wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2026 – 03:51 am BST

PDB ID	:	8RIU / pdb_00008riu
Title	:	Crystal structure of the F420-reducing carbon monoxide dehydrogenase component from the ethanotroph Candidatus Ethanoperedens thermophilum
Authors	:	Lemaire, O.N.; Wagner, T.
Deposited on	:	2023-12-19
Resolution	:	1.89 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

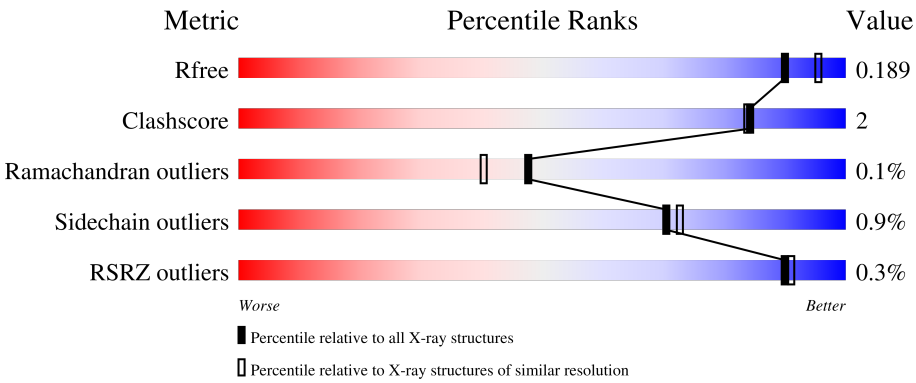
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.89 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	792	89% 6% •
1	D	792	89% 6% •
2	B	370	% 94% 6%
2	E	370	94% 6%
3	C	174	89% 10% •

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Mol	Chain	Length	Quality of chain
3	F	174	95% 5%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 21942 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 Acetyl-CoA decarbonylase/synthase complex subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	759	5859	3706	1011	1091	51	0	0	0
1	D	760	5902	3732	1023	1096	51	0	4	0

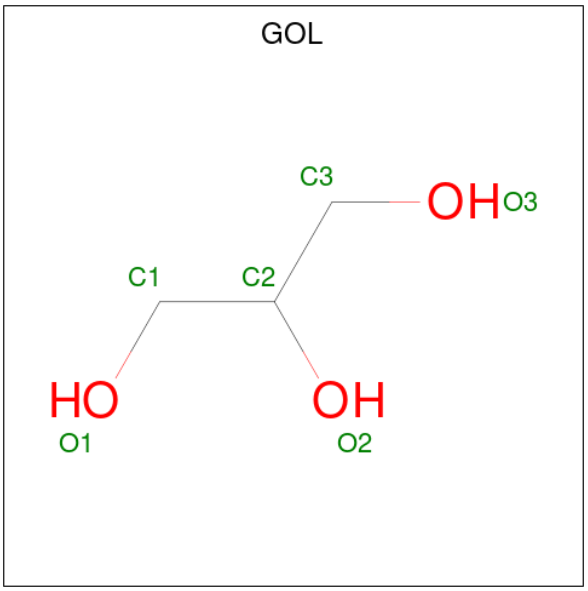
- Molecule 2 is a protein called Coenzyme F420 hydrogenase/dehydrogenase, beta subunit C terminus.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	370	2843	1791	475	553	24	0	0	0
2	E	370	2854	1797	479	554	24	0	1	0

- Molecule 3 is a protein called Acetyl-CoA decarbonylase/synthase complex subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	174	1352	859	233	253	7	0	2	0
3	F	174	1343	855	231	249	8	0	1	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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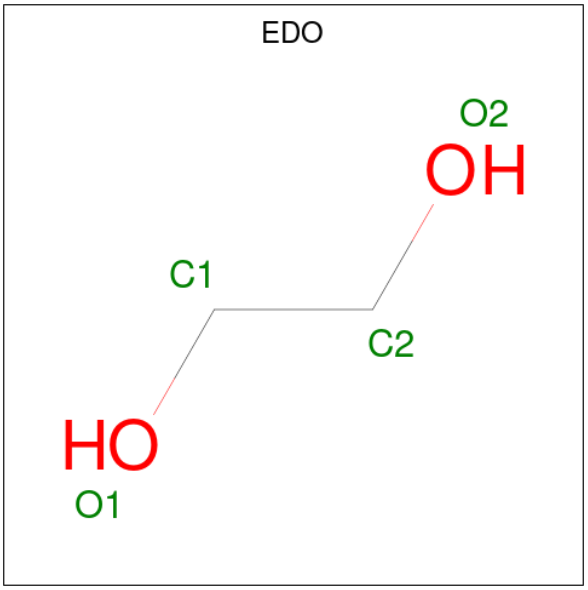
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	F	1	6	3	3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	B	1	4	2	2	0	0
5	D	1	4	2	2	0	0

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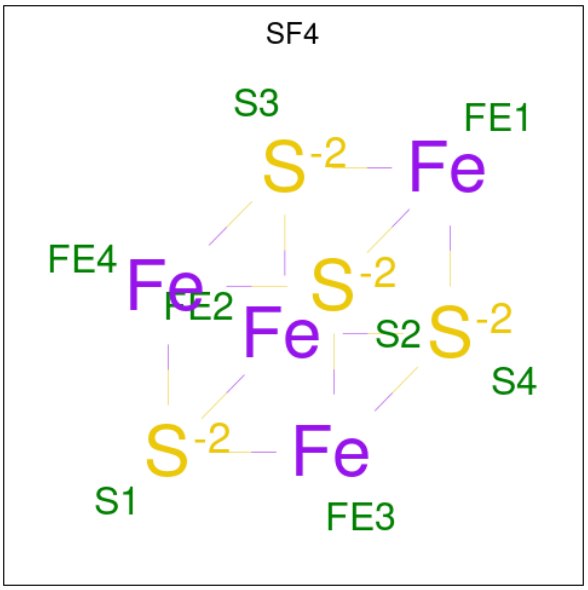
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	F	1	4	2	2	0	0

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

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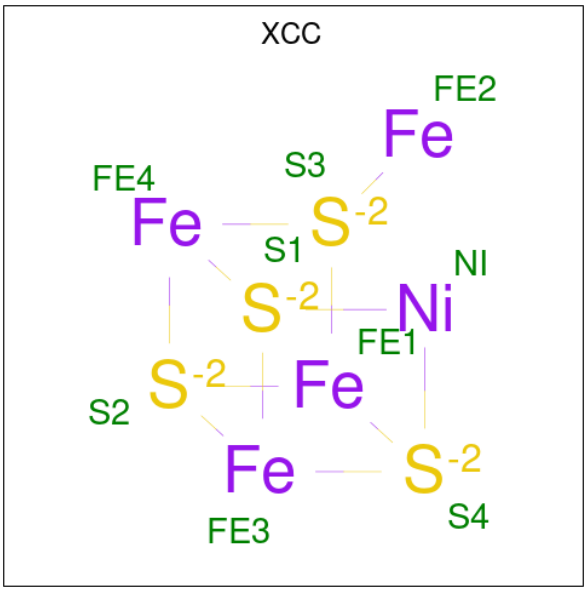
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
6	E	1	8	4	4	0	0
			Total	Fe	S		
6	E	1	8	4	4	0	0
			Total	Fe	S		
6	E	1	8	4	4	0	0

- Molecule 7 is FE(4)-NI(1)-S(4) CLUSTER (CCD ID: XCC) (formula: Fe_4NiS_4) (labeled as "Ligand of Interest" by depositor).



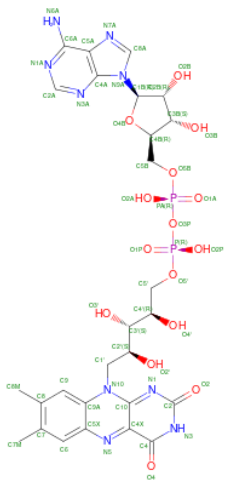
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Fe	Ni	S		
7	A	1	9	4	1	4	0	0
			Total	Fe	Ni	S		
7	D	1	9	4	1	4	0	0

- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
8	A	1	1	1	0	0
			Total	K		
8	D	1	1	1	0	0

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).

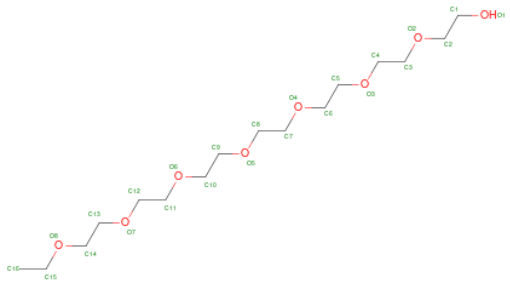
FAD



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

- Molecule 10 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: PE4) (formula: $C_{16}H_{34}O_8$).

PE4



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	D	1	6	4	2	0	0

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
11	D	1	1	1	0	1

- Molecule 12 is water.

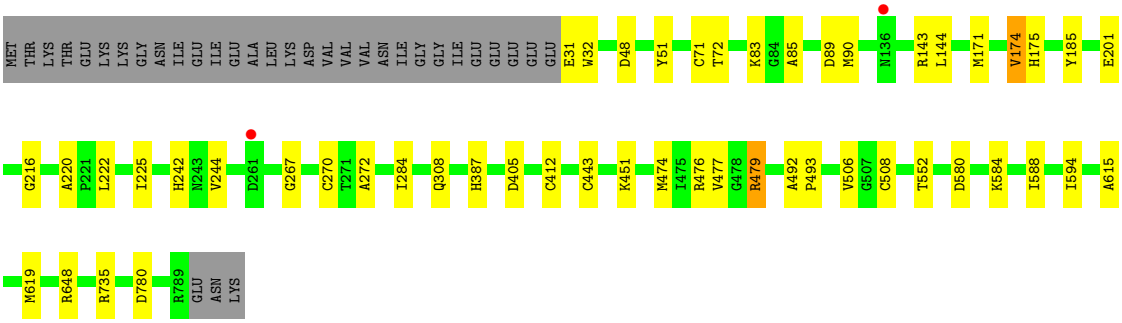
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	455	455	455	0	0
			Total	O		
12	B	140	140	140	0	0
			Total	O		
12	C	160	160	160	0	1
			Total	O		
12	D	351	351	351	0	0
			Total	O		
12	E	179	179	179	0	0
			Total	O		
12	F	133	133	133	0	1

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.

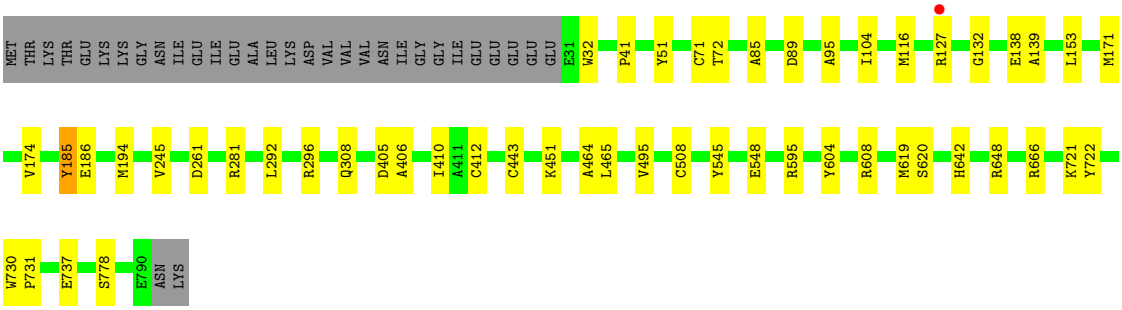
• Molecule 1: Acetyl-CoA decarbonylase/synthase complex subunit alpha

Chain A:



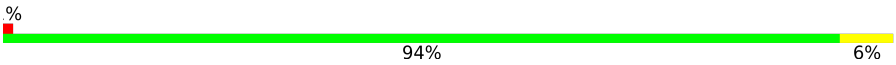
• Molecule 1: Acetyl-CoA decarbonylase/synthase complex subunit alpha

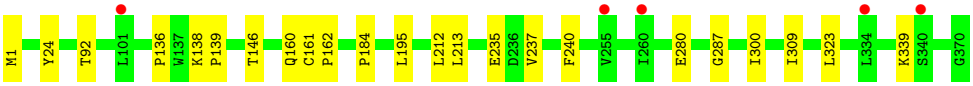
Chain D:



• Molecule 2: Coenzyme F420 hydrogenase/dehydrogenase, beta subunit C terminus

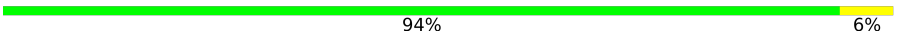
Chain B:





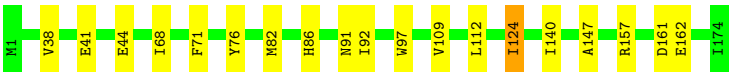
• Molecule 2: Coenzyme F420 hydrogenase/dehydrogenase, beta subunit C terminus

Chain E:



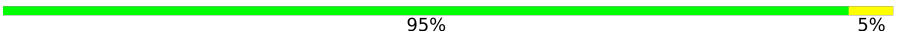
• Molecule 3: Acetyl-CoA decarbonylase/synthase complex subunit epsilon

Chain C:



• Molecule 3: Acetyl-CoA decarbonylase/synthase complex subunit epsilon

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.07Å 159.21Å 191.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.80 – 1.89 39.80 – 1.89	Depositor EDS
% Data completeness (in resolution range)	70.0 (39.80-1.89) 70.0 (39.80-1.89)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.165 , 0.187 0.170 , 0.189	Depositor DCC
R_{free} test set	8281 reflections (3.52%)	wwPDB-VP
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	21942	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, FAD, GOL, EDO, SF4, K, XCC, PE4

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	0.59	0/5972	0.81	2/8088 (0.0%)
1	D	0.54	0/6021	0.74	1/8152 (0.0%)
2	B	0.56	0/2886	0.81	1/3885 (0.0%)
2	E	0.50	0/2897	0.72	1/3899 (0.0%)
3	C	0.56	0/1379	0.79	1/1861 (0.1%)
3	F	0.53	0/1370	0.73	0/1848
All	All	0.55	0/20525	0.77	6/27733 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	80	SER	N-CA-C	-6.07	105.69	114.12
3	C	140	ILE	N-CA-C	-5.87	105.66	111.77
1	D	132	GLY	CA-C-O	-5.61	118.41	122.45
1	A	780	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	735	ARG	N-CA-C	-5.02	107.28	113.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5859	0	5870	32	0
1	D	5902	0	5922	33	0
2	B	2843	0	2852	11	0
2	E	2854	0	2864	14	0
3	C	1352	0	1370	9	0
3	F	1343	0	1368	3	0
4	A	42	0	56	3	0
4	B	6	0	8	0	0
4	C	18	0	24	0	0
4	D	6	0	8	1	0
4	E	6	0	8	0	0
4	F	12	0	16	0	0
5	A	32	0	48	0	0
5	B	4	0	6	0	0
5	D	4	0	6	0	0
5	F	4	0	6	0	0
6	A	32	0	0	1	0
6	B	24	0	0	0	0
6	D	24	0	0	1	0
6	E	24	0	0	0	0
7	A	9	0	0	1	0
7	D	9	0	0	0	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
9	B	53	0	31	0	0
9	E	53	0	31	1	0
10	D	6	0	9	0	0
11	D	1	0	0	0	0
12	A	455	0	0	1	0
12	B	140	0	0	0	0
12	C	160	0	0	1	0
12	D	351	0	0	0	0
12	E	179	0	0	2	0
12	F	133	0	0	0	0
All	All	21942	0	20503	96	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.

The worst 5 of 96 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)
7:A:812:XCC:FE4	7:A:812:XCC:S2	1.86	0.66
1:D:292:LEU:O	1:D:296[B]:ARG:HG3	2.04	0.57
3:C:41:GLU:O	3:C:44:GLU:HG2	2.10	0.51
1:A:51:TYR:CD2	4:A:813:GOL:H31	2.45	0.51
1:A:267:GLY:C	1:A:272:ALA:HB2	2.37	0.49

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	757/792 (96%)	739 (98%)	17 (2%)	1 (0%)	48	40
1	D	762/792 (96%)	743 (98%)	18 (2%)	1 (0%)	48	40
2	B	368/370 (100%)	359 (98%)	9 (2%)	0	100	100
2	E	369/370 (100%)	362 (98%)	7 (2%)	0	100	100
3	C	174/174 (100%)	172 (99%)	2 (1%)	0	100	100
3	F	173/174 (99%)	172 (99%)	1 (1%)	0	100	100
All	All	2603/2672 (97%)	2547 (98%)	54 (2%)	2 (0%)	48	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	GLN
1	D	308	GLN

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	628/657 (96%)	621 (99%)	7 (1%)	65	67
1	D	633/657 (96%)	628 (99%)	5 (1%)	73	75
2	B	308/308 (100%)	307 (100%)	1 (0%)	86	88
2	E	309/308 (100%)	306 (99%)	3 (1%)	68	70
3	C	143/141 (101%)	141 (99%)	2 (1%)	59	59
3	F	142/141 (101%)	140 (99%)	2 (1%)	59	59
All	All	2163/2212 (98%)	2143 (99%)	20 (1%)	70	73

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	508	CYS
2	E	256	ARG
3	F	124	ILE
3	F	86	HIS
1	A	508	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	90	ASN
2	E	177	ASN
1	D	402	GLN
1	D	376	GLN
1	D	453	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 47 ligands modelled in this entry, 3 are monoatomic - leaving 44 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	GOL	A	816	-	5,5,5	0.09	0	5,5,5	0.35	0
6	SF4	E	401	2	0,12,12	-	-	-		
4	GOL	A	801	-	5,5,5	0.86	0	5,5,5	1.02	0
6	SF4	D	803	1	0,12,12	-	-	-		
6	SF4	A	810	1	0,12,12	-	-	-		
6	SF4	E	404	2	0,12,12	-	-	-		
4	GOL	F	403	-	5,5,5	0.99	0	5,5,5	0.84	0
6	SF4	D	804	1	0,12,12	-	-	-		
5	EDO	A	818	-	3,3,3	0.06	0	2,2,2	0.23	0
4	GOL	A	814	-	5,5,5	1.01	0	5,5,5	0.85	0
4	GOL	B	406	-	5,5,5	0.08	0	5,5,5	0.36	0
4	GOL	E	405	-	5,5,5	0.92	0	5,5,5	0.91	0
5	EDO	A	807	-	3,3,3	0.14	0	2,2,2	0.27	0
5	EDO	A	802	-	3,3,3	0.10	0	2,2,2	0.10	0
10	PE4	D	807	-	5,5,23	0.34	0	4,4,22	0.41	0
5	EDO	A	805	-	3,3,3	0.16	0	2,2,2	0.23	0
5	EDO	D	802	-	3,3,3	0.06	0	2,2,2	0.20	0
6	SF4	A	811	1	0,12,12	-	-	-		
6	SF4	A	819	1	0,12,12	-	-	-		
5	EDO	A	808	-	3,3,3	0.08	0	2,2,2	0.23	0
6	SF4	B	402	2	0,12,12	-	-	-		
7	XCC	D	806	1	0,12,12	-	-	-		
9	FAD	E	403	-	56,58,58	0.57	0	81,89,89	0.56	0
5	EDO	F	402	-	3,3,3	0.13	0	2,2,2	0.25	0
4	GOL	C	201	-	5,5,5	0.08	0	5,5,5	0.38	0
6	SF4	B	405	2	0,12,12	-	-	-		
4	GOL	F	401	-	5,5,5	0.08	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	FAD	B	404	-	56,58,58	0.54	0	81,89,89	0.57	0
6	SF4	A	809	1	0,12,12	-	-	-		
6	SF4	E	402	2	0,12,12	-	-	-		
6	SF4	B	403	2	0,12,12	-	-	-		
5	EDO	B	401	-	3,3,3	0.11	0	2,2,2	0.21	0
5	EDO	A	803	-	3,3,3	0.09	0	2,2,2	0.18	0
4	GOL	A	815	-	5,5,5	0.10	0	5,5,5	0.35	0
4	GOL	A	820	-	5,5,5	0.08	0	5,5,5	0.41	0
5	EDO	A	804	-	3,3,3	0.12	0	2,2,2	0.15	0
4	GOL	A	813	-	5,5,5	0.08	0	5,5,5	0.33	0
4	GOL	C	203	-	5,5,5	0.94	0	5,5,5	0.88	0
6	SF4	D	805	1	0,12,12	-	-	-		
7	XCC	A	812	1	0,12,12	-	-	-		
4	GOL	D	801	-	5,5,5	0.09	0	5,5,5	0.32	0
4	GOL	C	202	-	5,5,5	0.82	0	5,5,5	0.97	0
5	EDO	A	806	-	3,3,3	0.07	0	2,2,2	0.16	0
4	GOL	A	817	-	5,5,5	0.95	0	5,5,5	0.95	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
4	GOL	A	816	-	-	3/4/4/4	-
6	SF4	E	401	2	-	-	0/6/5/5
4	GOL	A	801	-	-	0/4/4/4	-
6	SF4	D	803	1	-	-	0/6/5/5
6	SF4	A	810	1	-	-	0/6/5/5
6	SF4	E	404	2	-	-	0/6/5/5
4	GOL	F	403	-	-	3/4/4/4	-
6	SF4	D	804	1	-	-	0/6/5/5
5	EDO	A	818	-	-	1/1/1/1	-
4	GOL	A	814	-	-	0/4/4/4	-
4	GOL	B	406	-	-	2/4/4/4	-
4	GOL	E	405	-	-	3/4/4/4	-
5	EDO	A	807	-	-	0/1/1/1	-
5	EDO	A	802	-	-	1/1/1/1	-
10	PE4	D	807	-	-	2/3/3/21	-
5	EDO	A	805	-	-	0/1/1/1	-
5	EDO	D	802	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SF4	A	811	1	-	-	0/6/5/5
6	SF4	A	819	1	-	-	0/6/5/5
5	EDO	A	808	-	-	0/1/1/1	-
6	SF4	B	402	2	-	-	0/6/5/5
7	XCC	D	806	1	-	-	0/4/4/4
9	FAD	E	403	-	-	1/34/50/50	0/6/6/6
5	EDO	F	402	-	-	0/1/1/1	-
4	GOL	C	201	-	-	2/4/4/4	-
6	SF4	B	405	2	-	-	0/6/5/5
4	GOL	F	401	-	-	0/4/4/4	-
9	FAD	B	404	-	-	1/34/50/50	0/6/6/6
6	SF4	A	809	1	-	-	0/6/5/5
6	SF4	E	402	2	-	-	0/6/5/5
6	SF4	B	403	2	-	-	0/6/5/5
5	EDO	B	401	-	-	0/1/1/1	-
5	EDO	A	803	-	-	1/1/1/1	-
4	GOL	A	815	-	-	2/4/4/4	-
4	GOL	A	820	-	-	3/4/4/4	-
5	EDO	A	804	-	-	0/1/1/1	-
4	GOL	A	813	-	-	4/4/4/4	-
4	GOL	C	203	-	-	0/4/4/4	-
6	SF4	D	805	1	-	-	0/6/5/5
7	XCC	A	812	1	-	-	0/4/4/4
4	GOL	D	801	-	-	3/4/4/4	-
4	GOL	C	202	-	-	2/4/4/4	-
5	EDO	A	806	-	-	1/1/1/1	-
4	GOL	A	817	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	813	GOL	C1-C2-C3-O3
4	A	816	GOL	C1-C2-C3-O3
4	A	817	GOL	O1-C1-C2-C3
4	A	820	GOL	C1-C2-C3-O3
4	C	201	GOL	O1-C1-C2-C3

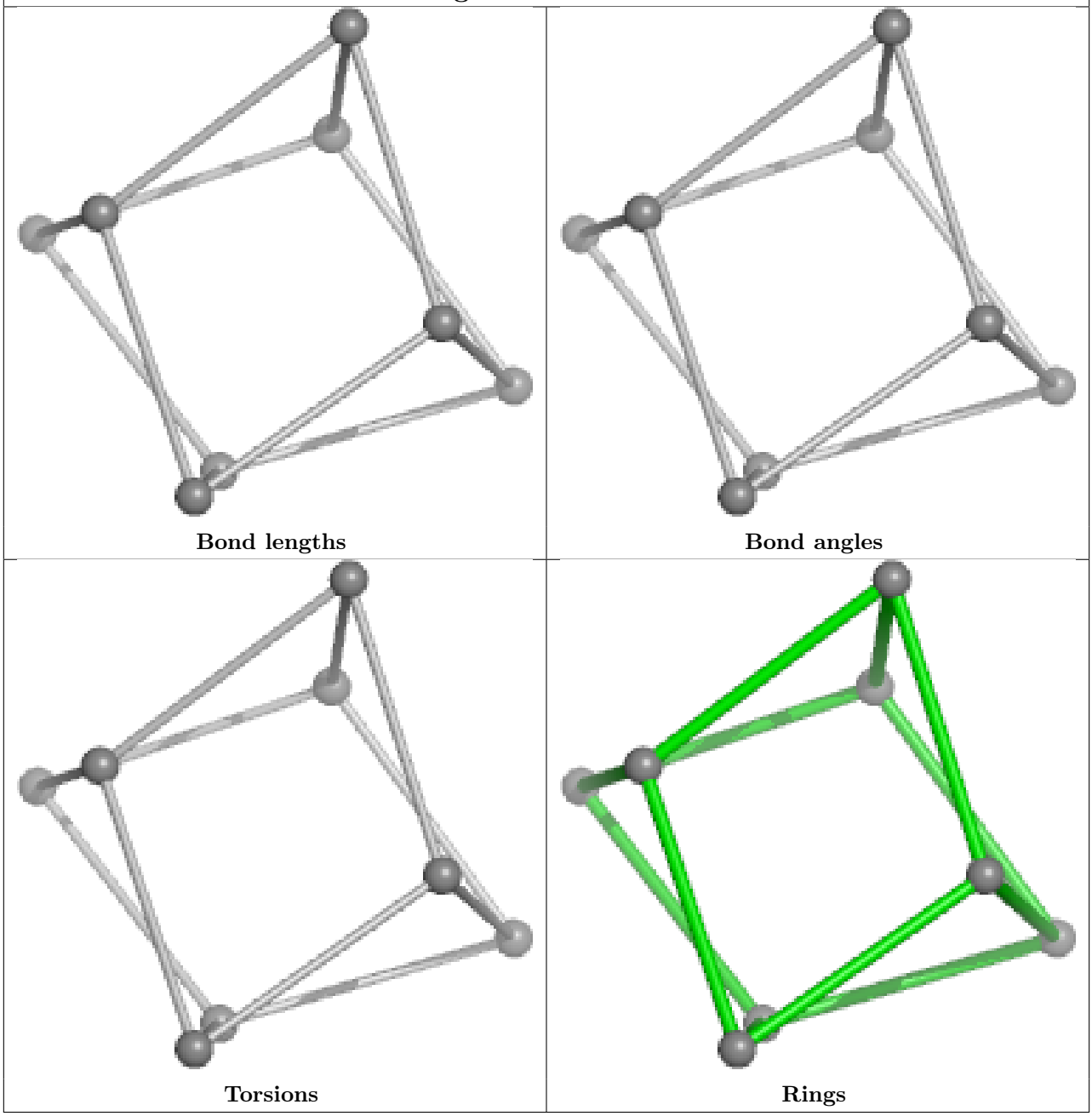
There are no ring outliers.

8 monomers are involved in 8 short contacts:

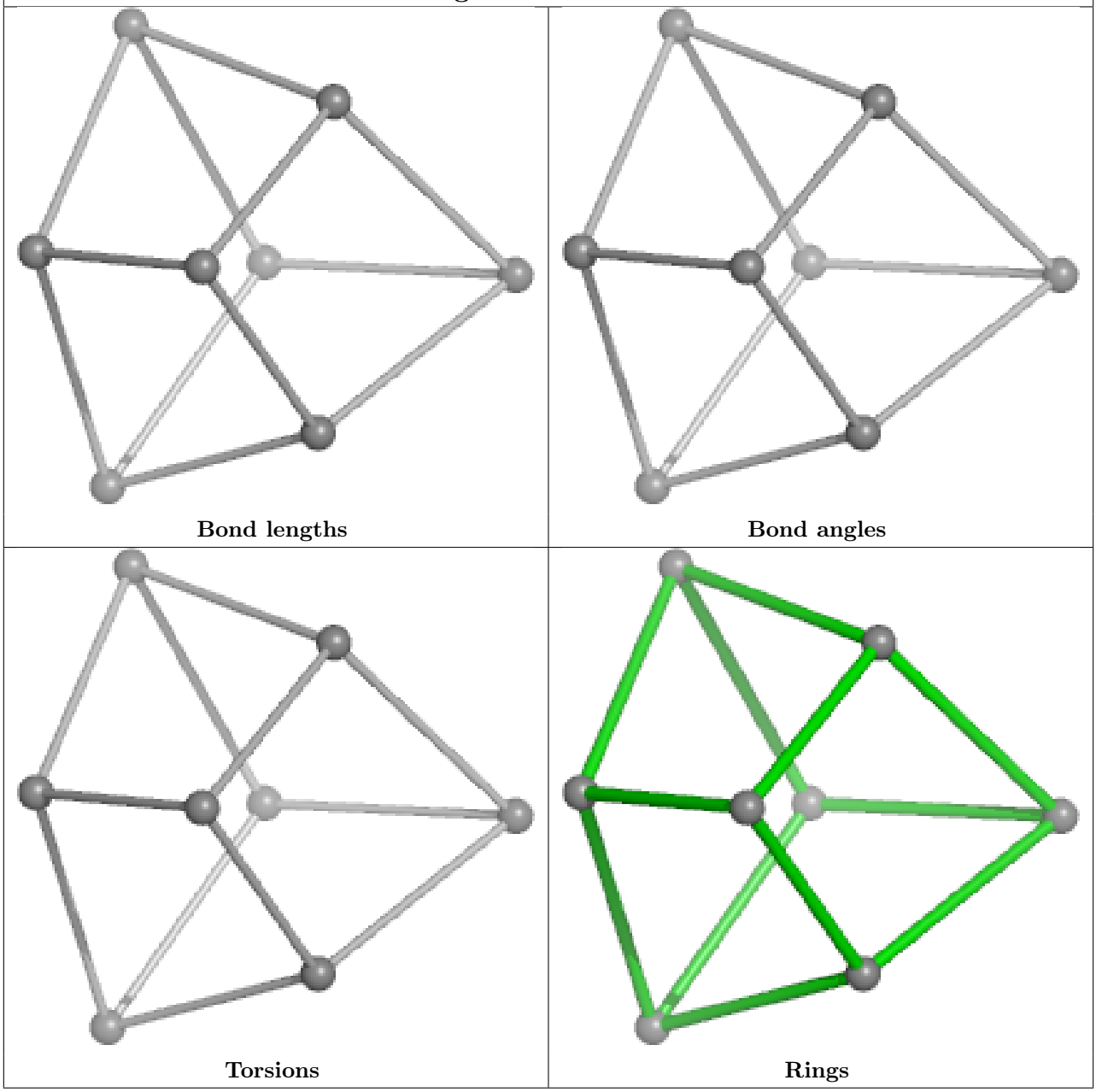
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	816	GOL	1	0
6	A	810	SF4	1	0
6	D	804	SF4	1	0
9	E	403	FAD	1	0
4	A	820	GOL	1	0
4	A	813	GOL	1	0
7	A	812	XCC	1	0
4	D	801	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 SF4 E 401



Ligand SF4 D 803



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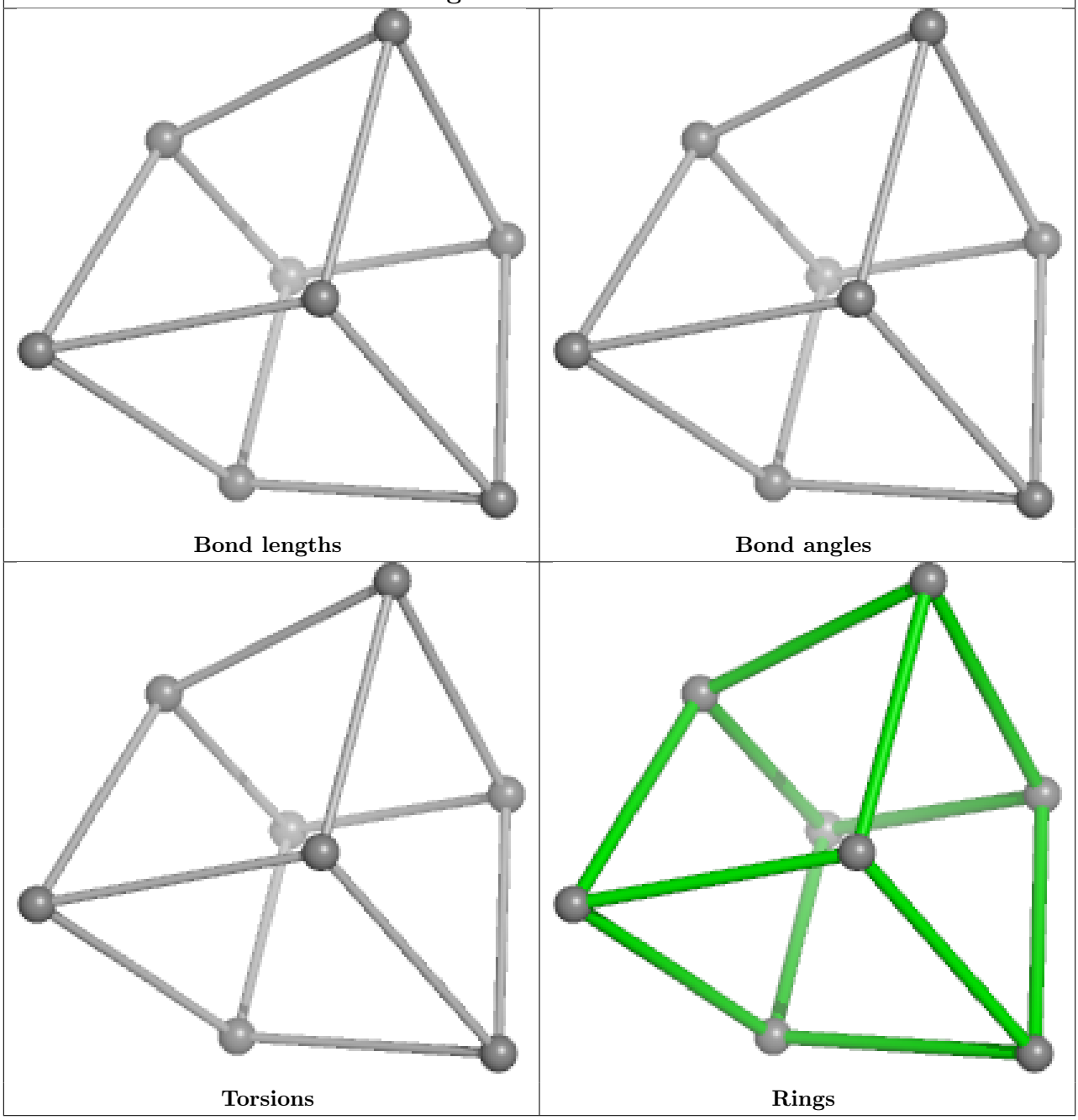

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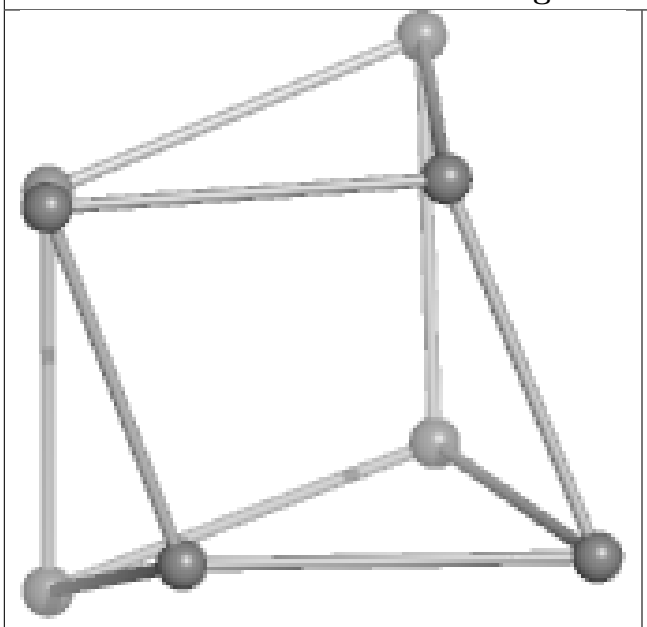
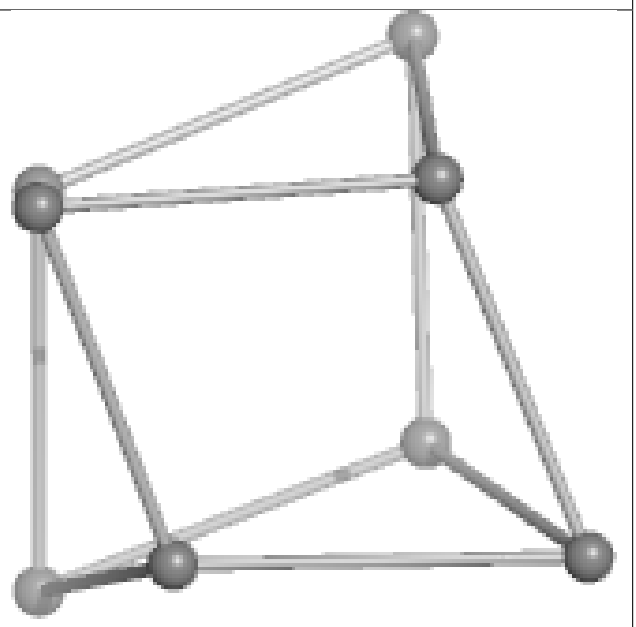
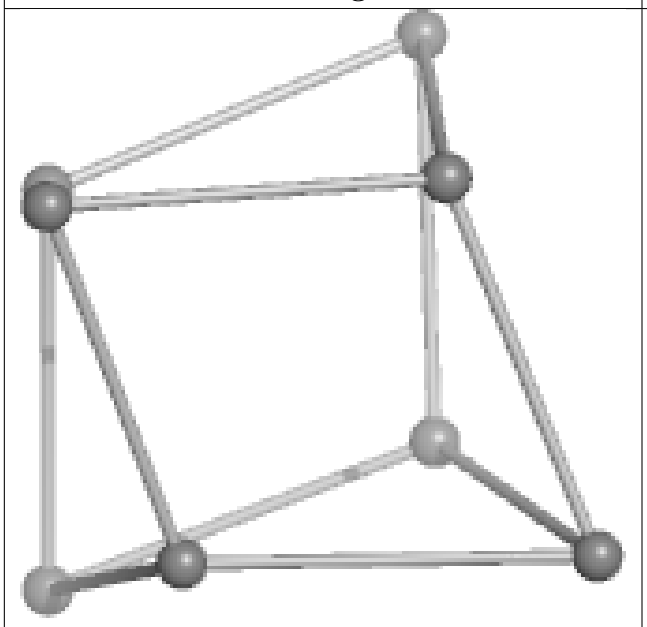


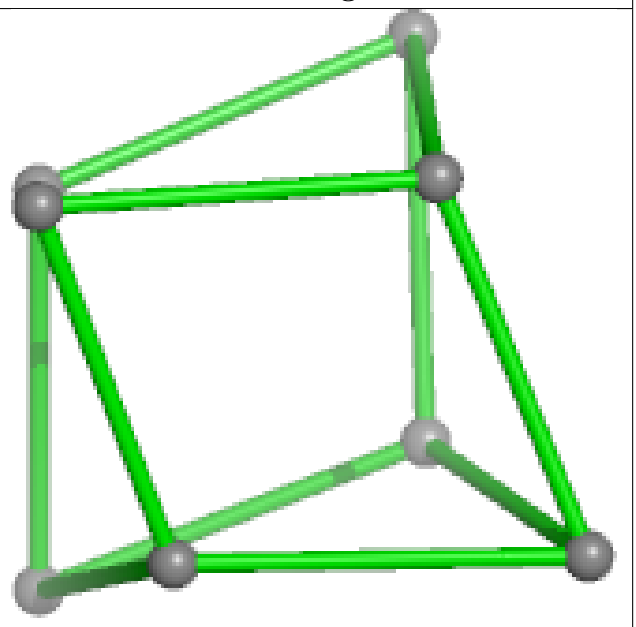
Bond lengths



Bond angles

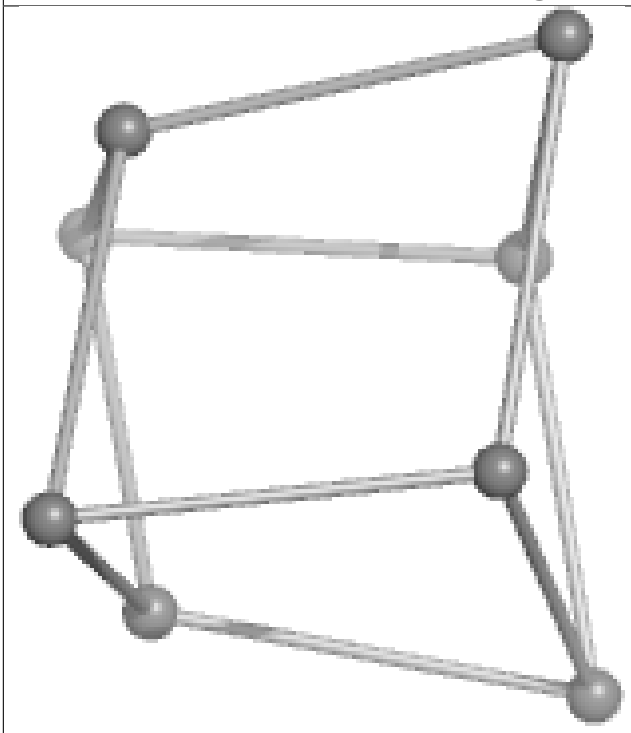


Torsions



Rings

Ligand SF4 D 804



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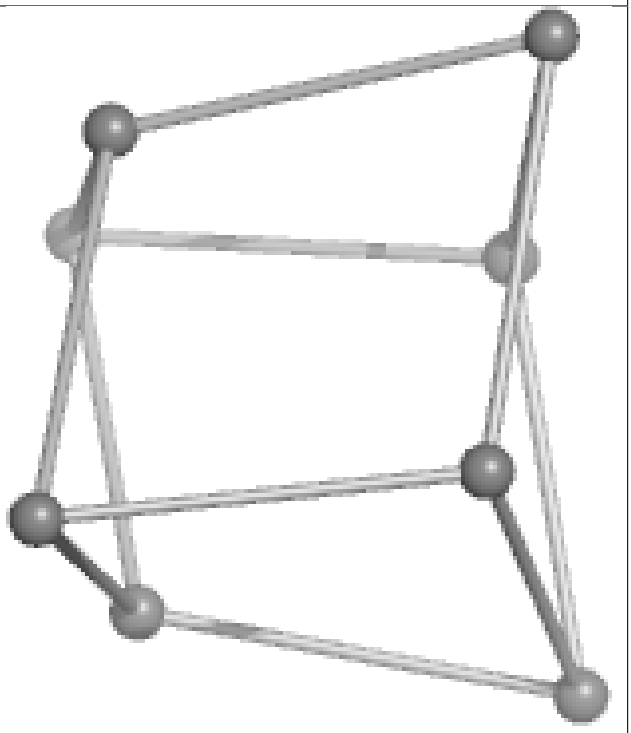

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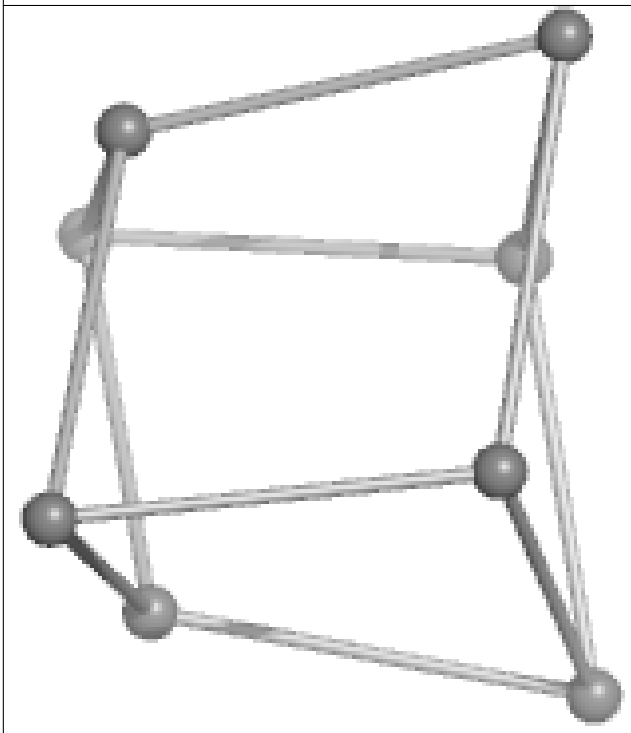
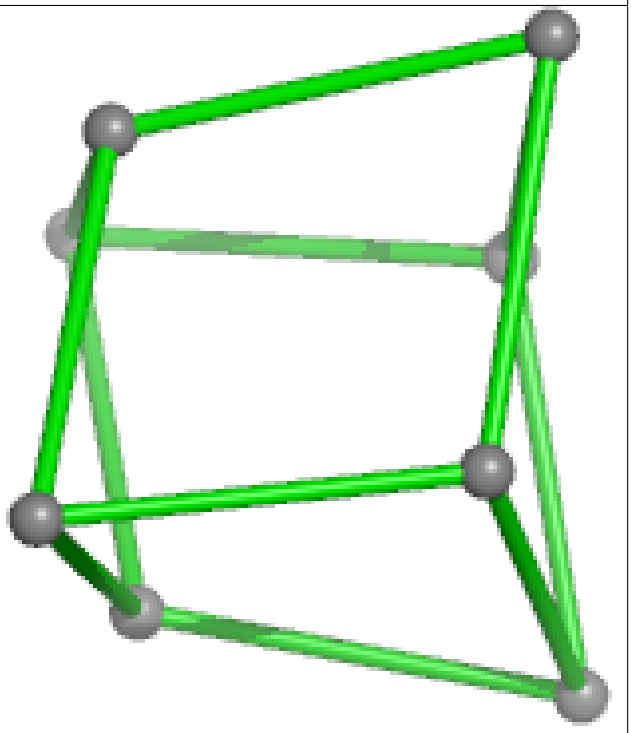
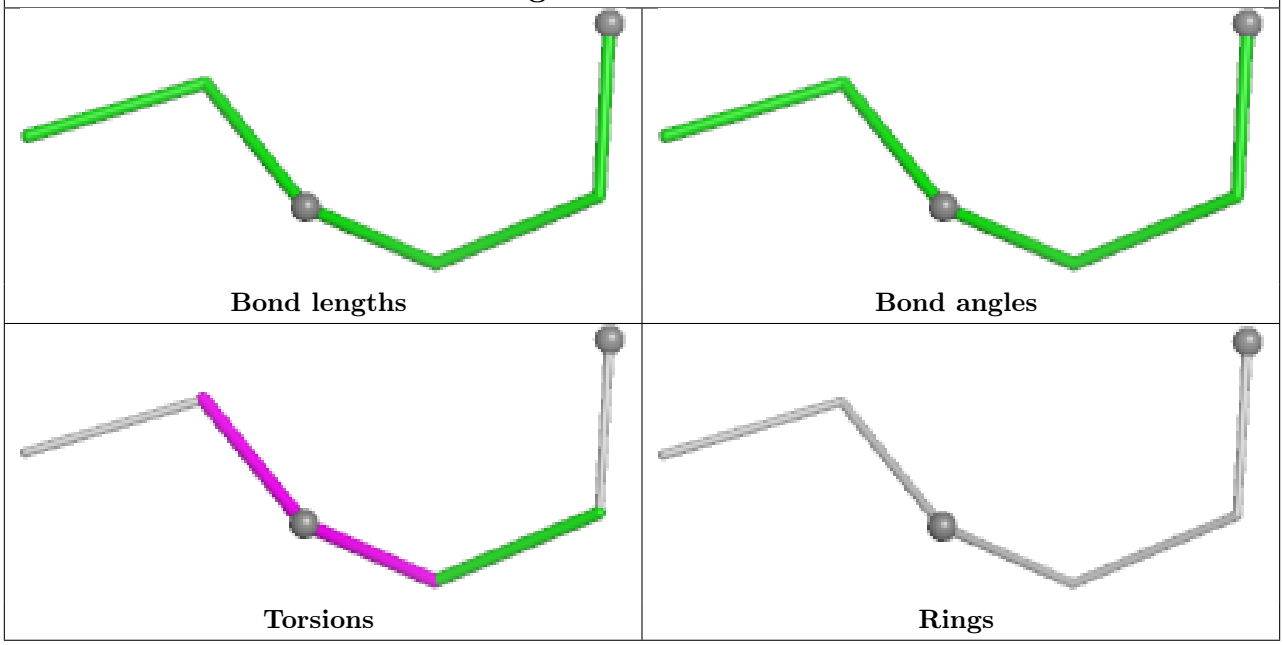


Torsions

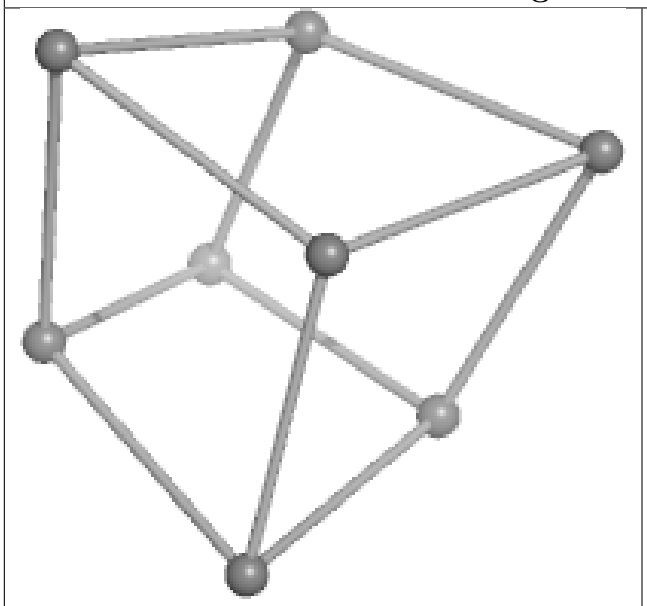


Rings

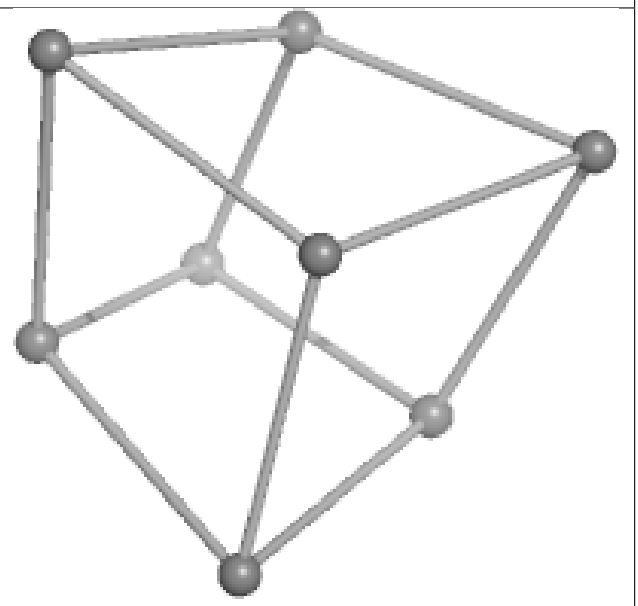
Ligand PE4 D 807



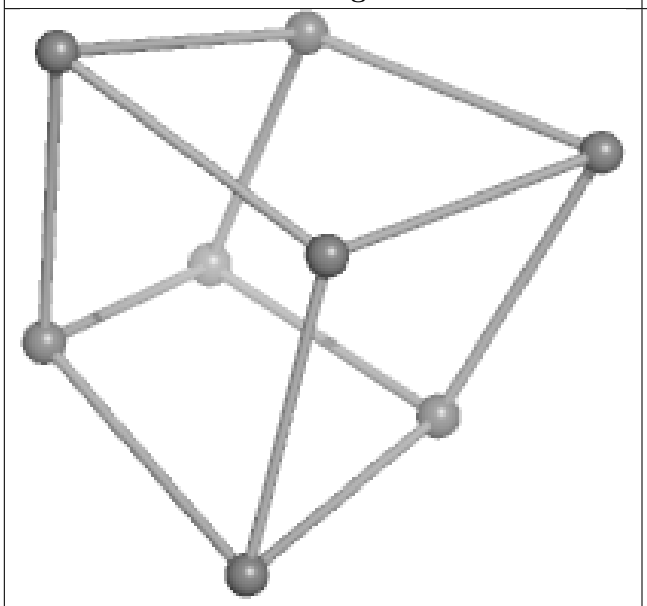
Ligand SF4 A 811



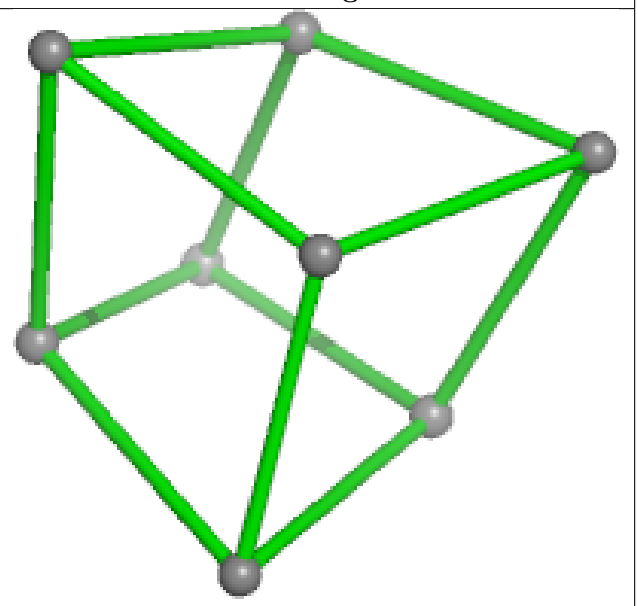
Bond lengths



Bond angles

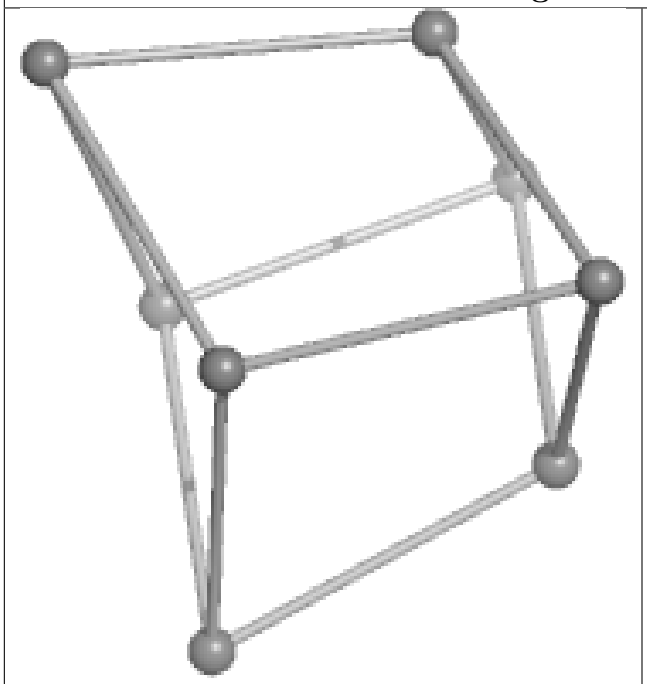


Torsions

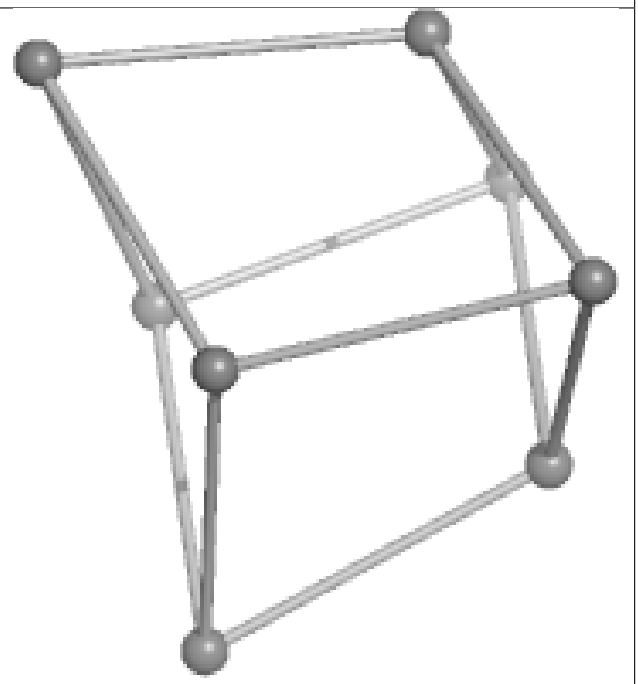


Rings

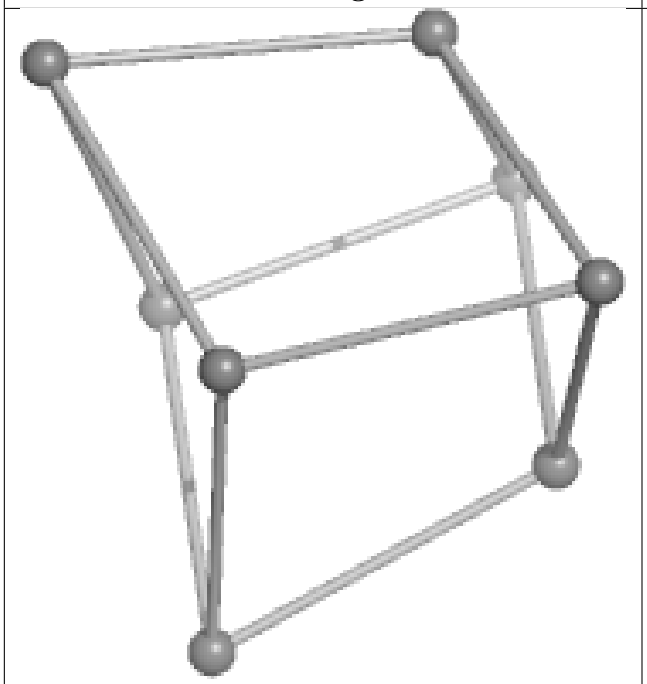
Ligand SF4 A 819



Bond lengths



Bond angles



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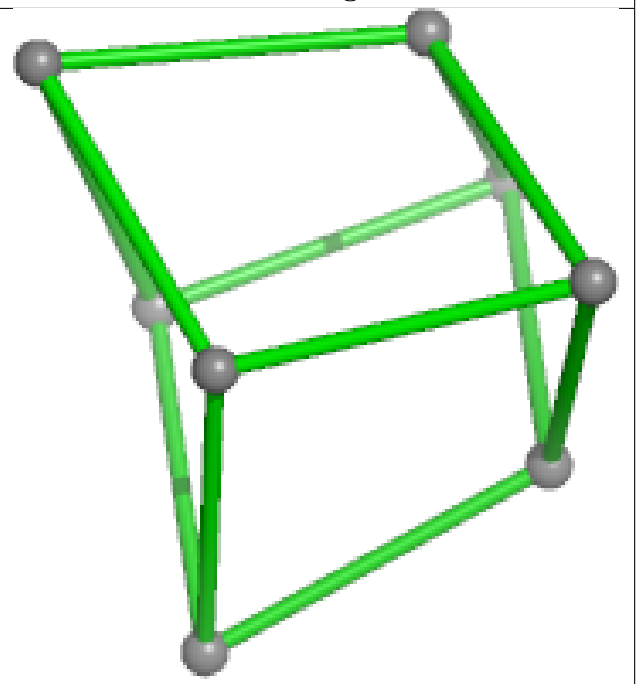
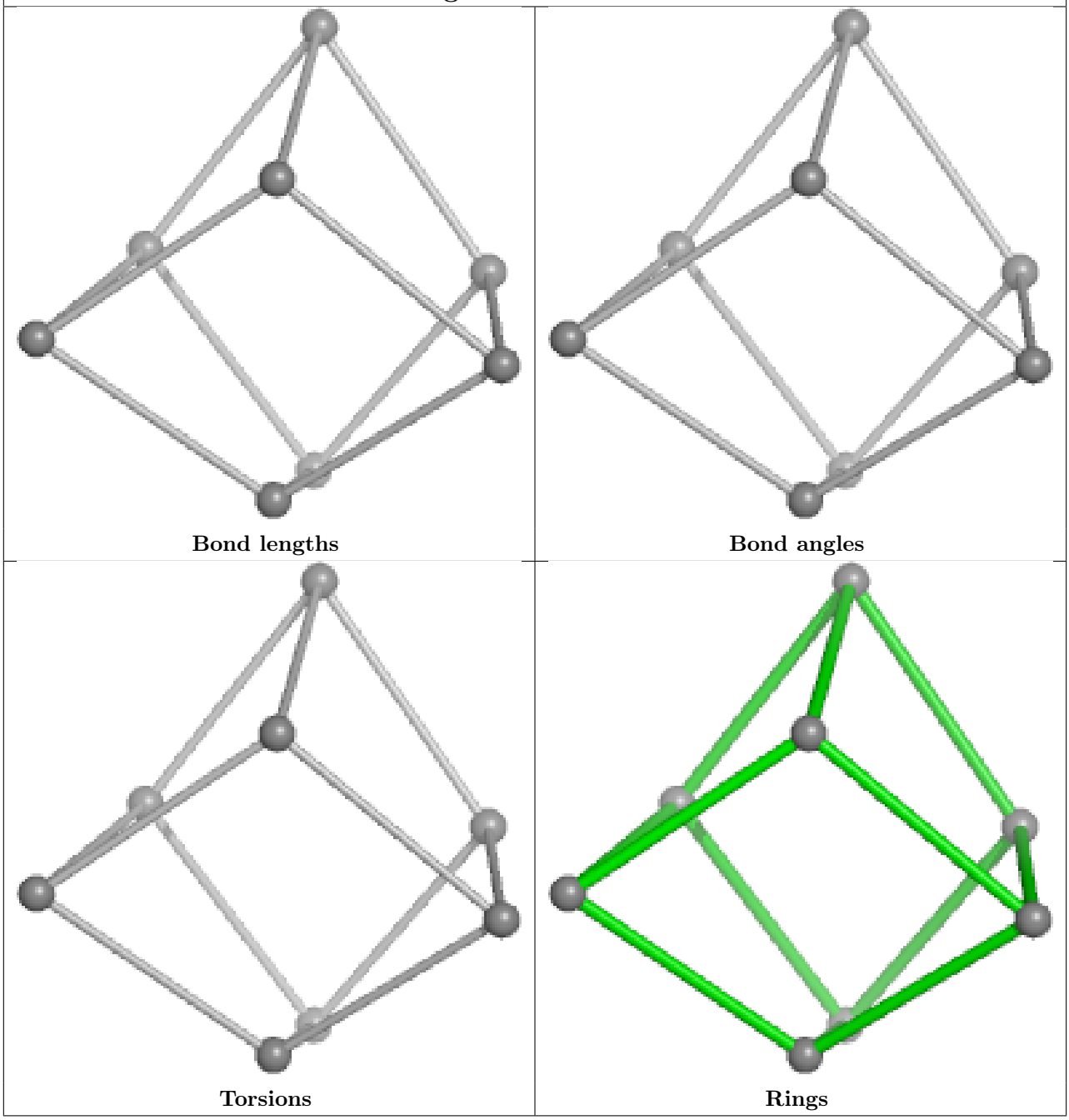
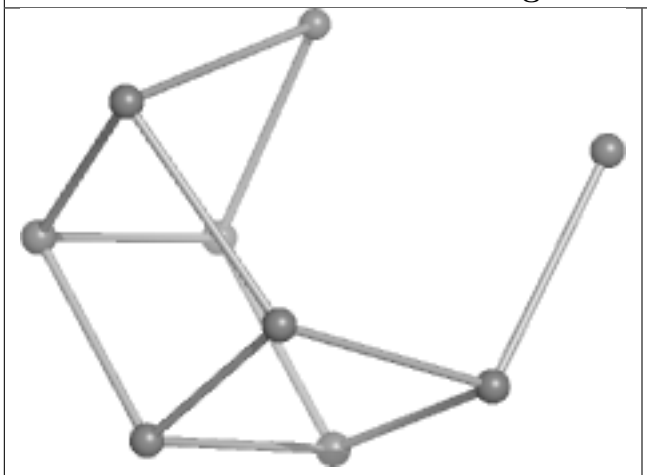


Rings

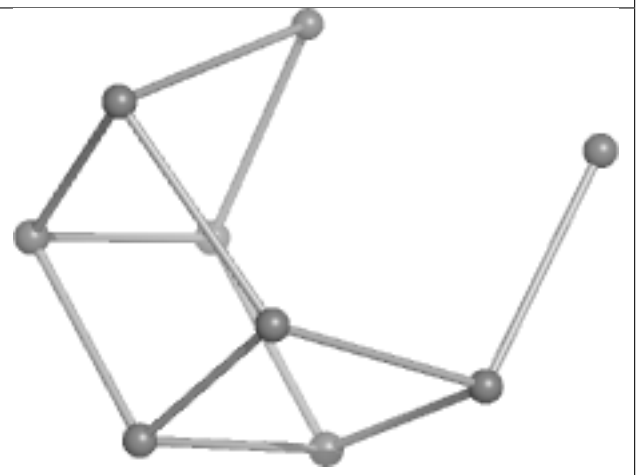
Ligand SF4 B 402



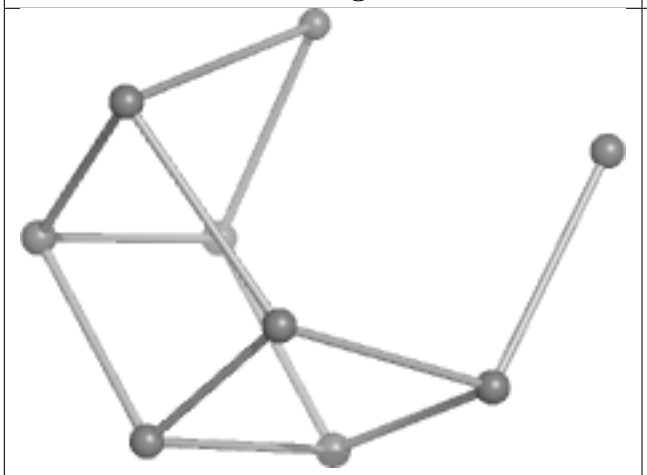
Ligand XCC D 806



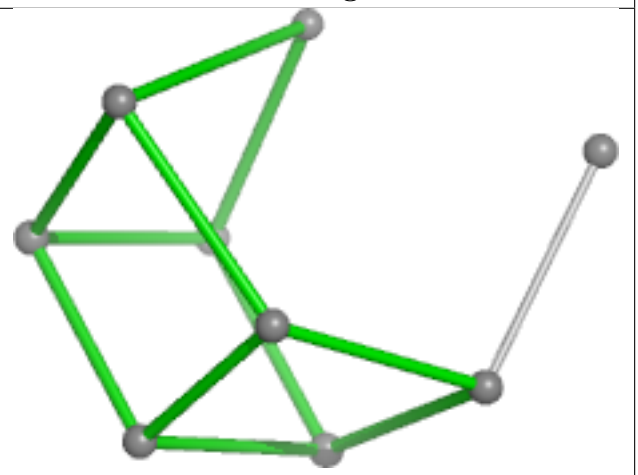
Bond lengths



Bond angles

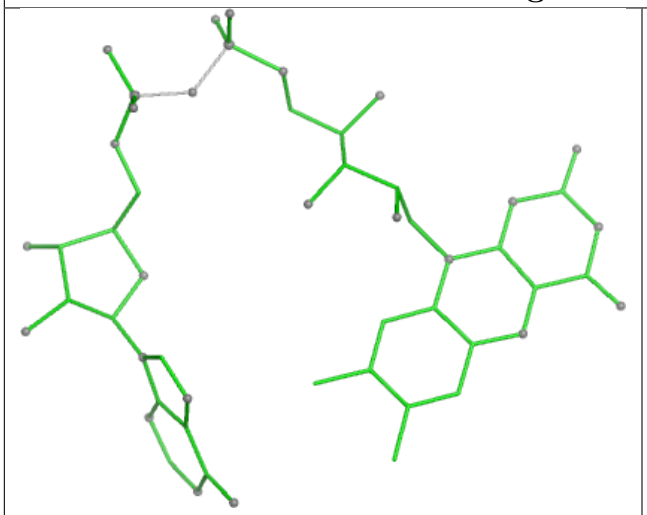


Torsions

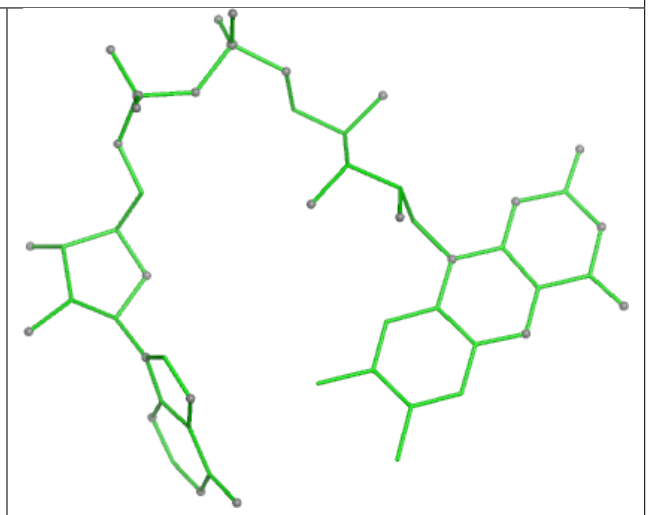


Rings

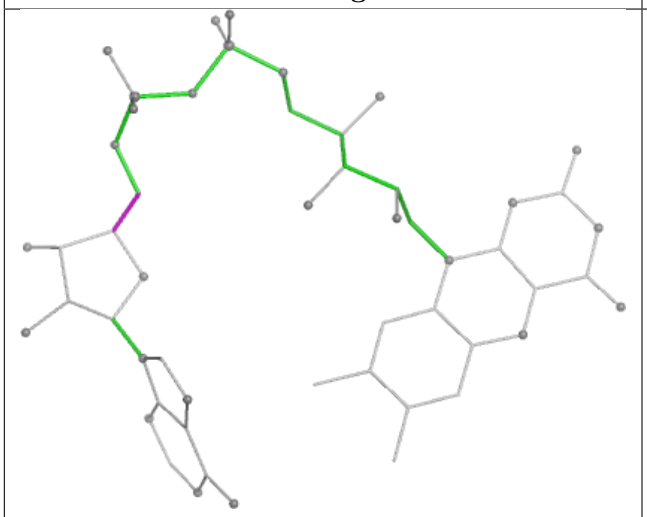
Ligand FAD E 403



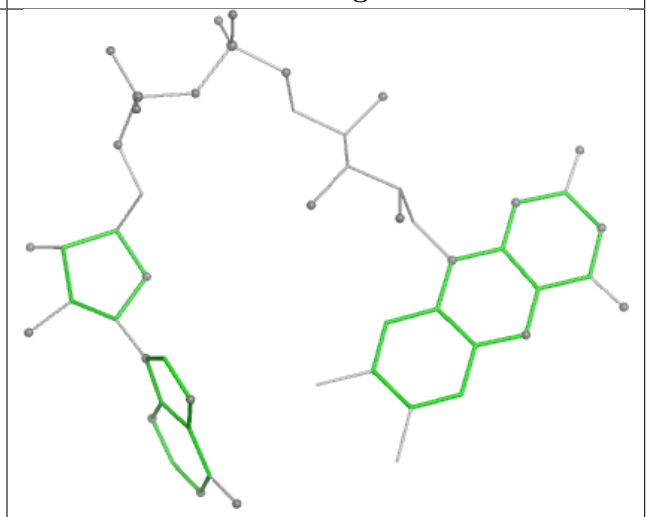
Bond lengths



Bond angles

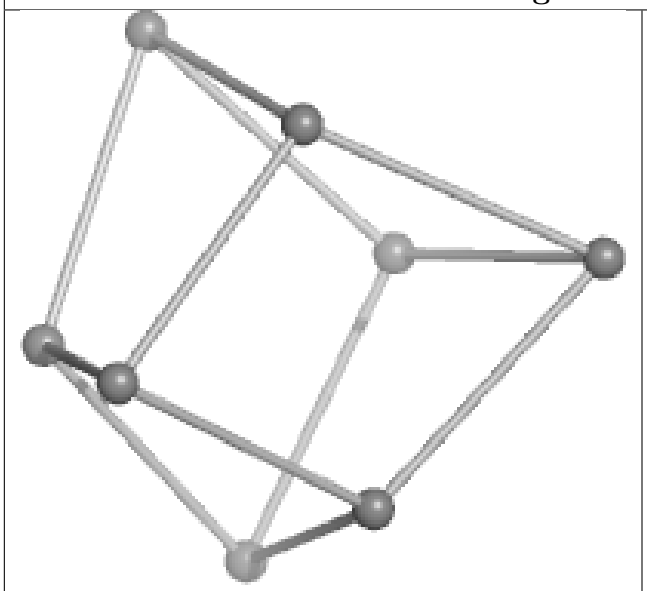


Torsions

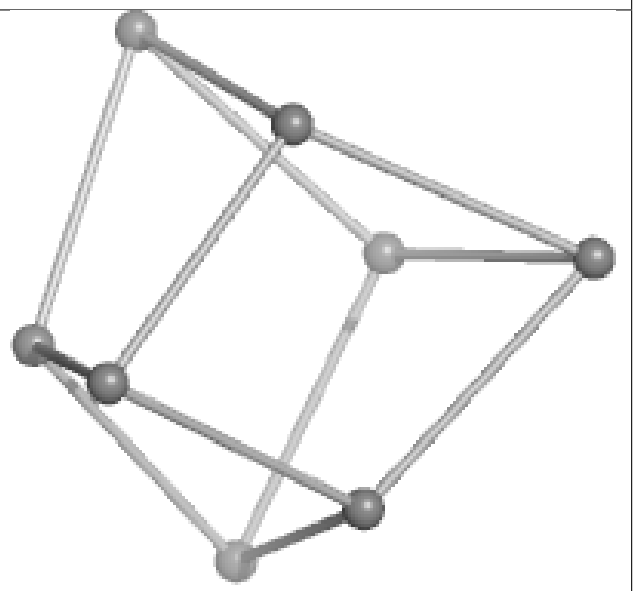


Rings

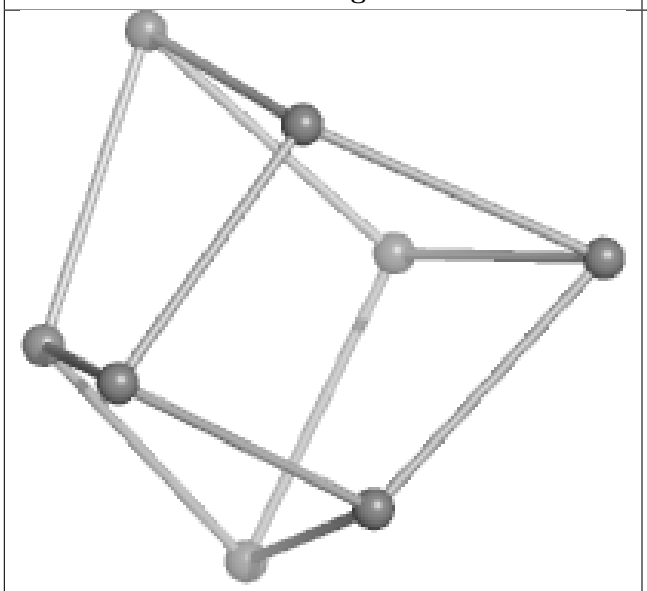
Ligand SF4 B 405



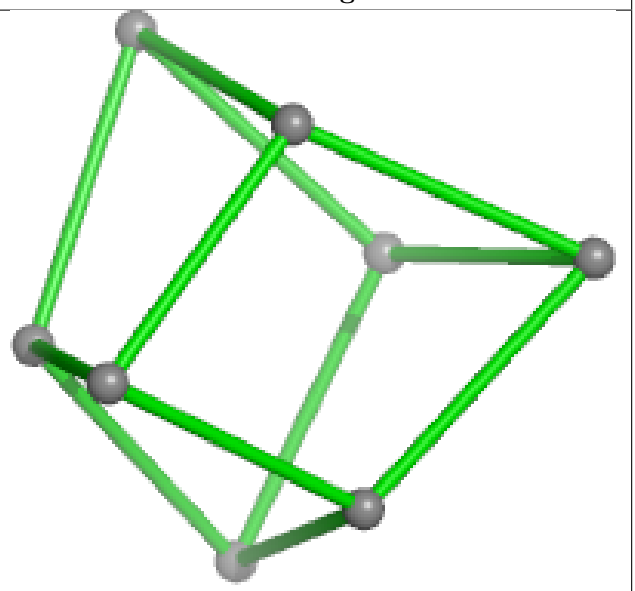
Bond lengths



Bond angles

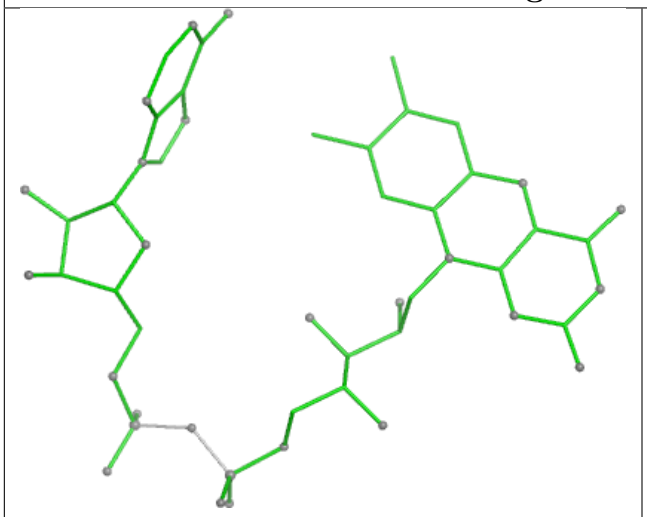


Torsions

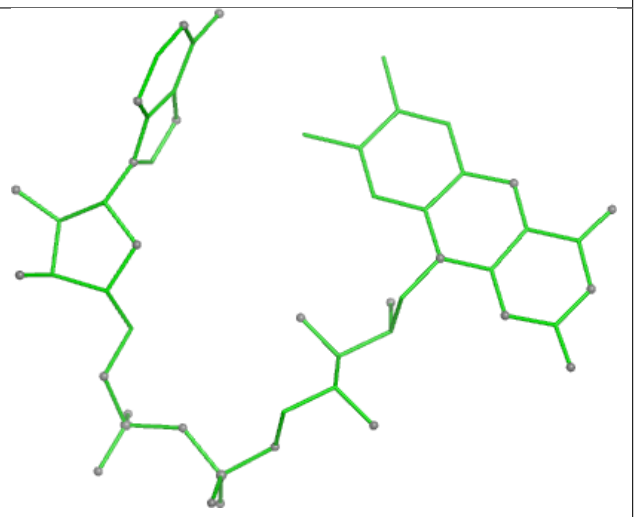


Rings

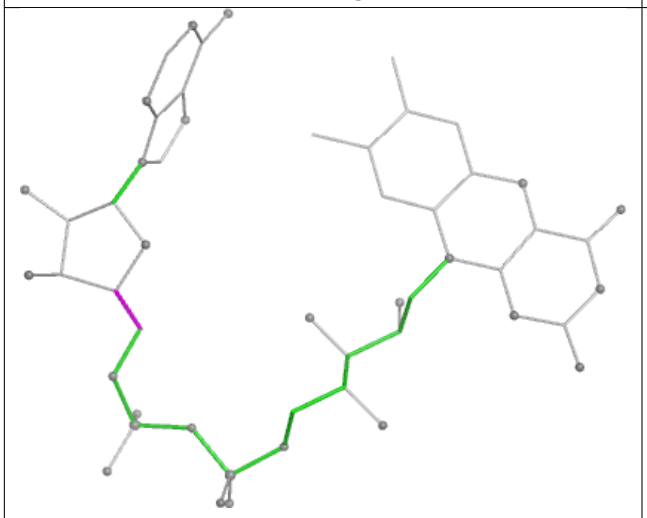
Ligand FAD B 404



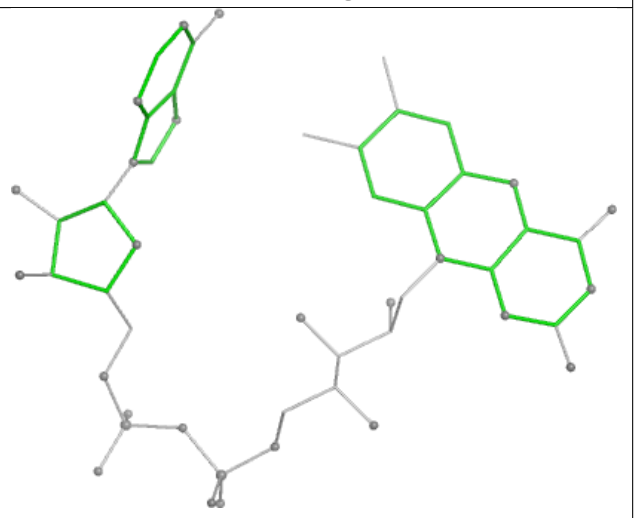
Bond lengths



Bond angles

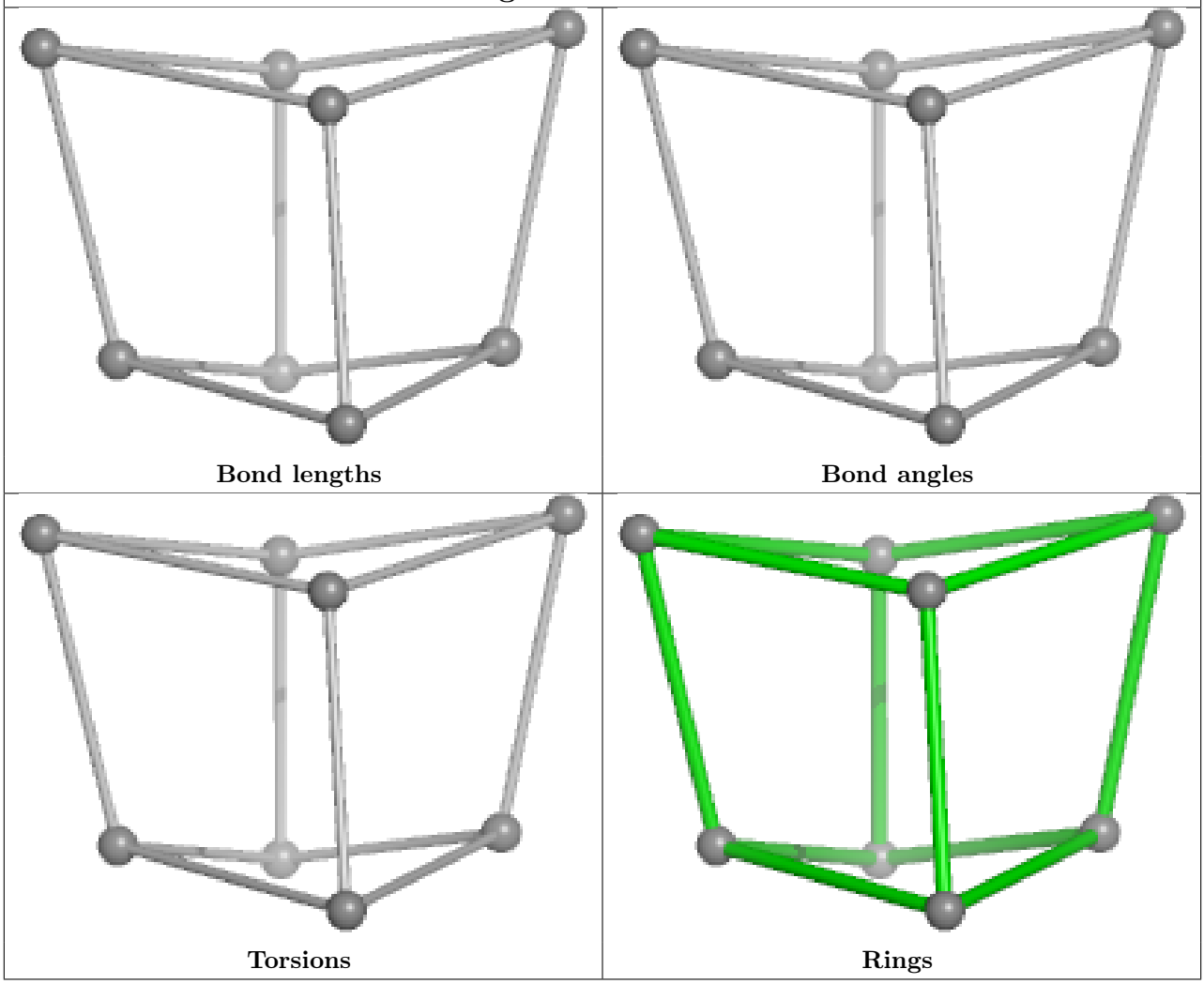


Torsions

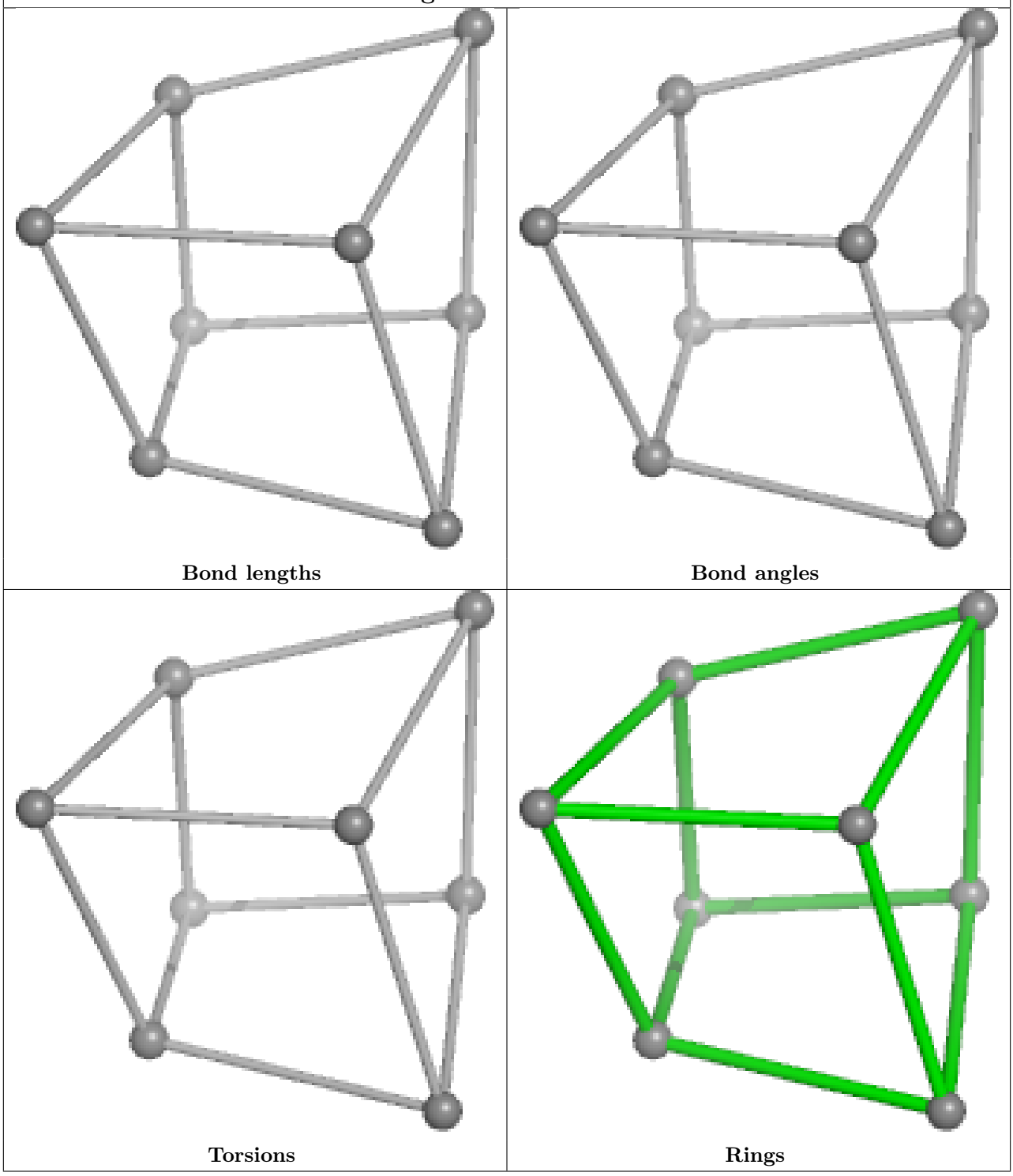


Rings

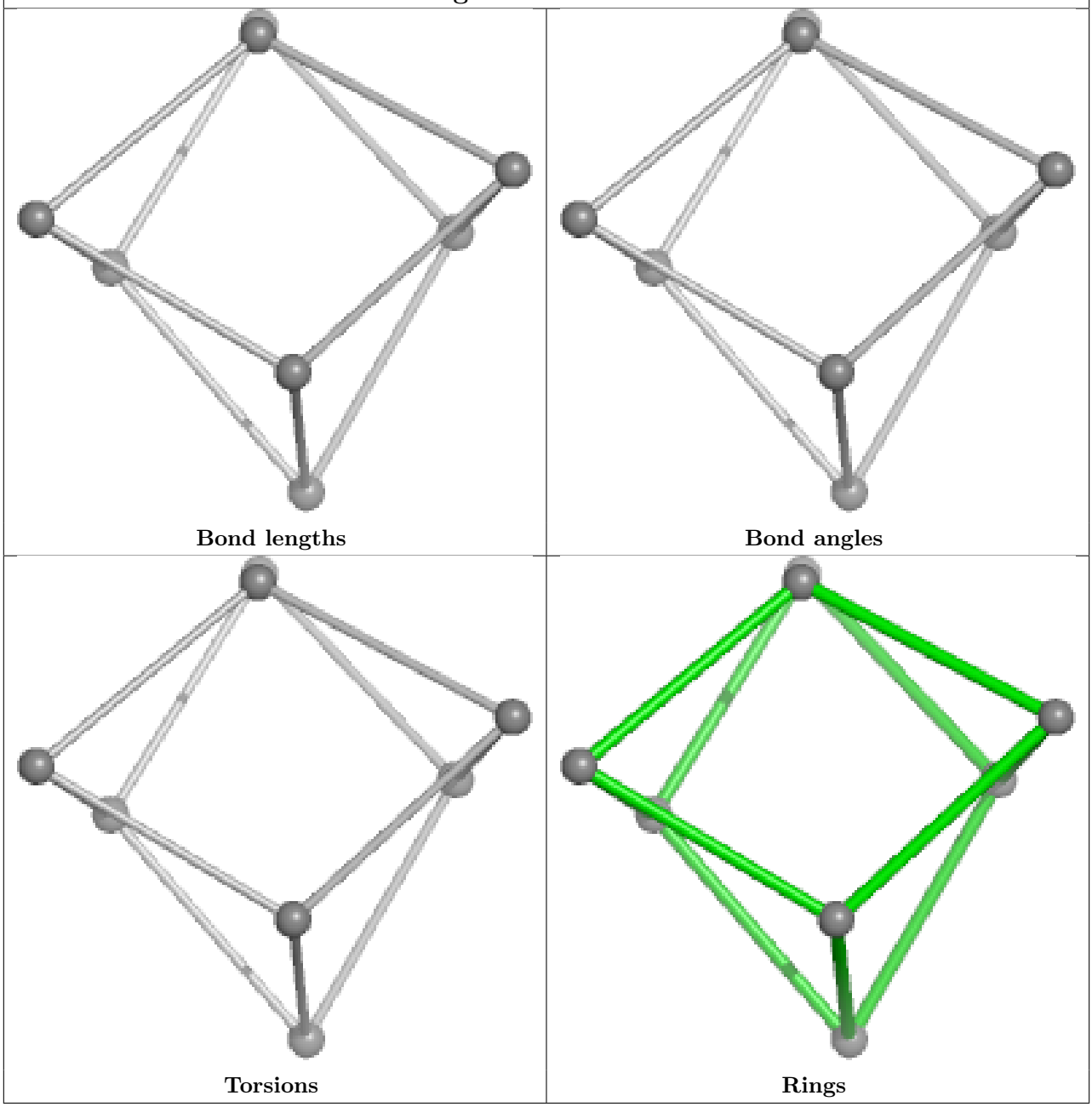
Ligand SF4 A 809



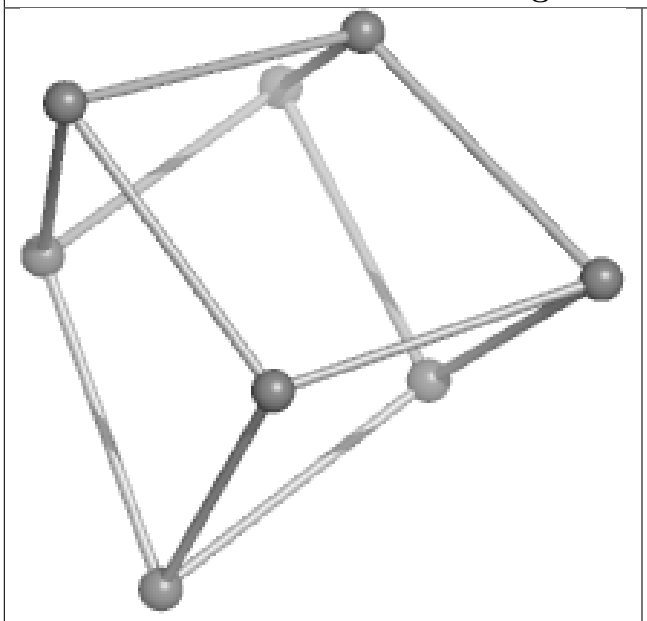
Ligand SF4 E 402



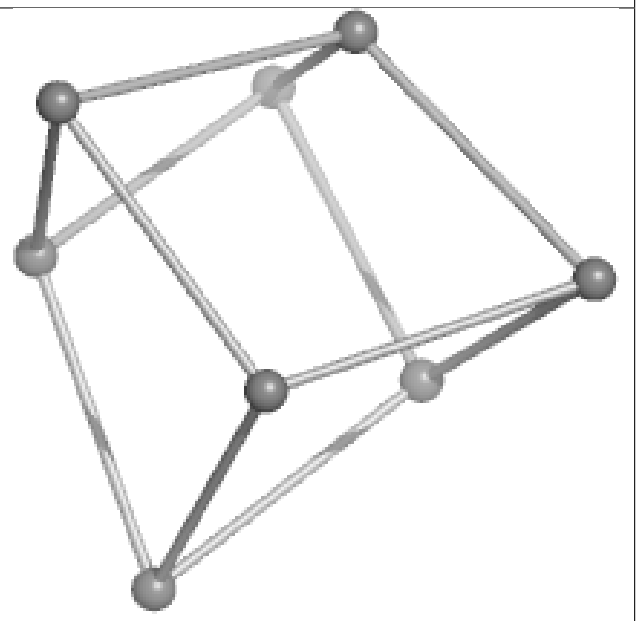
Ligand SF4 B 403



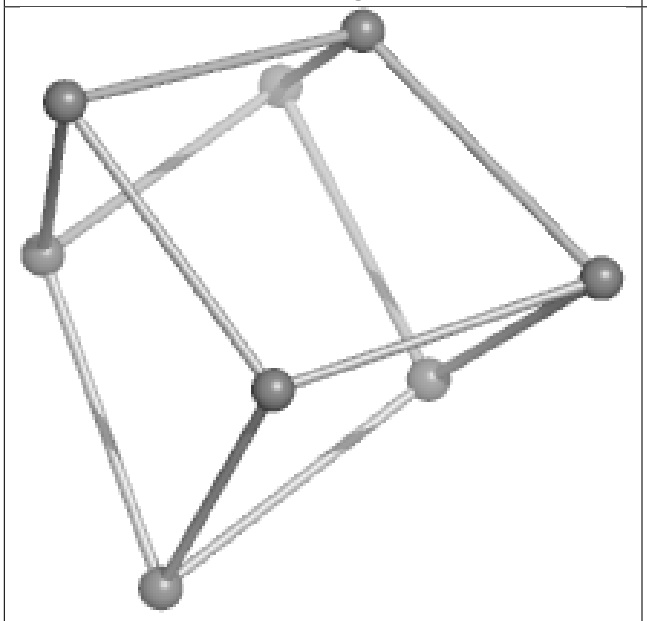
Ligand SF4 D 805



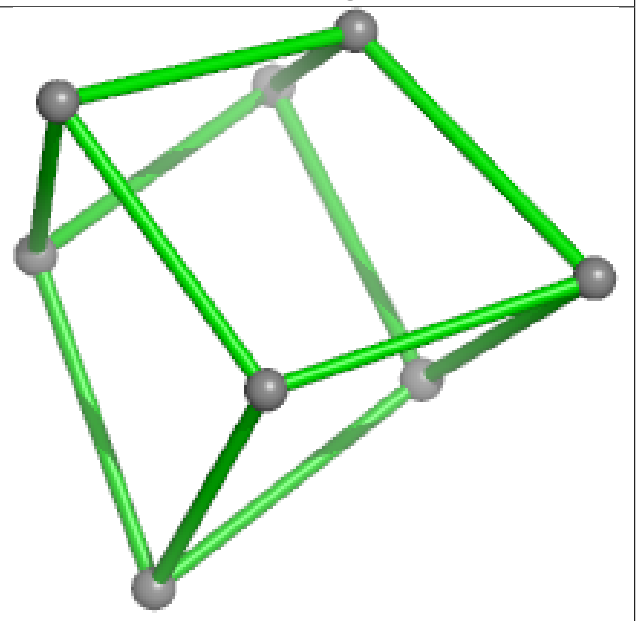
Bond lengths



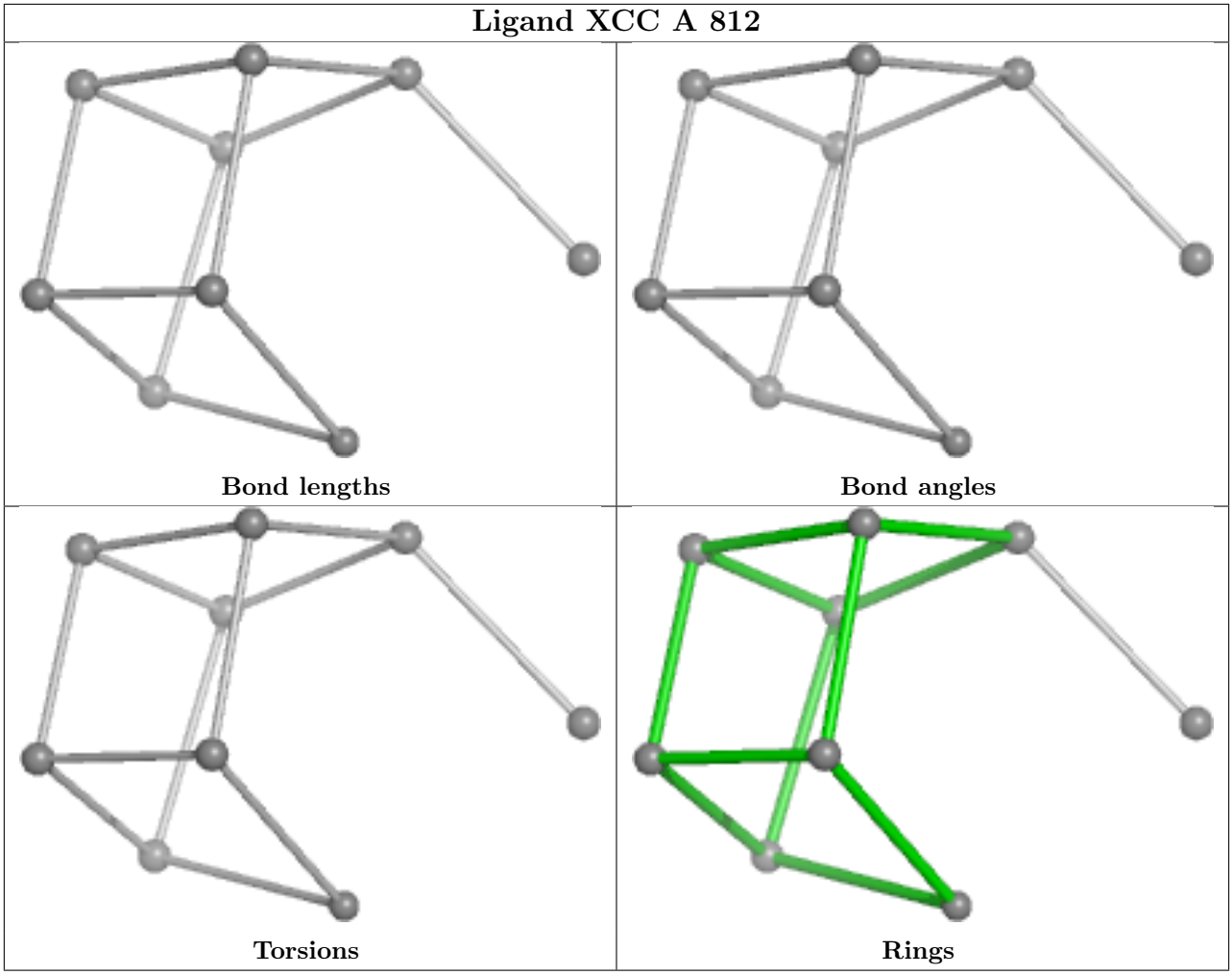
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	759/792 (95%)	-0.20	2 (0%)	90	91	28, 38, 56, 90	0
1	D	760/792 (95%)	-0.06	1 (0%)	92	92	16, 43, 62, 92	4 (0%)
2	B	370/370 (100%)	0.26	5 (1%)	73	76	31, 53, 84, 114	0
2	E	370/370 (100%)	0.04	0	100	100	21, 44, 70, 104	1 (0%)
3	C	174/174 (100%)	-0.32	0	100	100	22, 34, 45, 52	2 (1%)
3	F	174/174 (100%)	-0.24	0	100	100	26, 38, 49, 62	1 (0%)
All	All	2607/2672 (97%)	-0.07	8 (0%)	90	91	16, 41, 67, 114	8 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	260	ILE	2.5
1	A	136	ASN	2.3
1	D	127	ARG	2.2
2	B	340	SER	2.1
2	B	101	LEU	2.1

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	A	808	4/4	0.55	0.21	51,58,59,63	0
4	GOL	A	815	6/6	0.64	0.19	55,57,57,58	0
5	EDO	B	401	4/4	0.65	0.20	51,53,55,57	0
5	EDO	A	818	4/4	0.69	0.18	53,55,57,59	0
5	EDO	D	802	4/4	0.70	0.18	66,69,69,70	0
5	EDO	A	807	4/4	0.72	0.17	59,59,60,63	0
5	EDO	A	805	4/4	0.73	0.14	57,64,67,67	0
4	GOL	A	814	6/6	0.73	0.17	51,55,57,58	0
4	GOL	C	201	6/6	0.74	0.15	50,57,62,65	0
10	PE4	D	807	6/24	0.74	0.19	51,54,57,59	0
5	EDO	A	806	4/4	0.75	0.14	63,66,67,67	0
5	EDO	A	803	4/4	0.79	0.14	52,53,58,58	0
4	GOL	D	801	6/6	0.79	0.12	50,55,57,62	0
4	GOL	F	403	6/6	0.79	0.15	47,53,54,57	0
4	GOL	A	816	6/6	0.80	0.12	52,57,60,65	0
4	GOL	E	405	6/6	0.80	0.13	47,50,53,58	0
4	GOL	A	801	6/6	0.81	0.12	60,62,66,67	0
4	GOL	C	203	6/6	0.81	0.12	40,52,55,55	0
5	EDO	A	802	4/4	0.82	0.12	49,49,52,56	0
4	GOL	A	817	6/6	0.82	0.14	57,62,65,67	0
4	GOL	C	202	6/6	0.84	0.12	44,54,59,60	0
4	GOL	F	401	6/6	0.85	0.12	44,49,50,53	0
11	CL	D	808[A]	1/1	0.85	0.34	55,55,55,55	1
4	GOL	B	406	6/6	0.87	0.10	44,52,56,58	0
5	EDO	F	402	4/4	0.87	0.10	52,54,55,60	0
5	EDO	A	804	4/4	0.88	0.12	49,51,51,57	0
4	GOL	A	813	6/6	0.89	0.09	38,39,44,46	0
9	FAD	B	404	53/53	0.94	0.08	40,47,55,59	0
4	GOL	A	820	6/6	0.94	0.07	38,40,41,42	0
7	XCC	D	806	9/9	0.94	0.07	32,36,41,42	0
7	XCC	A	812	9/9	0.96	0.06	31,34,38,40	0
9	FAD	E	403	53/53	0.96	0.06	33,37,42,44	0
8	K	A	821	1/1	0.98	0.08	35,35,35,35	0
8	K	D	809	1/1	0.98	0.08	36,36,36,36	0
6	SF4	B	405	8/8	0.98	0.04	36,38,39,40	0
6	SF4	D	805	8/8	0.99	0.03	31,32,34,34	0
6	SF4	E	401	8/8	0.99	0.03	30,32,33,34	0

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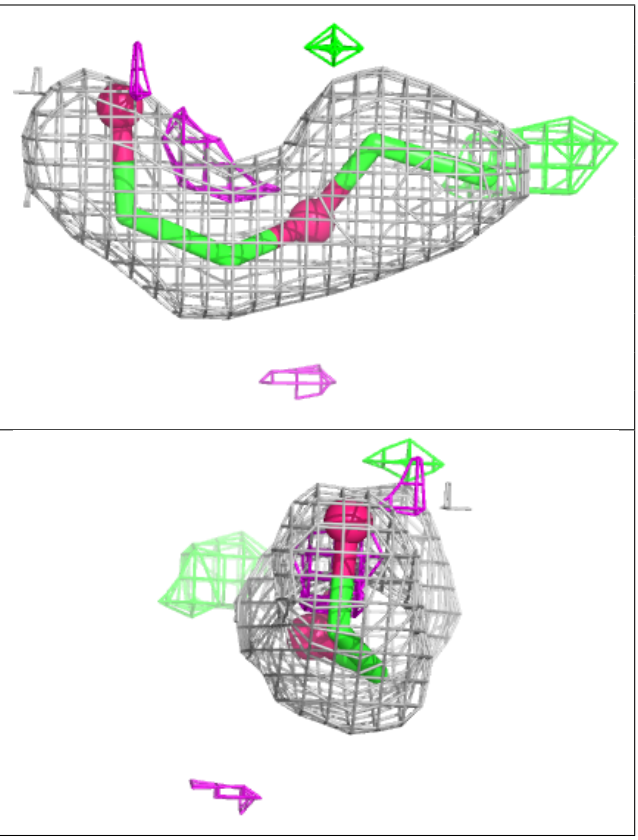
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SF4	E	402	8/8	0.99	0.03	29,31,31,33	0
6	SF4	E	404	8/8	0.99	0.03	33,34,35,37	0
6	SF4	A	810	8/8	0.99	0.02	27,29,29,30	0
6	SF4	A	811	8/8	0.99	0.03	28,30,31,31	0
6	SF4	A	819	8/8	0.99	0.03	28,29,30,30	0
6	SF4	B	402	8/8	0.99	0.03	30,33,34,34	0
6	SF4	B	403	8/8	0.99	0.03	31,31,32,33	0
6	SF4	A	809	8/8	0.99	0.03	28,29,31,32	0
6	SF4	D	803	8/8	0.99	0.03	26,28,29,30	0
6	SF4	D	804	8/8	0.99	0.03	30,31,32,33	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.

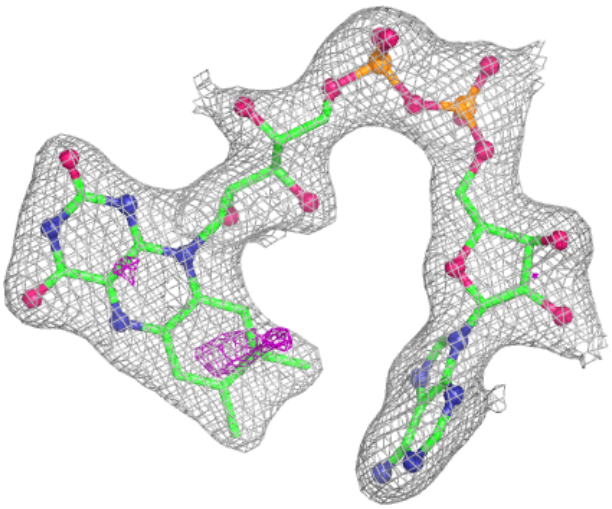
Electron density around PE4 D 807:

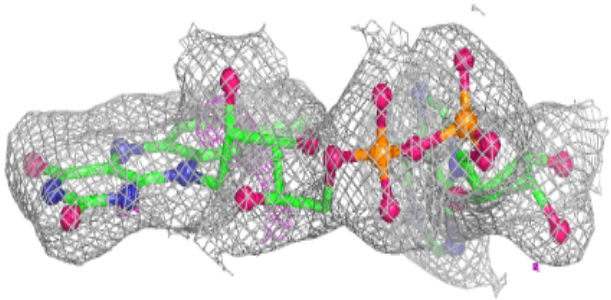
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

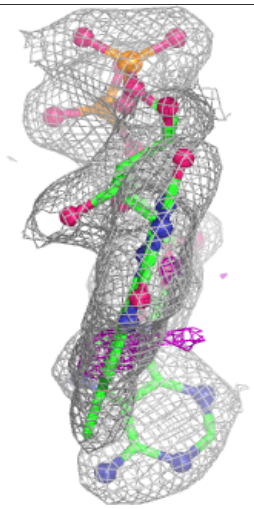


Electron density around FAD B 404:

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

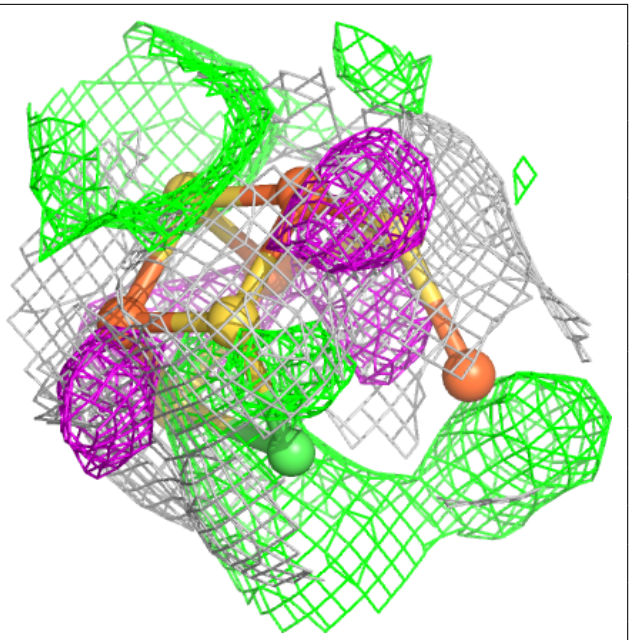


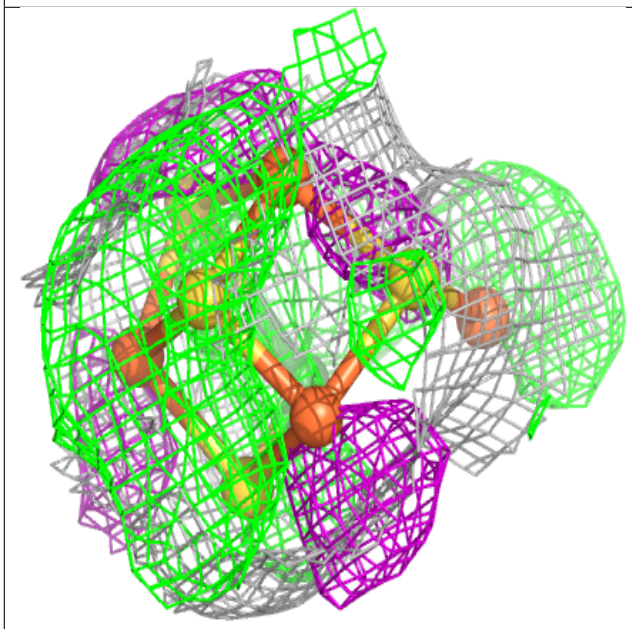


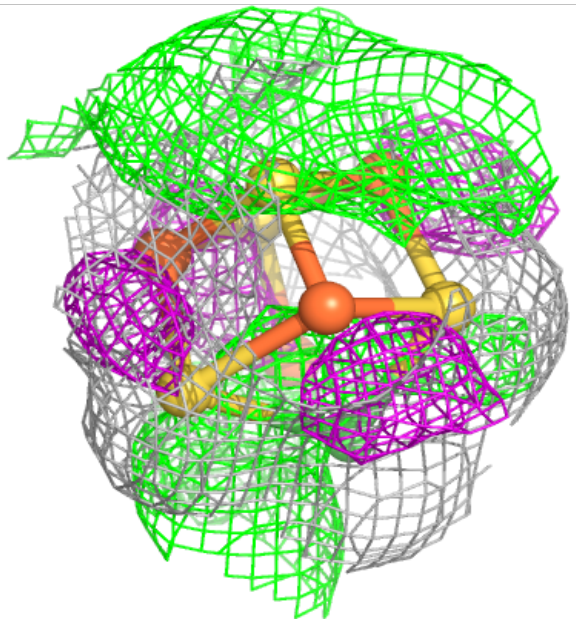


Electron density around XCC D 806:

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

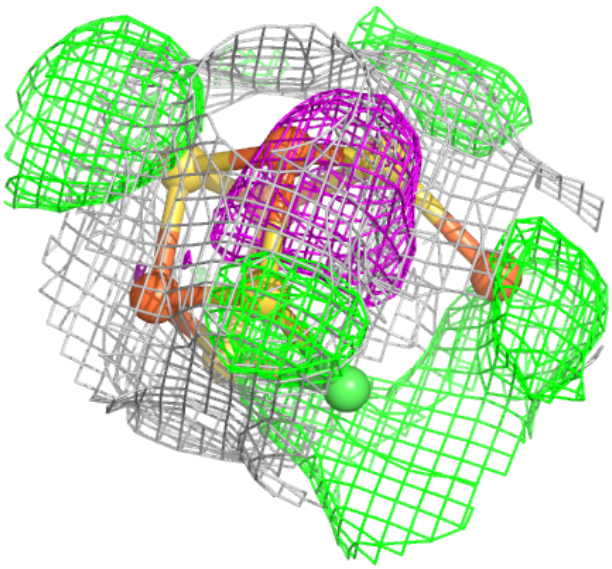


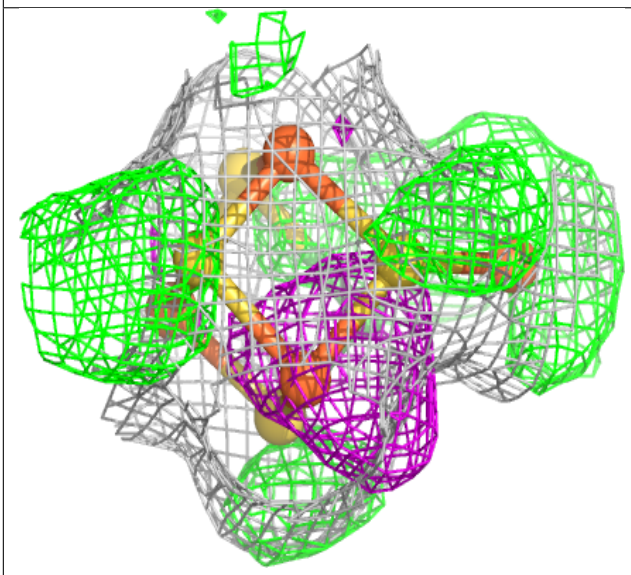


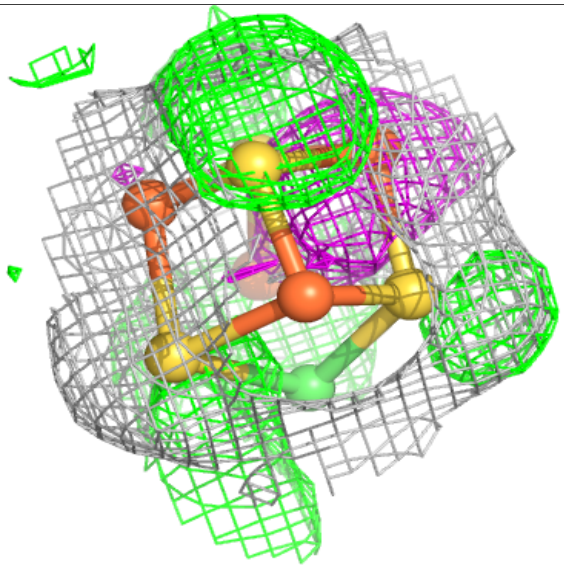


Electron density around XCC A 812:

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

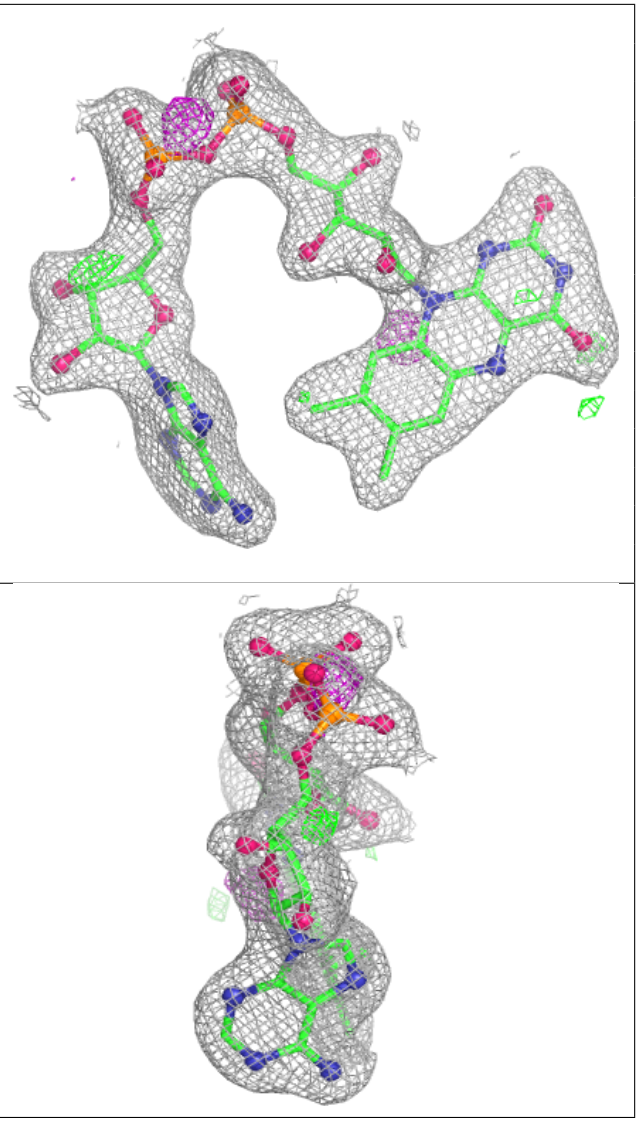






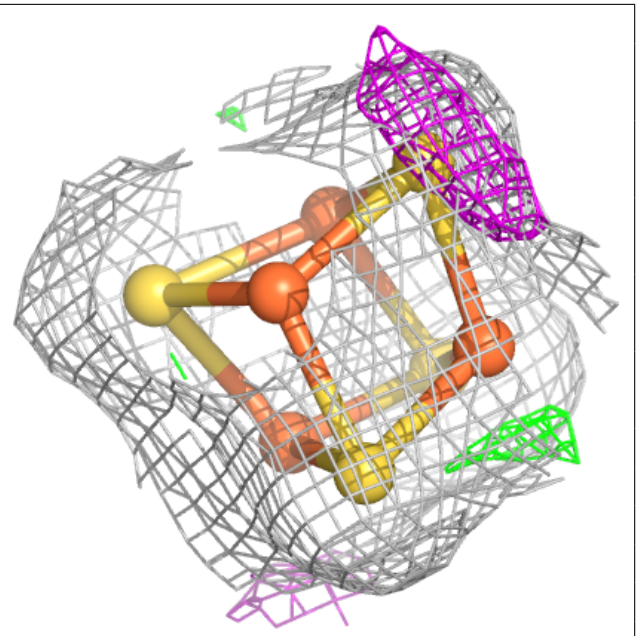
Electron density around FAD E 403:

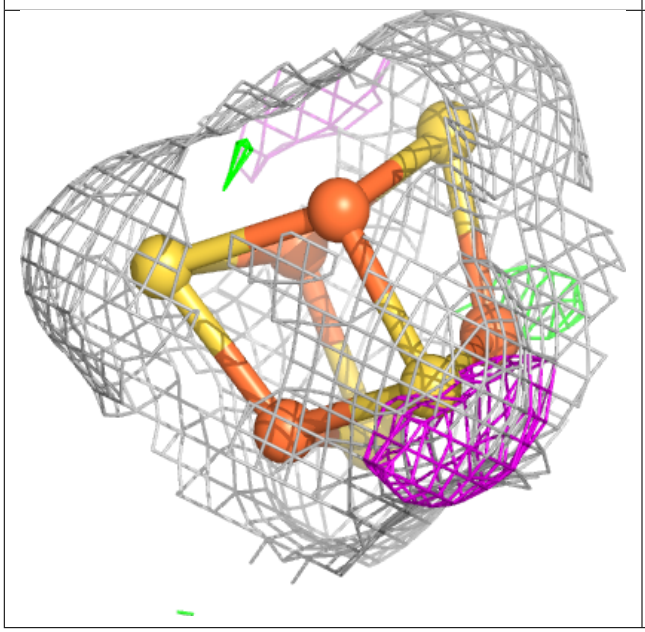
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

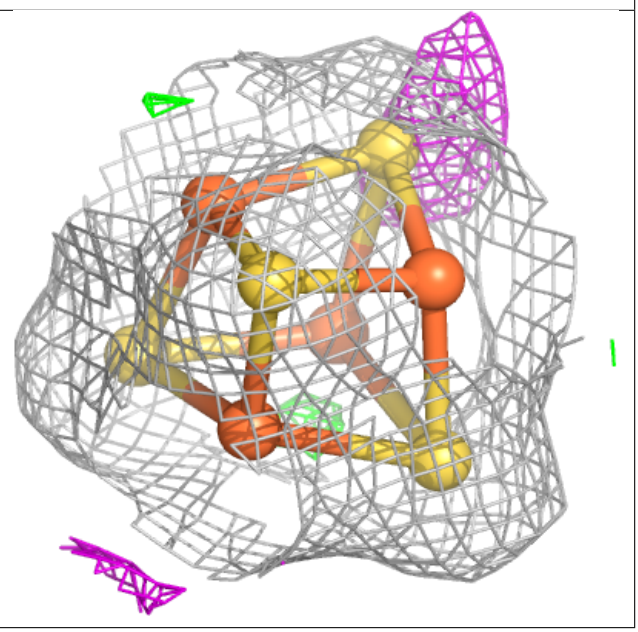


Electron density around SF4 B 405:

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

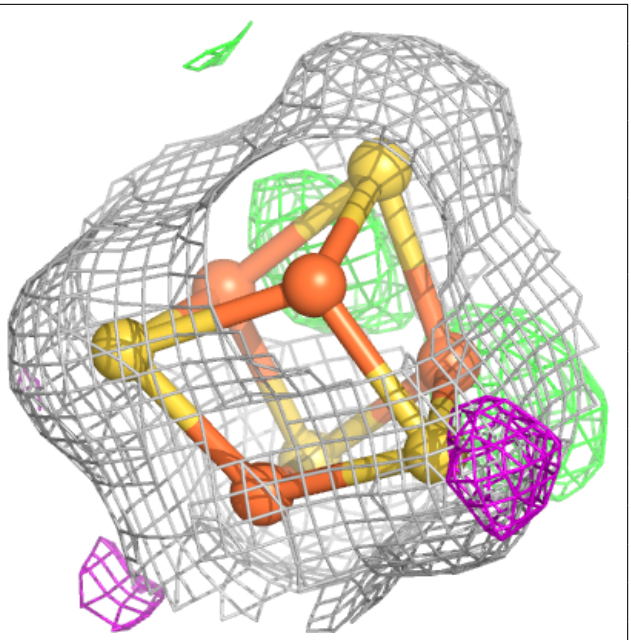


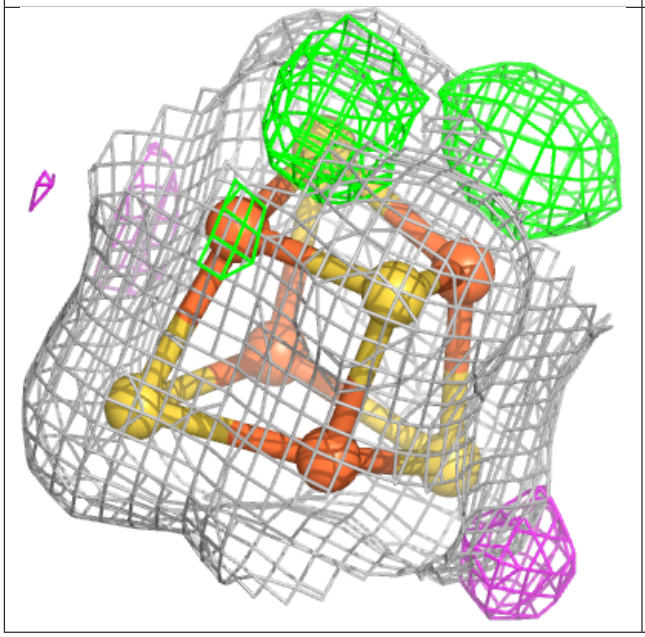


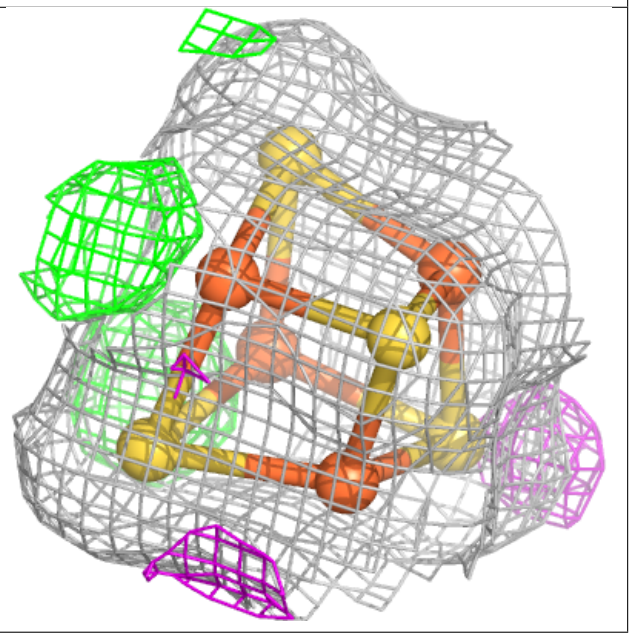


Electron density around SF4 D 805:

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

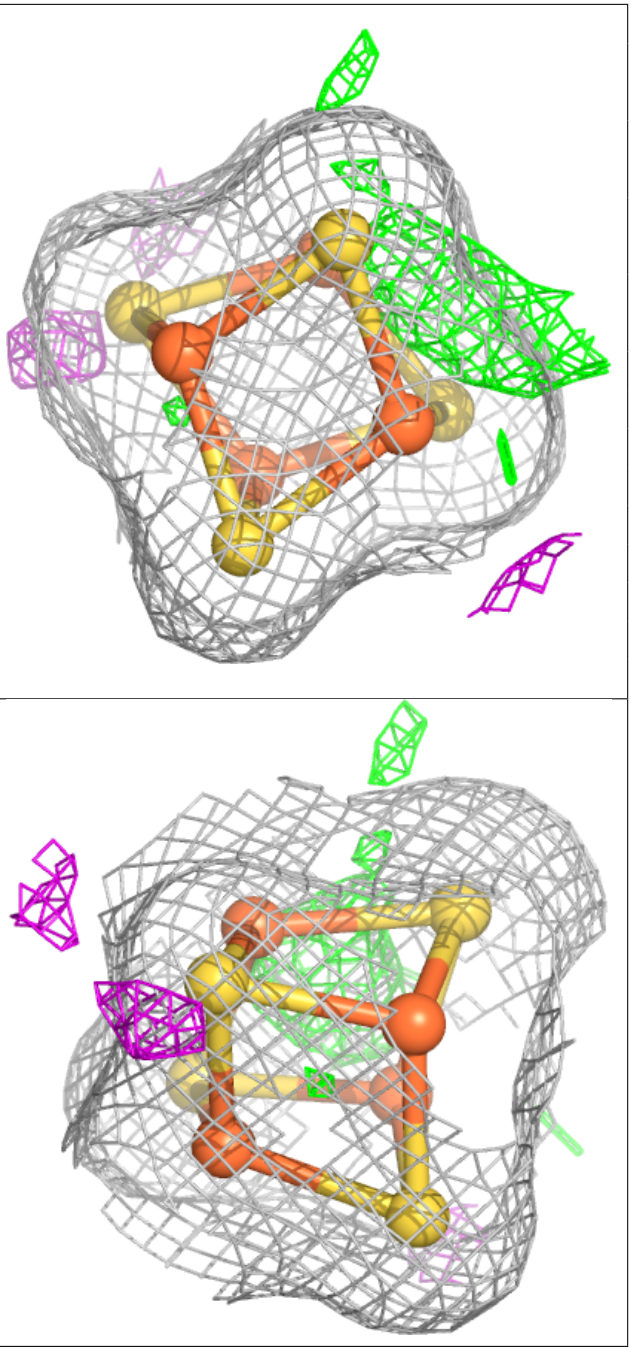






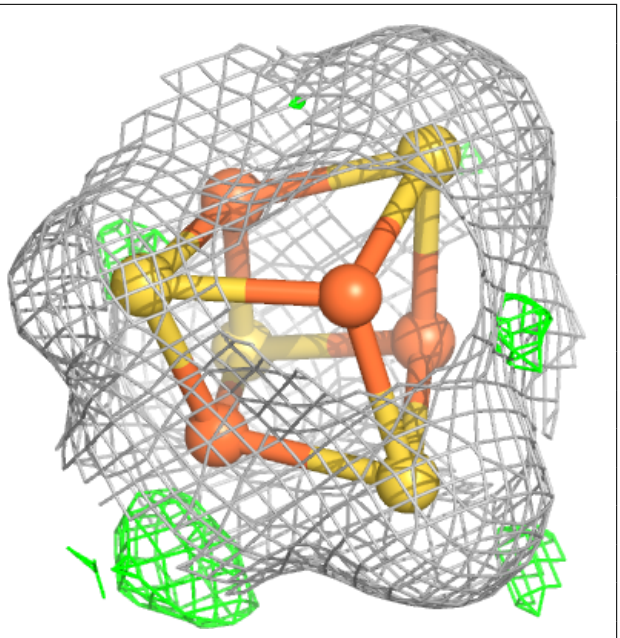
Electron density around SF4 E 401:

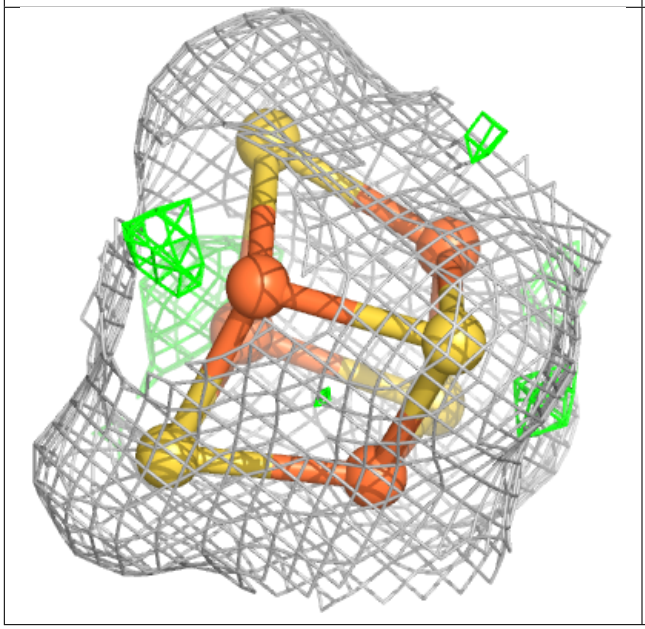
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

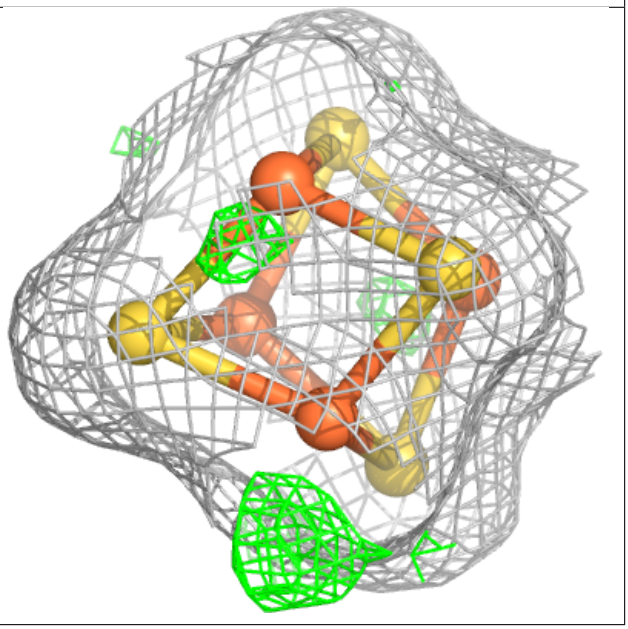


Electron density around SF4 E 402:

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

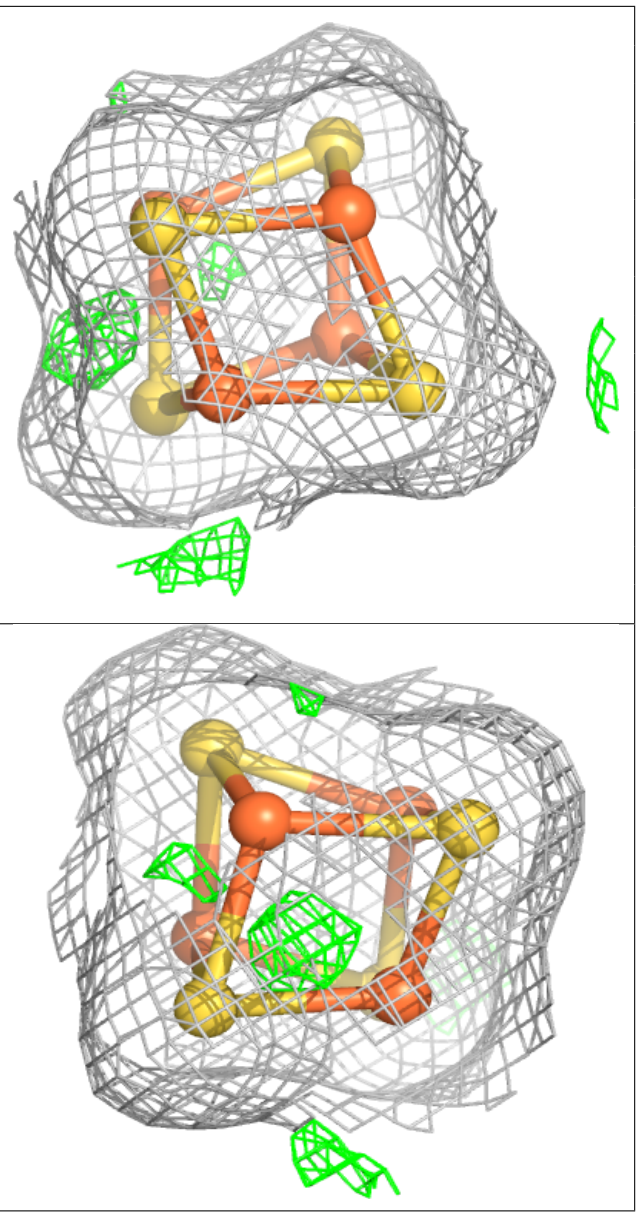






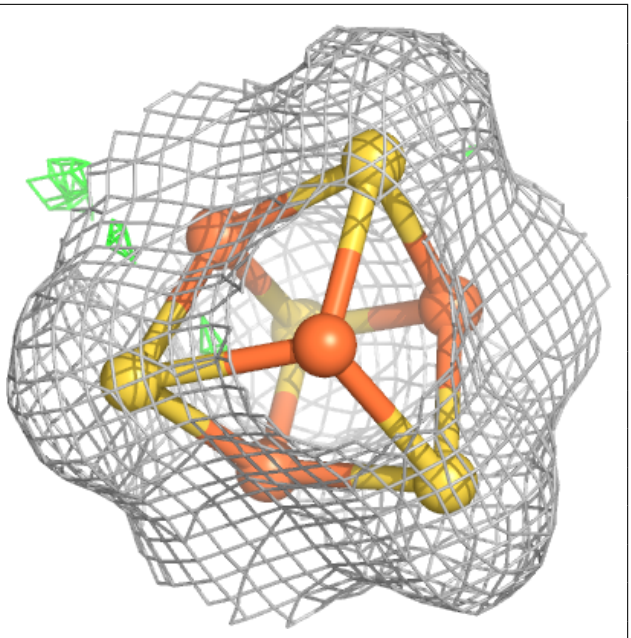
Electron density around SF4 E 404:

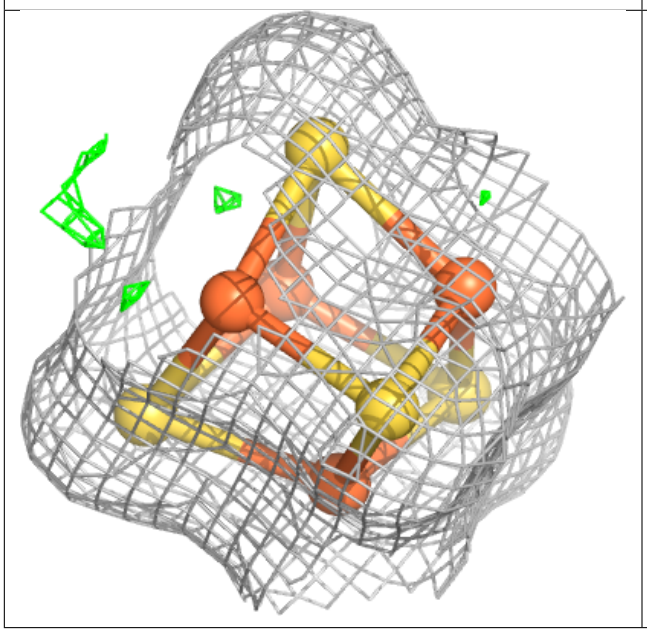
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

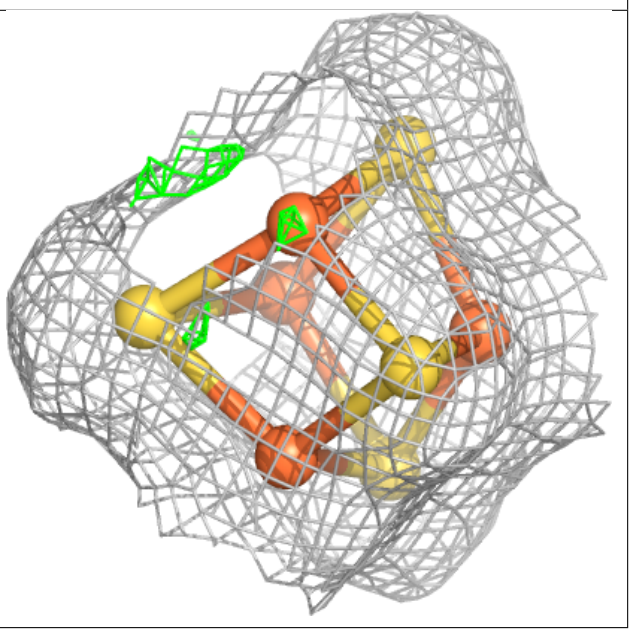


Electron density around SF4 A 810:

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

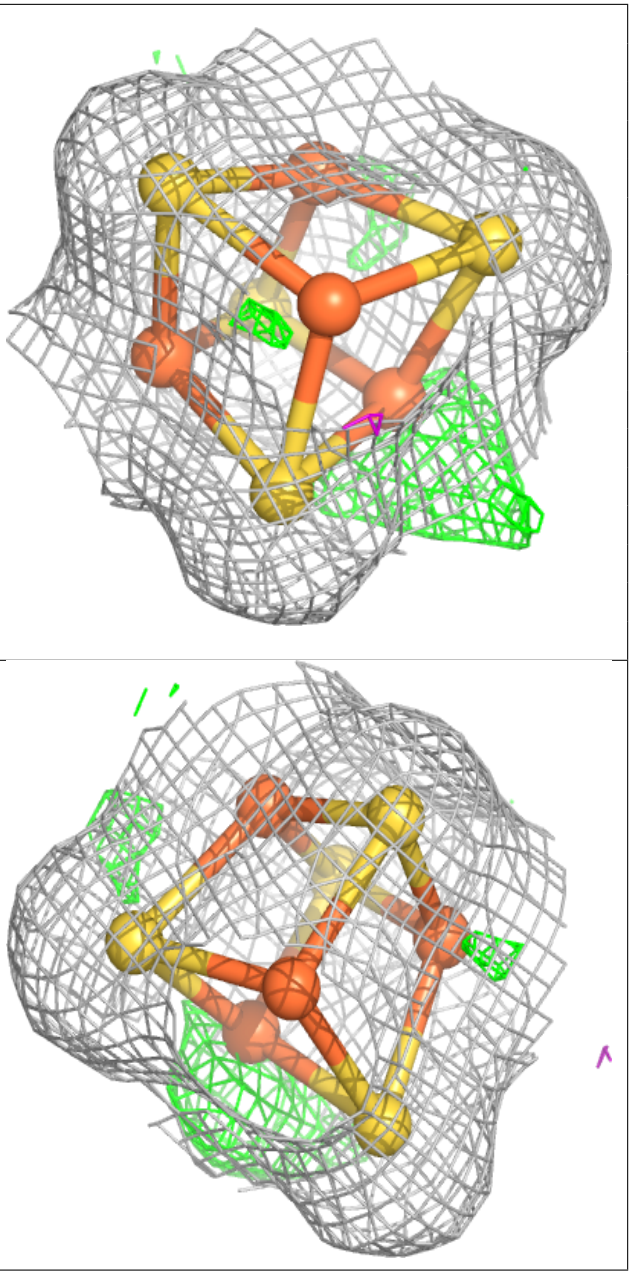






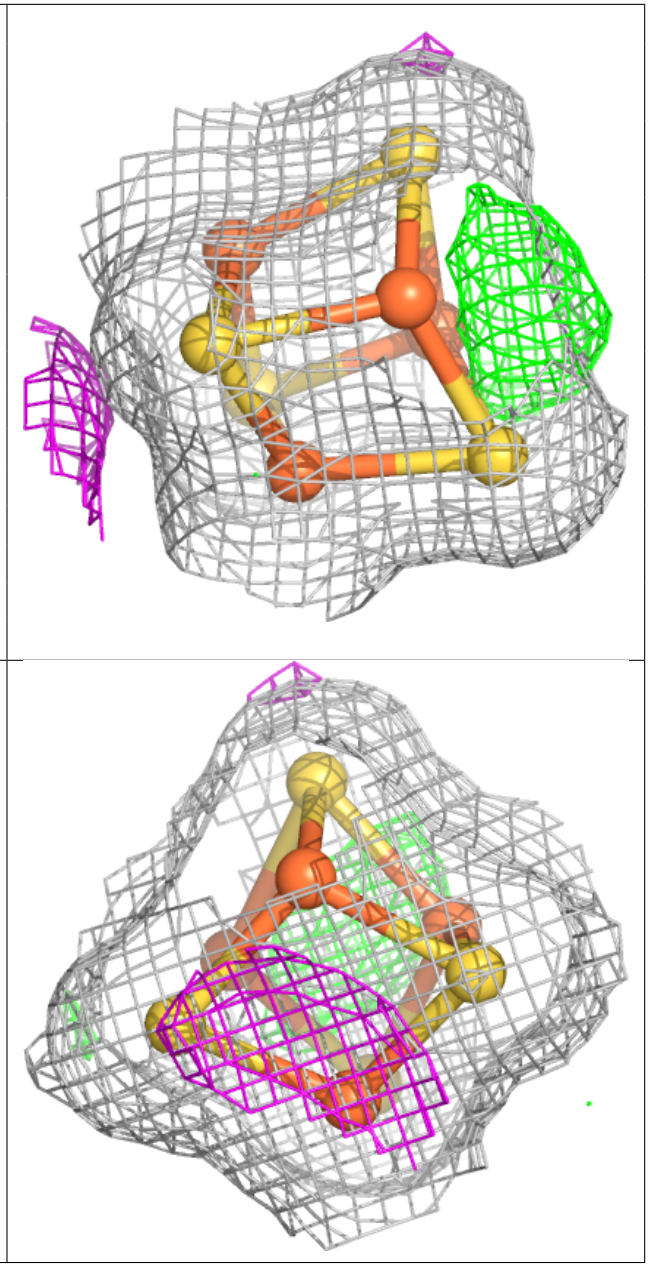
Electron density around SF4 A 811:

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



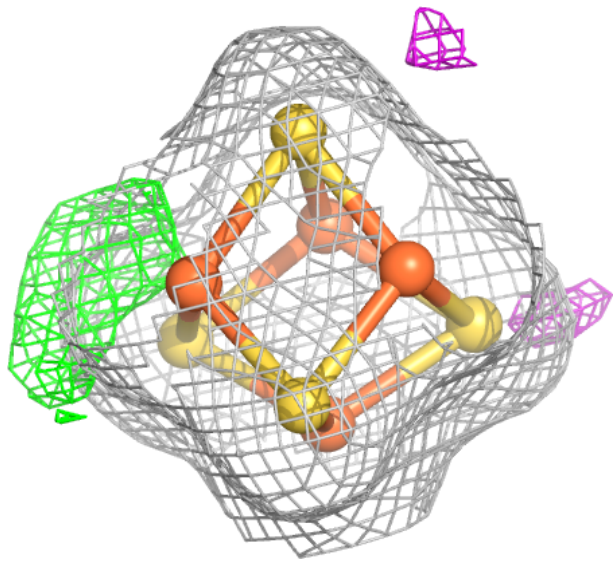
Electron density around SF4 A 819:

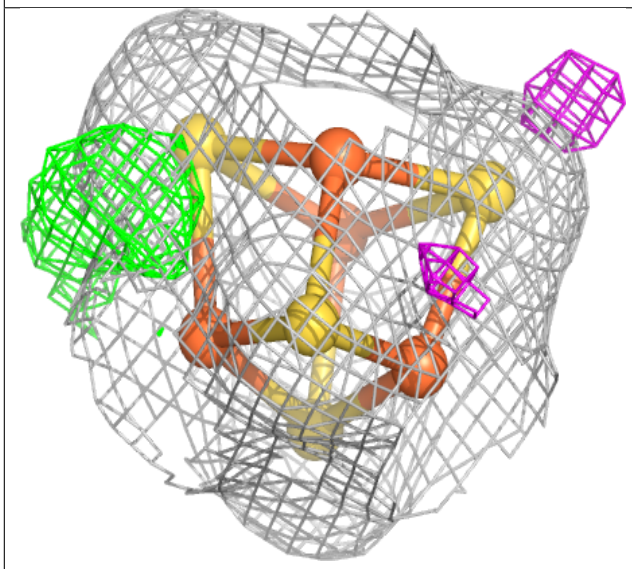
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

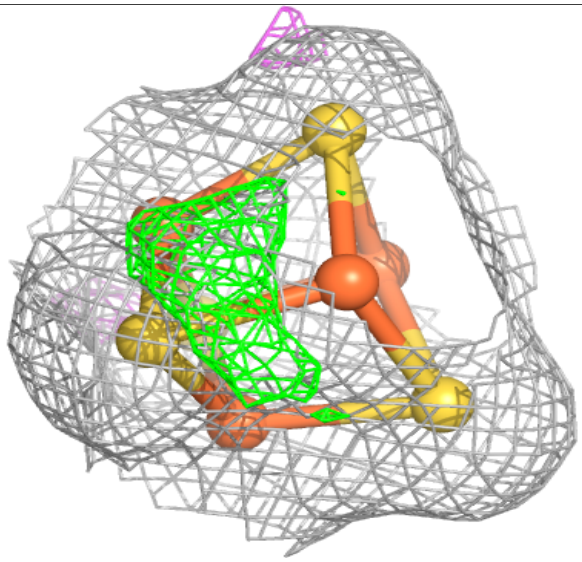


Electron density around SF4 B 402:

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

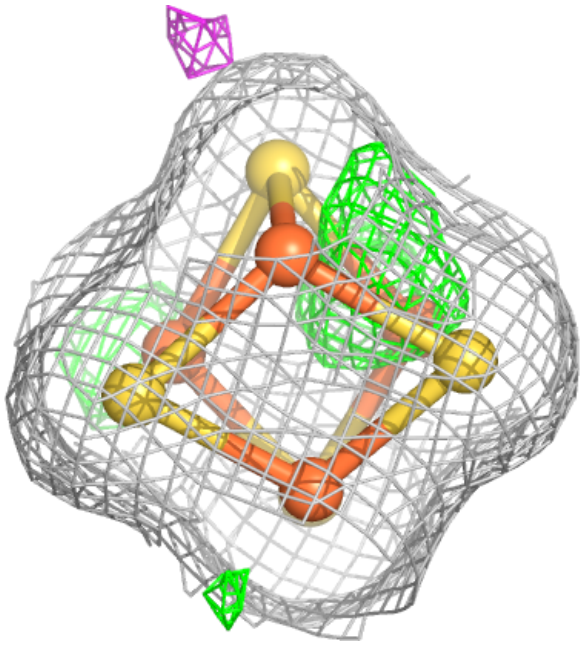


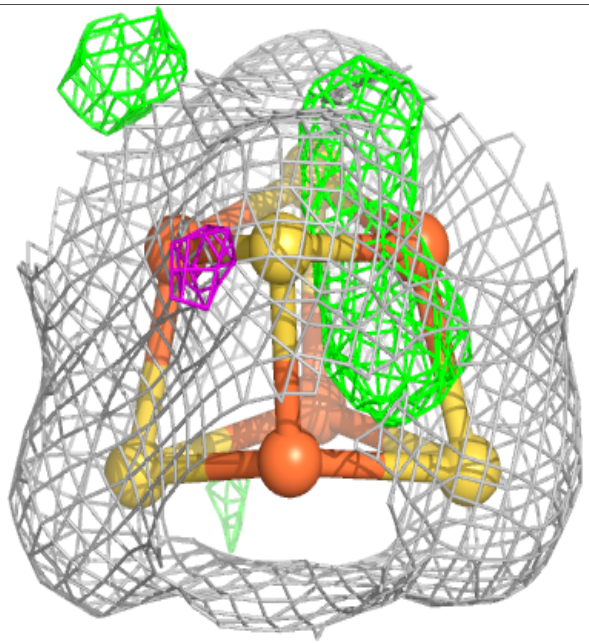


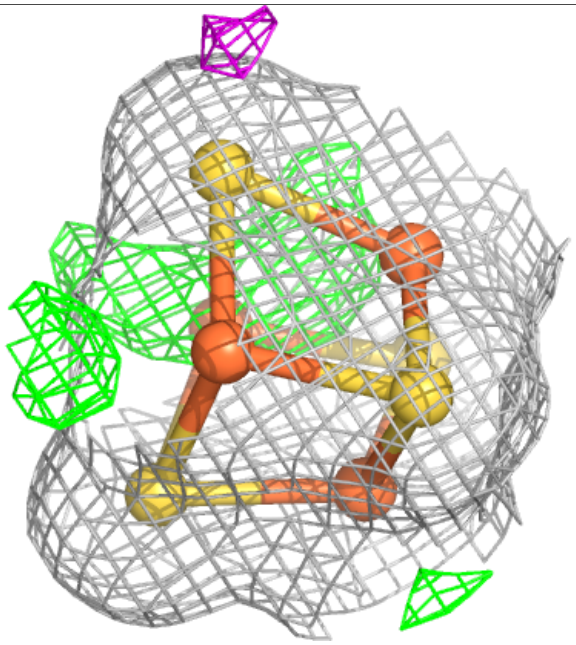


Electron density around SF4 B 403:

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

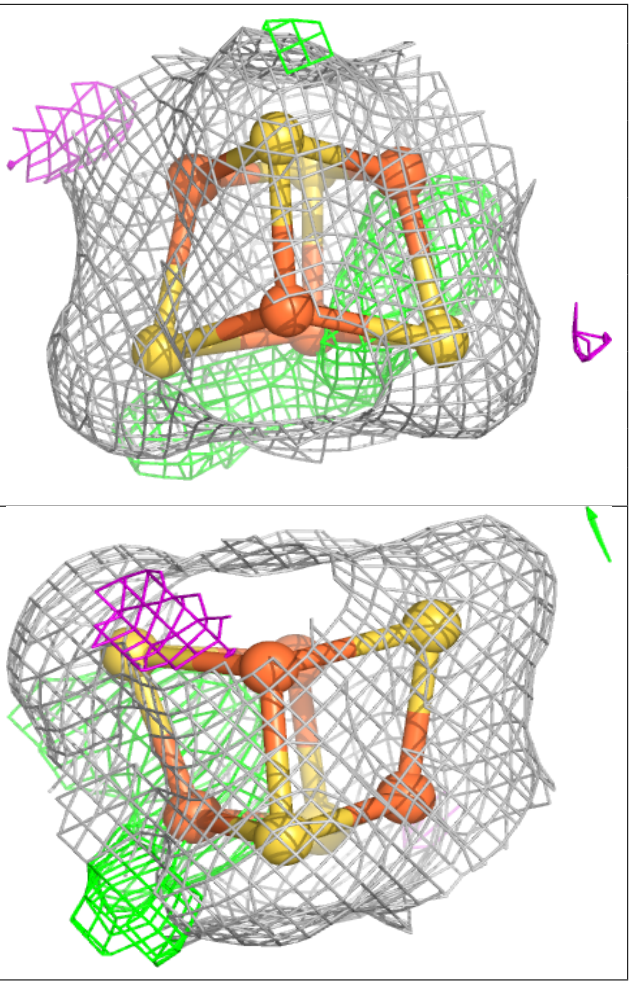






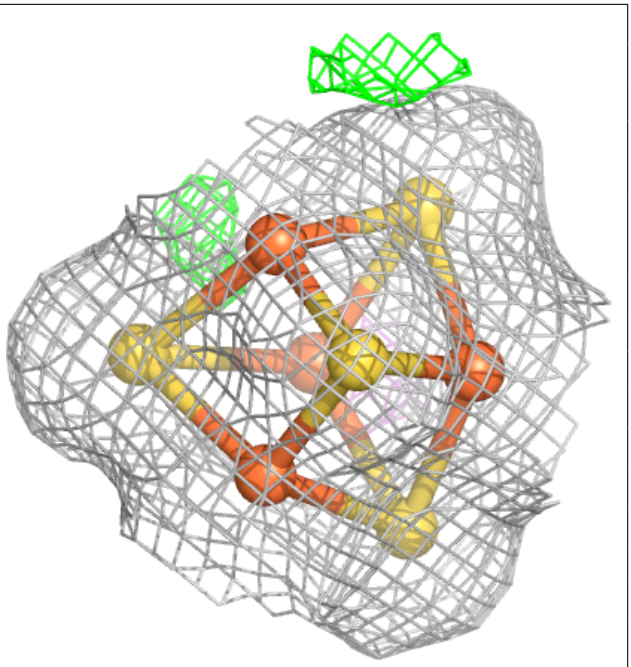
Electron density around SF4 A 809:

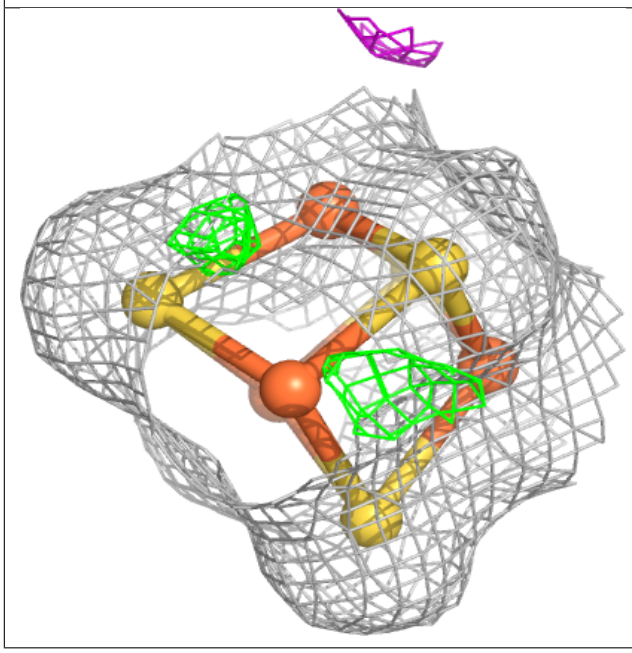
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

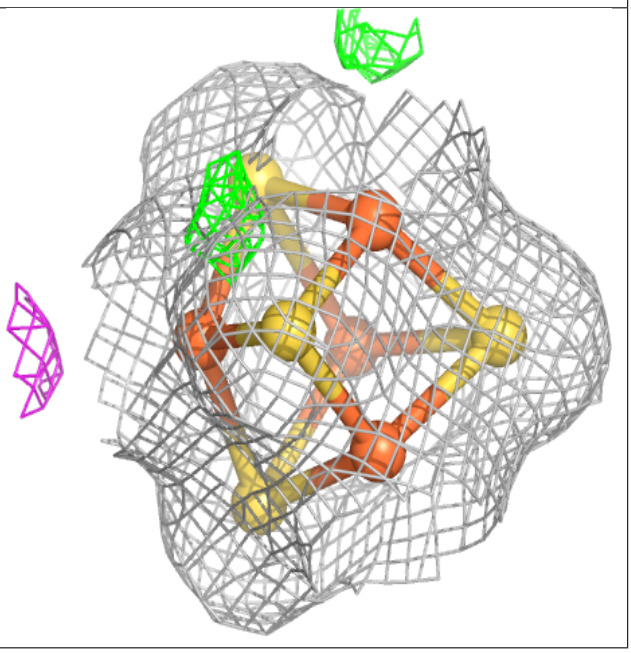


Electron density around SF4 D 803:

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

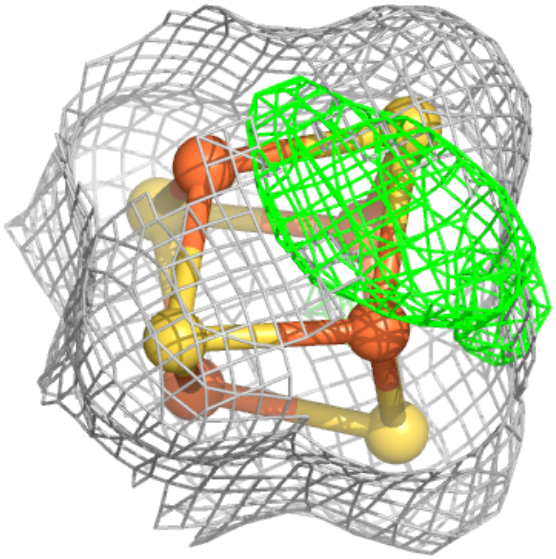


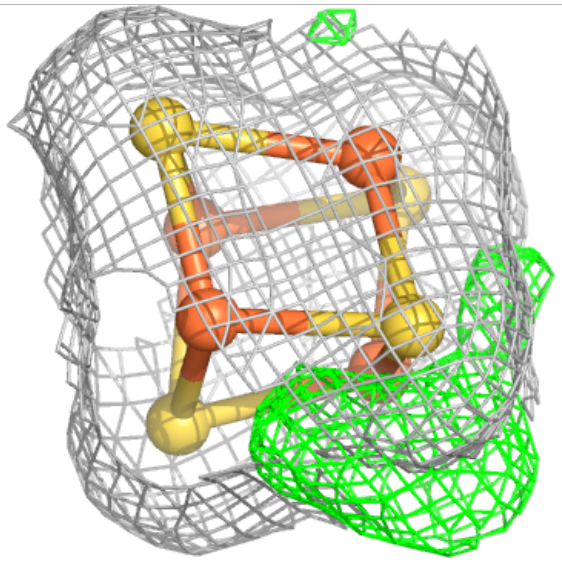


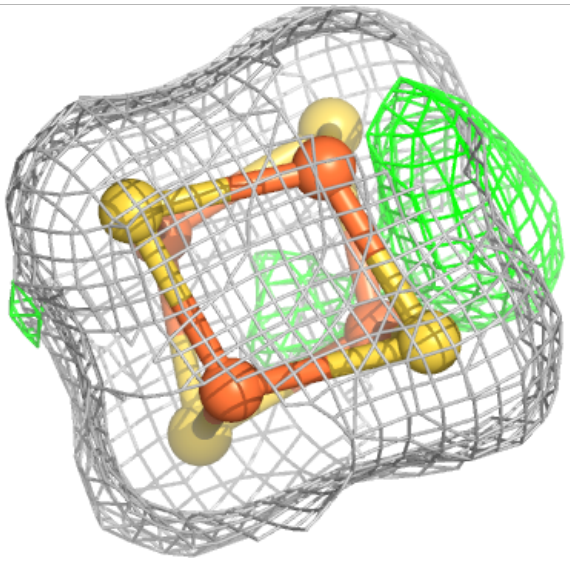


Electron density around SF4 D 804:

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







6.5 Other polymers (i)

There are no such residues in this entry.