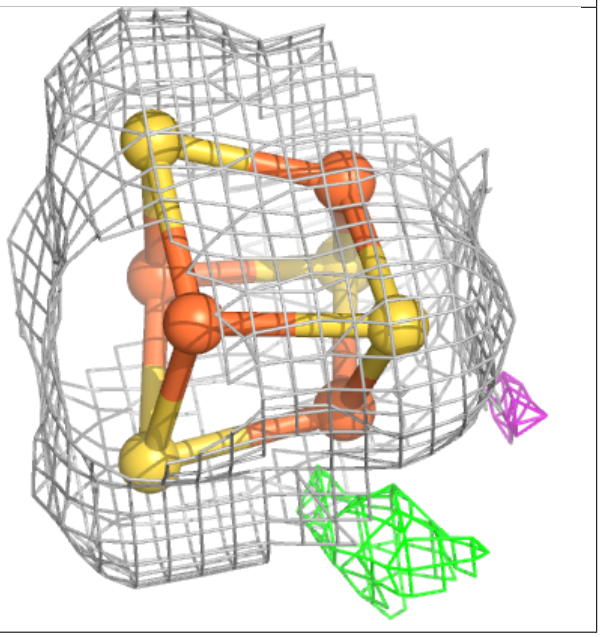


Electron density around SF4 C 1104:

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

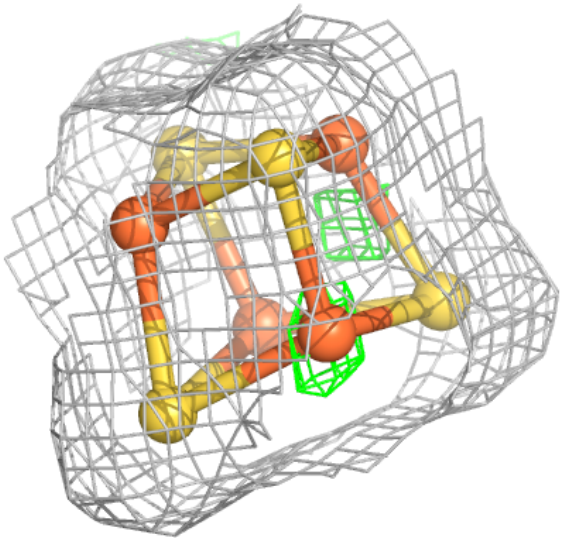


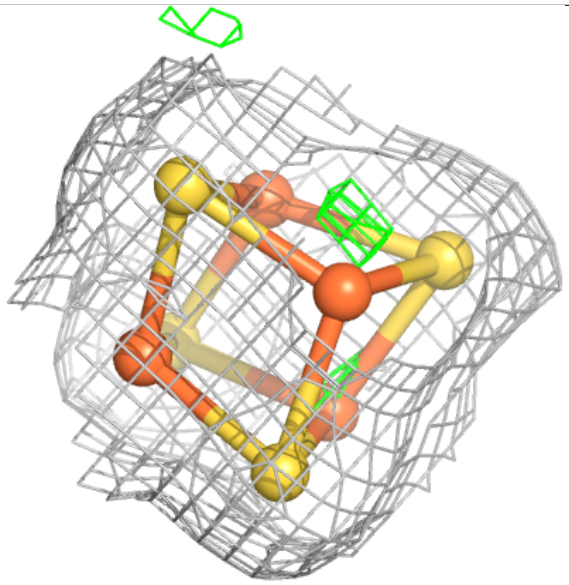


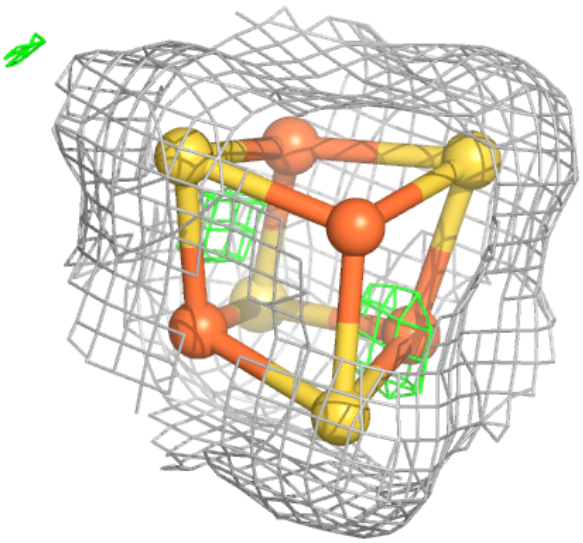


Electron density around SF4 C 1105:

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

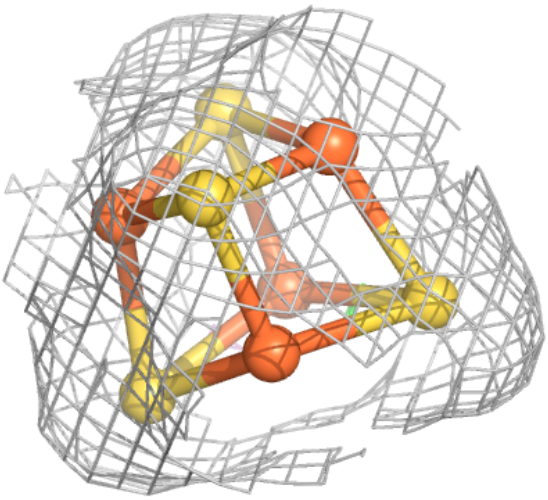


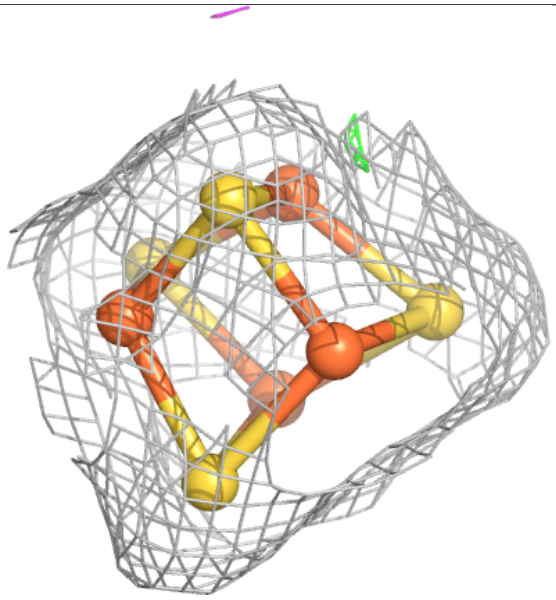


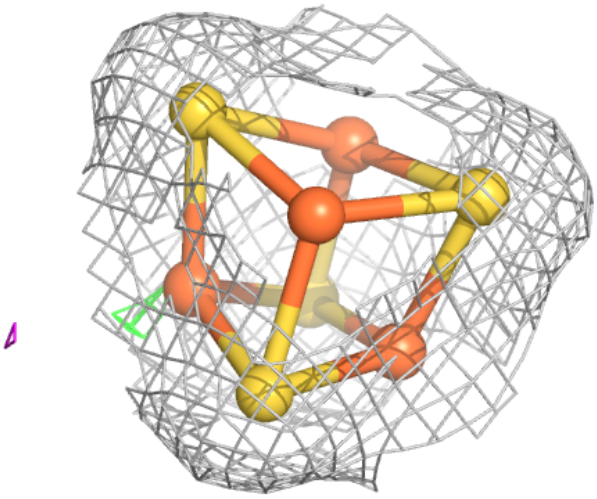


Electron density around SF4 C 1106:

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

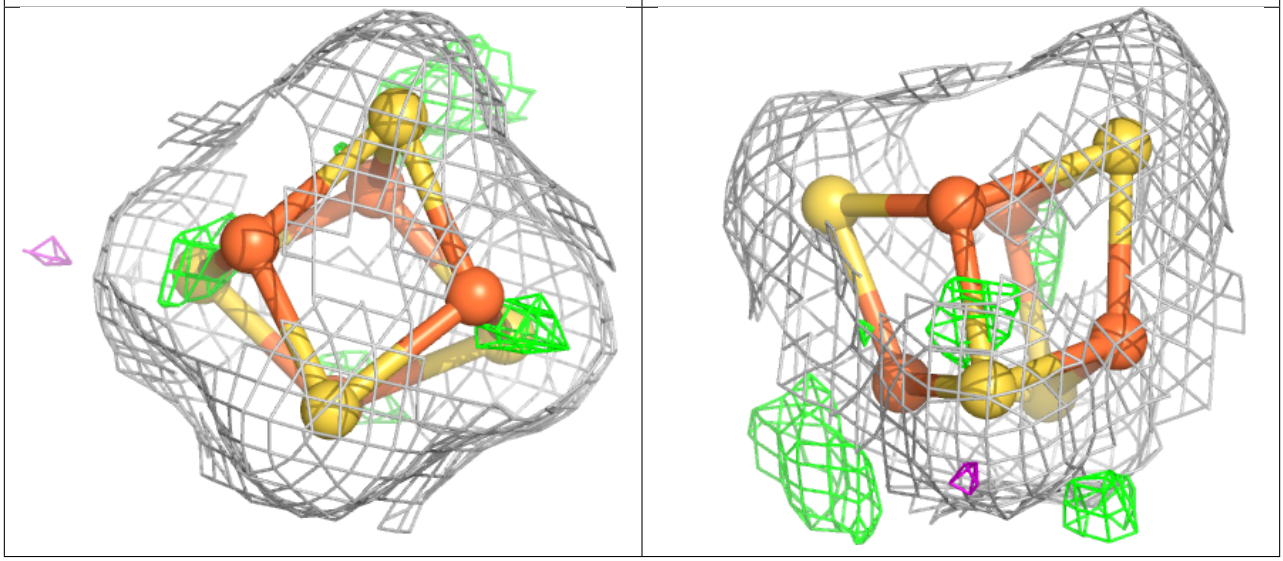






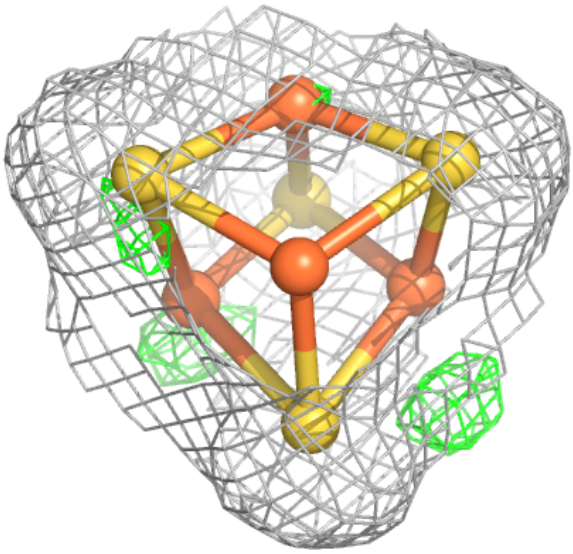
Electron density around SF4 D 1101:

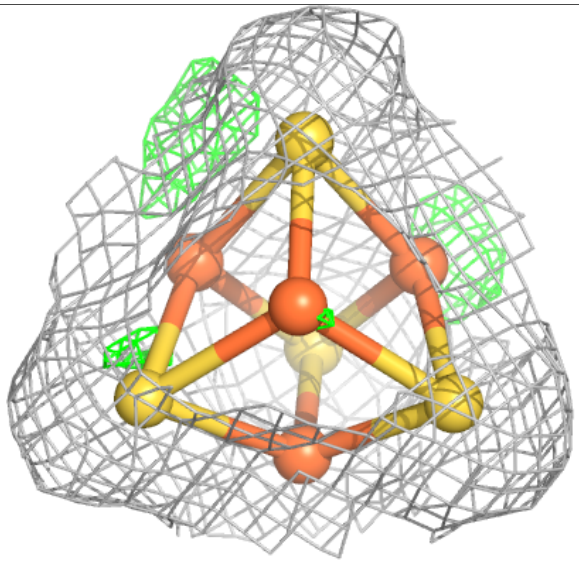
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

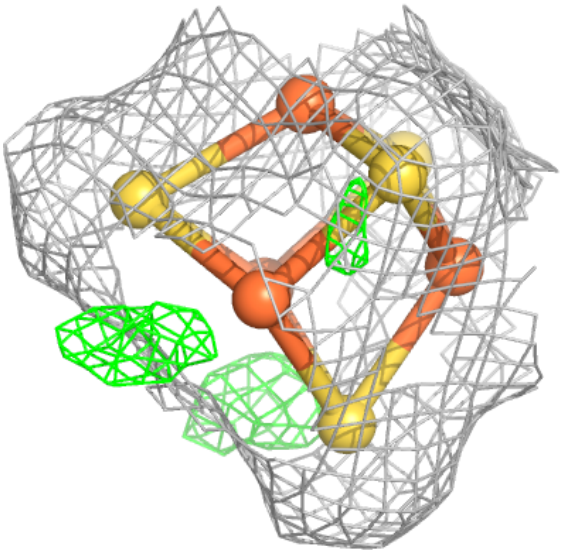


Electron density around SF4 D 1102:

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

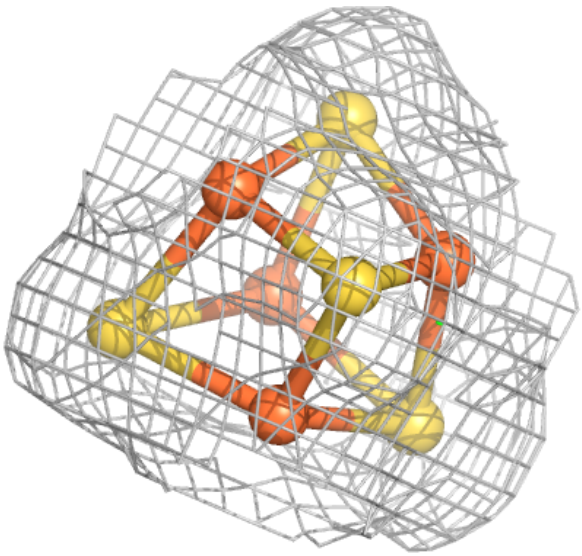


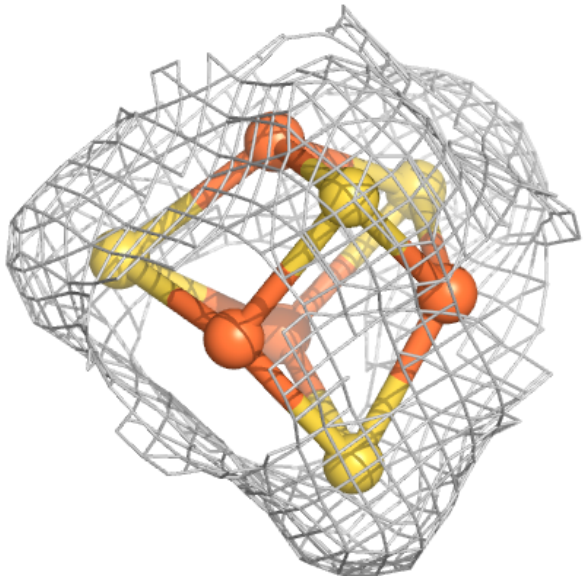


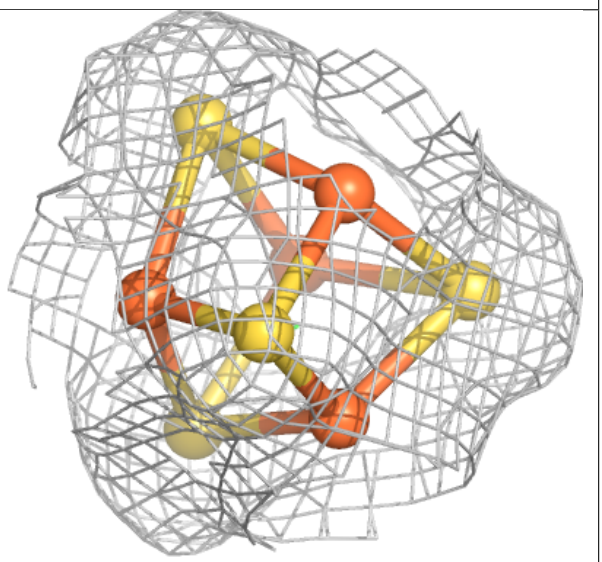


Electron density around SF4 D 1103:

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

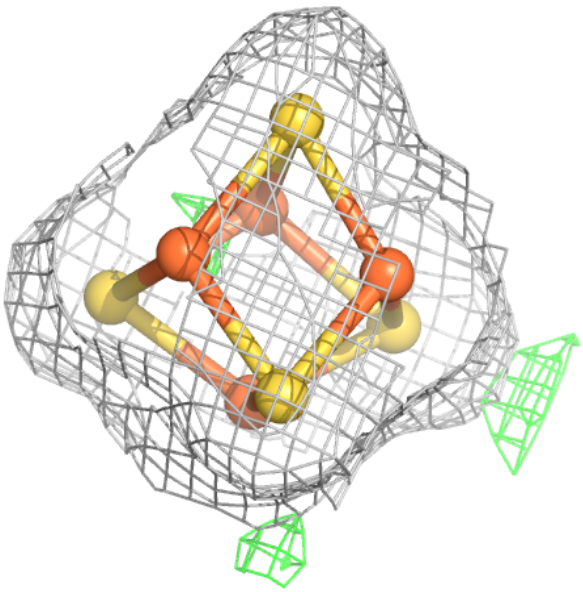


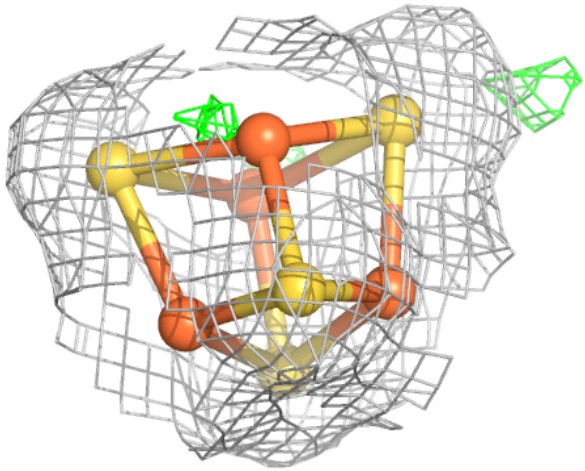


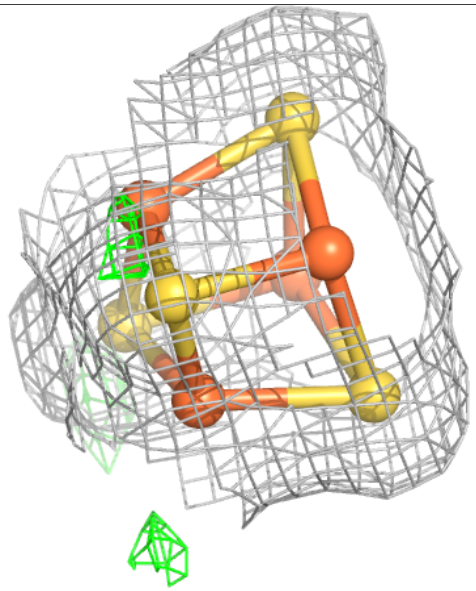


Electron density around SF4 D 1104:

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

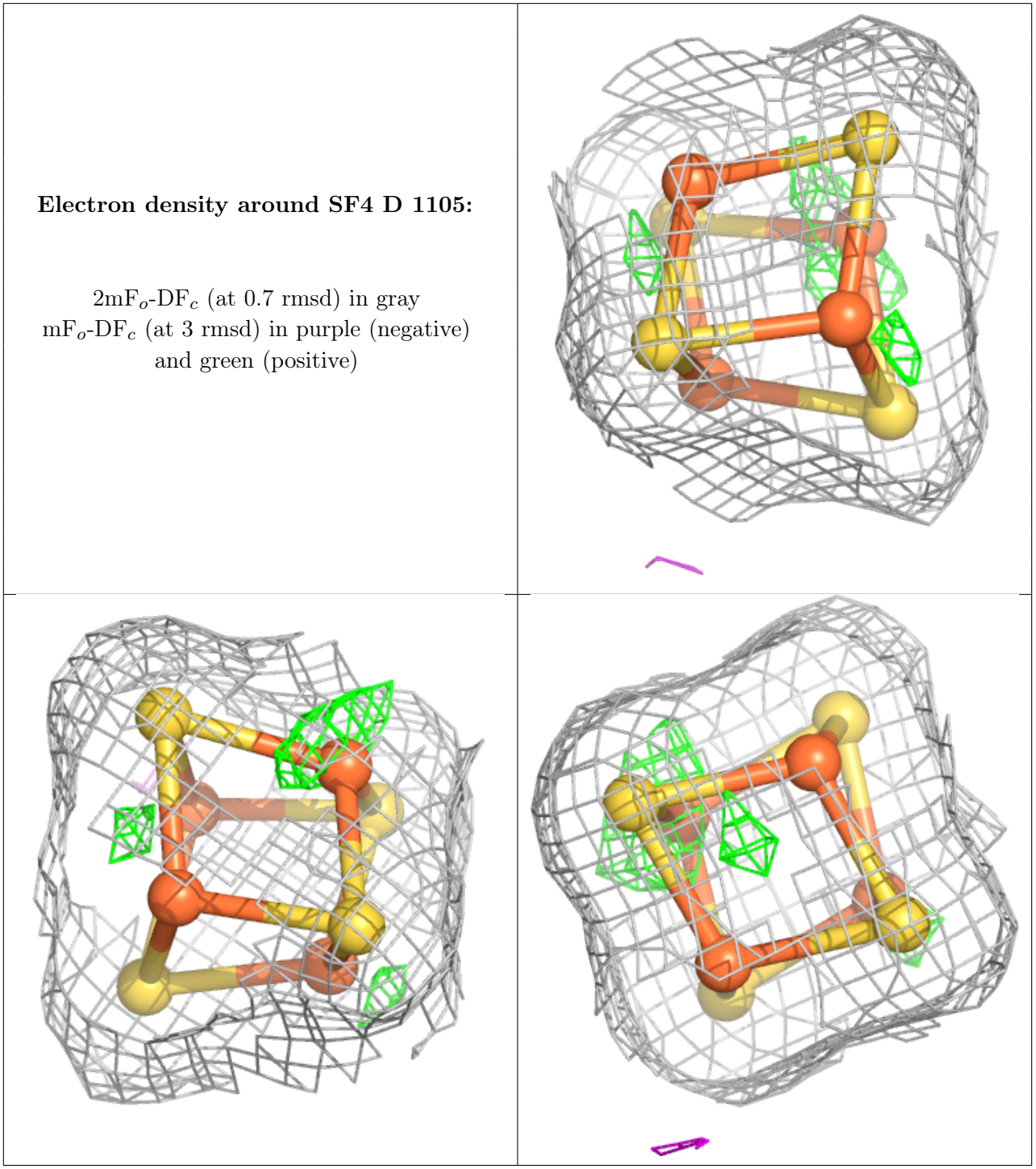






Electron density around SF4 D 1105:

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



6.5 Other polymers

There are no such residues in this entry.