wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2026 – 12:11 am BST

PDB ID	:	7B04 / pdb_00007b04
Title	:	Structure of Nitrite oxidoreductase (Nxr) from the anammox bacterium Kuenenia stuttgartiensis.
Authors	:	Moreno-Chicano, T.; Dietl, A.; Akram, M.; Barends, T.R.M.
Deposited on	:	2020-11-18
Resolution	:	2.97 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:

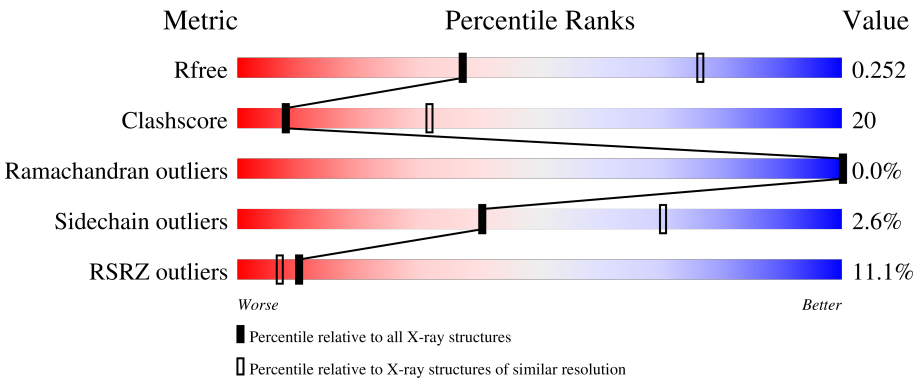
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.97 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	410	74% 25% •
1	D	410	58% 64% 35%
1	G	410	% 74% 26%
1	J	410	77% 22%
1	M	410	2% 64% 34% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	P	410	4% 69% 29%
1	S	410	73% 27%
1	V	410	21% 51% 43% 5%
2	B	1148	3% 60% 35%
2	E	1148	79% 70% 25%
2	H	1148	% 68% 29%
2	K	1148	% 65% 31%
2	N	1148	% 65% 31%
2	Q	1148	4% 55% 39%
2	T	1148	% 67% 29%
2	W	1148	5% 60% 35%
3	C	322	2% 70% 19% 9%
3	F	322	17% 57% 33% 9%
3	I	322	8% 58% 29% 9%
3	L	322	% 70% 19% 9%
3	O	322	17% 58% 29% 10%
3	R	322	% 69% 20% 10%
3	U	322	2% 69% 20% 9%
3	X	322	13% 56% 30% 9%

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	SF4	D	501	-	-	X	-
4	SF4	D	502	-	-	X	-
4	SF4	G	503	-	-	X	-
4	SF4	J	503	-	-	X	-
4	SF4	M	503	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	N	5804	-	-	X	-
4	SF4	P	503	-	-	X	-
4	SF4	Q	5804	-	-	X	-
4	SF4	S	503	-	-	X	-
4	SF4	T	5804	-	-	X	-
4	SF4	V	501	-	-	X	-
4	SF4	V	503	-	-	X	-
4	SF4	W	5804	-	-	X	-
5	F3S	D	504	-	-	X	-
5	F3S	M	504	-	-	X	-
5	F3S	V	504	-	-	X	-
6	MD1	E	5801	X	-	-	-
8	HEM	F	401	-	-	X	-
8	HEM	I	401	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 115931 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 Nitrite oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	409	3349	2138	579	606	26	0	0	0
1	D	408	2872	1805	508	534	25	0	0	0
1	G	409	3344	2138	578	602	26	0	0	0
1	J	409	3361	2147	580	608	26	0	0	0
1	M	409	3309	2114	572	597	26	0	0	0
1	P	409	3321	2121	573	601	26	0	0	0
1	S	409	3333	2131	577	599	26	0	0	0
1	V	409	3239	2063	556	594	26	0	0	0

- Molecule 2 is a protein called Nitrite oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1120	9003	5748	1551	1662	42	0	1	0
2	E	1111	6871	4264	1247	1334	26	0	1	0
2	H	1118	9028	5760	1561	1665	42	0	1	0
2	K	1119	9046	5777	1559	1668	42	0	1	0
2	N	1117	9052	5773	1564	1672	43	0	3	0
2	Q	1116	8902	5678	1533	1649	42	0	1	0

Continued on next page...

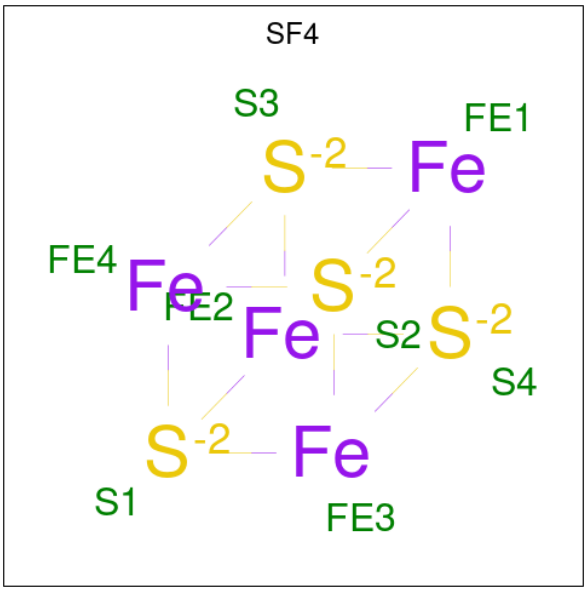
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	T	1119	9034	5766	1555	1671	42	0	0	0
			Total	C	N	O	S			
2	W	1118	8920	5688	1532	1658	42	0	1	0

- Molecule 3 is a protein called Nitrite oxidoreductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	292	2281	1435	400	438	8	0	1	0
			Total	C	N	O	S			
3	F	292	2068	1305	358	398	7	0	0	0
			Total	C	N	O	S			
3	I	292	2216	1401	385	422	8	0	0	0
			Total	C	N	O	S			
3	L	292	2274	1431	396	439	8	0	1	0
			Total	C	N	O	S			
3	O	291	2124	1337	369	410	8	0	0	0
			Total	C	N	O	S			
3	R	291	2261	1423	392	438	8	0	0	0
			Total	C	N	O	S			
3	U	292	2267	1428	393	438	8	0	0	0
			Total	C	N	O	S			
3	X	292	2225	1401	387	429	8	0	0	0

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



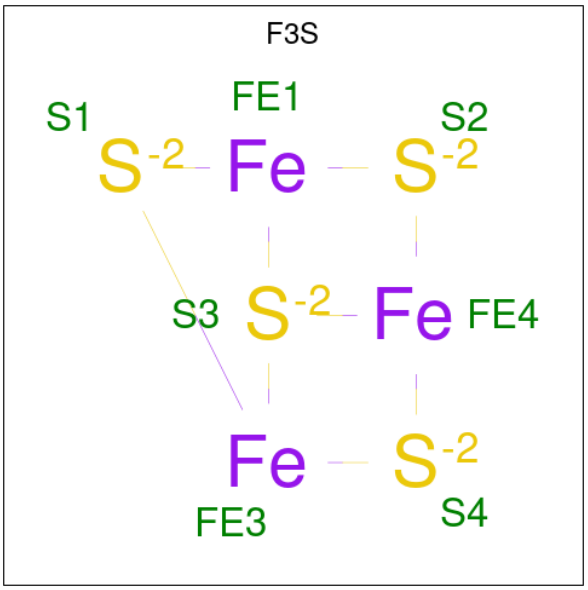
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	A	1	8	4	4	0	0
4	A	1	8	4	4	0	0
4	A	1	8	4	4	0	0
4	B	1	8	4	4	0	0
4	D	1	8	4	4	0	0
4	D	1	8	4	4	0	0
4	D	1	8	4	4	0	0
4	E	1	8	4	4	0	0
4	G	1	8	4	4	0	0
4	G	1	8	4	4	0	0
4	G	1	8	4	4	0	0
4	H	1	8	4	4	0	0
4	J	1	8	4	4	0	0
4	J	1	8	4	4	0	0
4	J	1	8	4	4	0	0
4	K	1	8	4	4	0	0
4	M	1	8	4	4	0	0
4	M	1	8	4	4	0	0
4	M	1	8	4	4	0	0
4	N	1	8	4	4	0	0
4	P	1	8	4	4	0	0
4	P	1	8	4	4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	P	1	8	4	4	0	0
4	Q	1	8	4	4	0	0
4	S	1	8	4	4	0	0
4	S	1	8	4	4	0	0
4	S	1	8	4	4	0	0
4	T	1	8	4	4	0	0
4	V	1	8	4	4	0	0
4	V	1	8	4	4	0	0
4	V	1	8	4	4	0	0
4	W	1	8	4	4	0	0

- Molecule 5 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4) (labeled as "Ligand of Interest" by depositor).



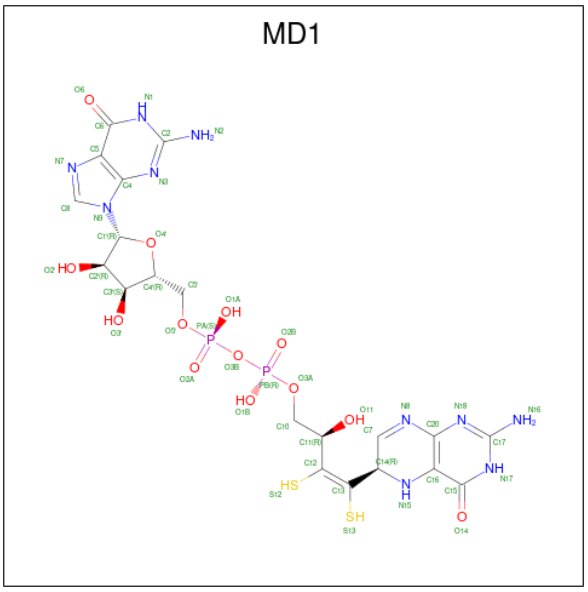
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
5	A	1	7	3	4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
5	D	1	7	3	4	0	0
5	G	1	7	3	4	0	0
5	J	1	7	3	4	0	0
5	M	1	7	3	4	0	0
5	P	1	7	3	4	0	0
5	S	1	7	3	4	0	0
5	V	1	7	3	4	0	0

- Molecule 6 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTERIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (CCD ID: MD1) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
6	B	1	47	20	10	13	2	2	0	0
6	B	1	47	20	10	13	2	2	0	0
6	E	1	47	20	10	13	2	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
6	E	1	47	20	10	13	2	2	0	0
6	H	1	47	20	10	13	2	2	0	0
6	H	1	47	20	10	13	2	2	0	0
6	K	1	47	20	10	13	2	2	0	0
6	K	1	47	20	10	13	2	2	0	0
6	N	1	47	20	10	13	2	2	0	0
6	N	1	47	20	10	13	2	2	0	0
6	Q	1	47	20	10	13	2	2	0	0
6	Q	1	47	20	10	13	2	2	0	0
6	T	1	47	20	10	13	2	2	0	0
6	T	1	47	20	10	13	2	2	0	0
6	W	1	47	20	10	13	2	2	0	0
6	W	1	47	20	10	13	2	2	0	0

- Molecule 7 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

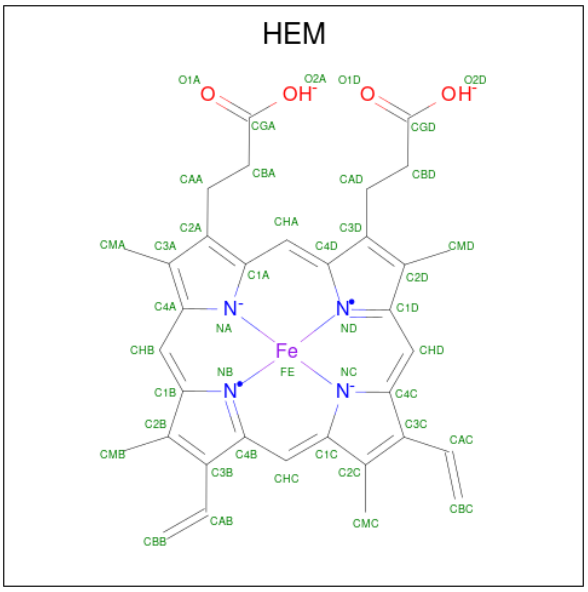
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mo		
7	B	1	1	1	0	0
7	E	1	1	1	0	0
7	H	1	1	1	0	0
7	K	1	1	1	0	0
7	N	1	1	1	0	0
7	Q	1	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	T	1	Total Mo 1 1	0	0
7	W	1	Total Mo 1 1	0	0

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C Fe N O 43 34 1 4 4	0	0
8	F	1	Total C Fe N O 43 34 1 4 4	0	0
8	I	1	Total C Fe N O 43 34 1 4 4	0	0
8	L	1	Total C Fe N O 43 34 1 4 4	0	0
8	O	1	Total C Fe N O 43 34 1 4 4	0	0
8	R	1	Total C Fe N O 43 34 1 4 4	0	0
8	U	1	Total C Fe N O 43 34 1 4 4	0	0
8	X	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
9	C	2	2	2	0	0
9	F	2	2	2	0	0
9	I	2	2	2	0	0
9	L	2	2	2	0	0
9	O	2	2	2	0	0
9	R	2	2	2	0	0
9	U	2	2	2	0	0
9	X	2	2	2	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	37	37	37	0	0
10	B	72	72	72	0	0
10	C	35	35	35	0	0
10	D	6	6	6	0	0
10	E	13	13	13	0	0
10	F	8	8	8	0	0
10	G	25	25	25	0	0
10	H	83	83	83	0	0
10	I	20	20	20	0	0
10	J	28	28	28	0	0
10	K	74	74	74	0	0
10	L	30	30	30	0	0

Continued on next page...

Continued from previous page...

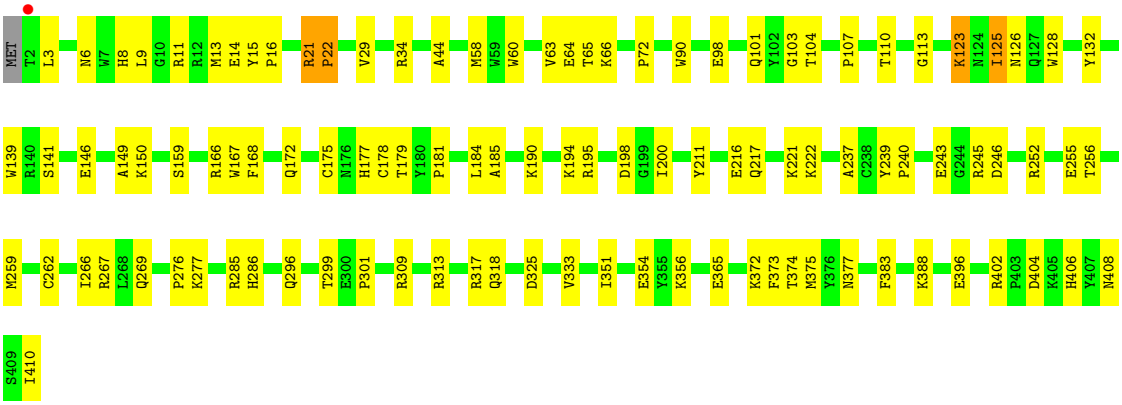
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	M	10	10	10	0	0
			Total	O		
10	N	76	76	76	0	0
			Total	O		
10	O	17	17	17	0	0
			Total	O		
10	P	16	16	16	0	0
			Total	O		
10	Q	43	43	43	0	0
			Total	O		
10	R	22	22	22	0	0
			Total	O		
10	S	20	20	20	0	0
			Total	O		
10	T	62	62	62	0	0
			Total	O		
10	U	25	25	25	0	0
			Total	O		
10	V	12	12	12	0	0
			Total	O		
10	W	41	41	41	0	0
			Total	O		
10	X	24	24	24	0	0

3 Residue-property plots (i)

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

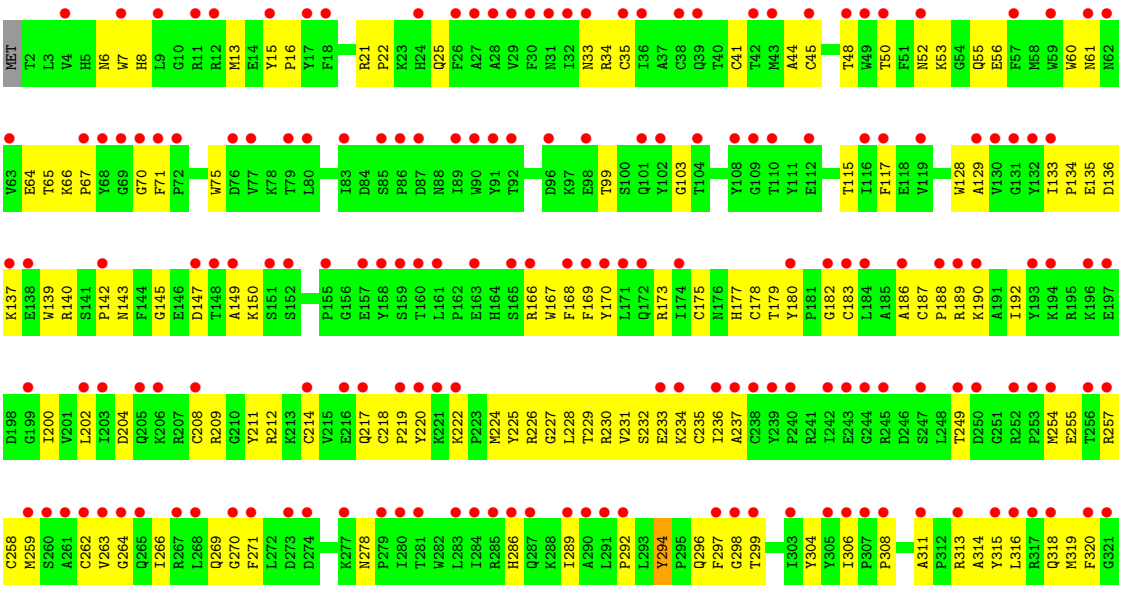
• Molecule 1: Nitrite oxidoreductase subunit B

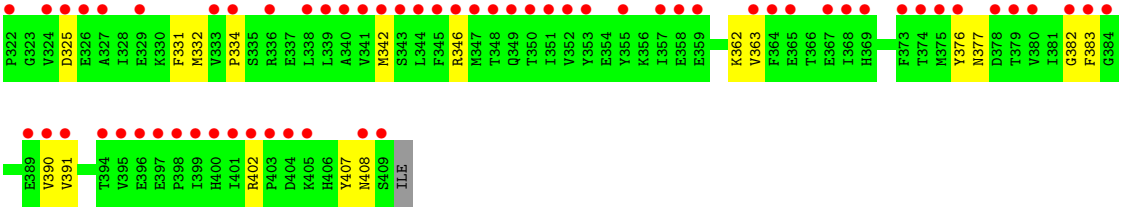
Chain A:



• Molecule 1: Nitrite oxidoreductase subunit B

Chain D:



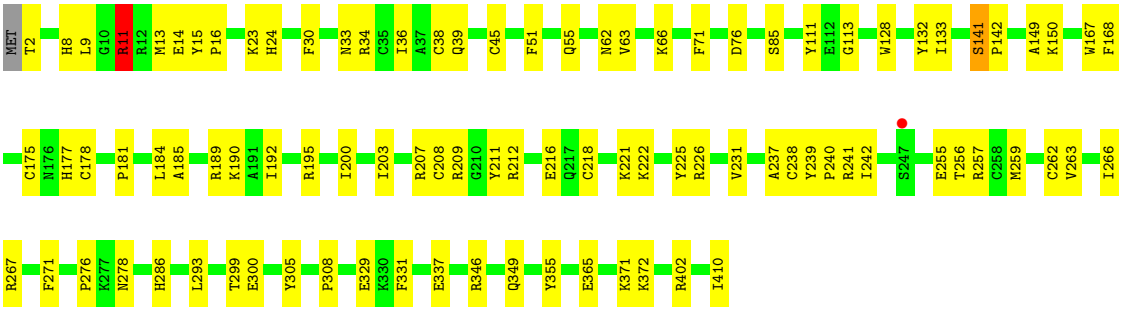


- Molecule 1: Nitrite oxidoreductase subunit B

Chain G:

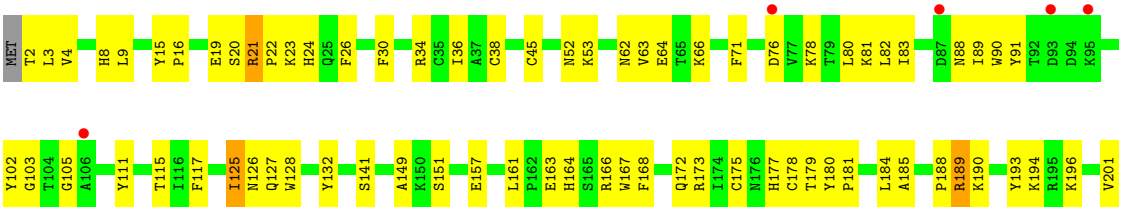
- Molecule 1: Nitrite oxidoreductase subunit B

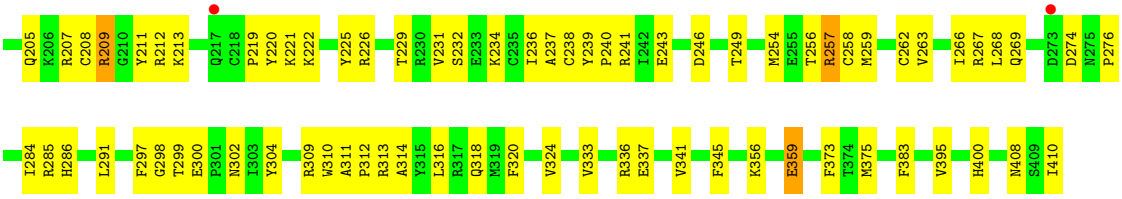
Chain J:



- Molecule 1: Nitrite oxidoreductase subunit B

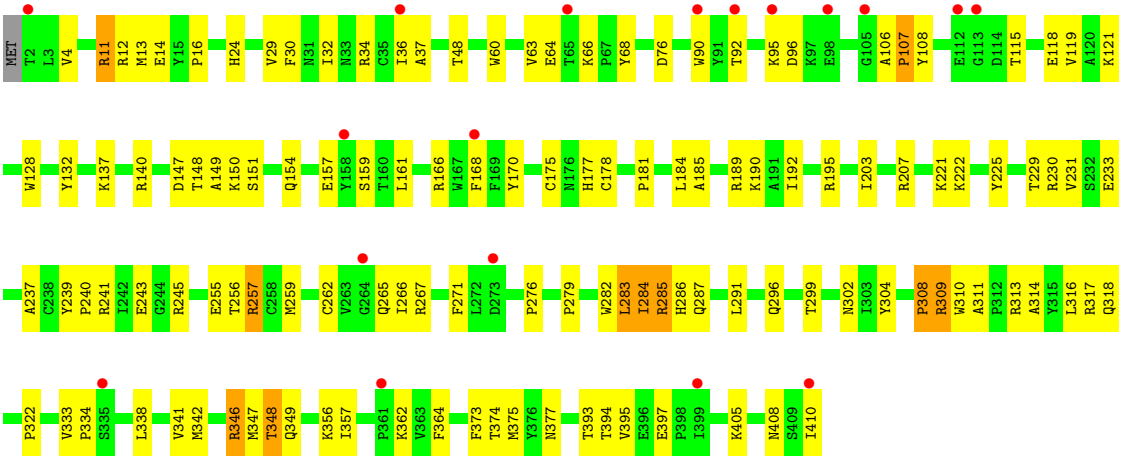
Chain M:





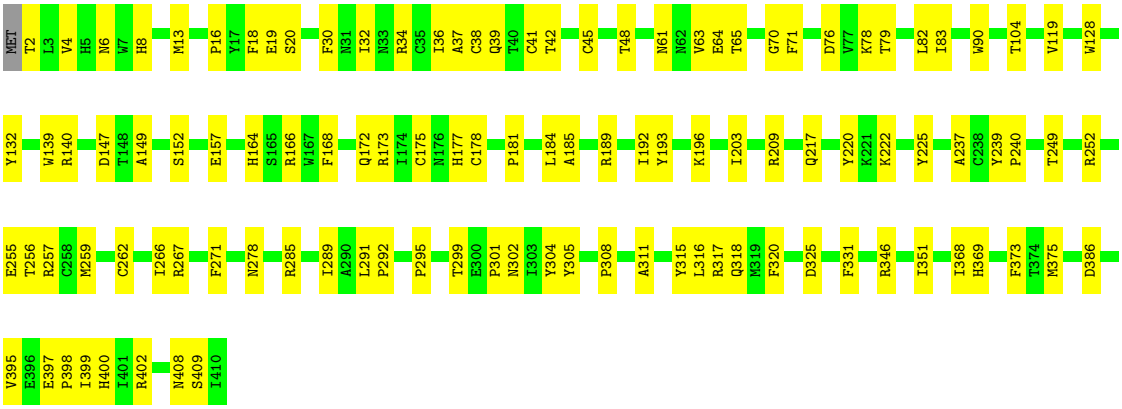
• Molecule 1: Nitrite oxidoreductase subunit B

Chain P:



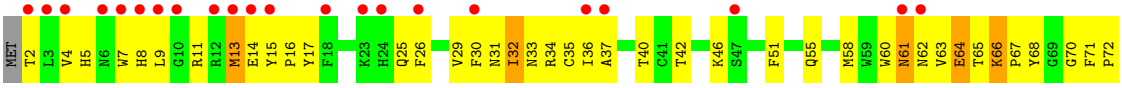
• Molecule 1: Nitrite oxidoreductase subunit B

Chain S:



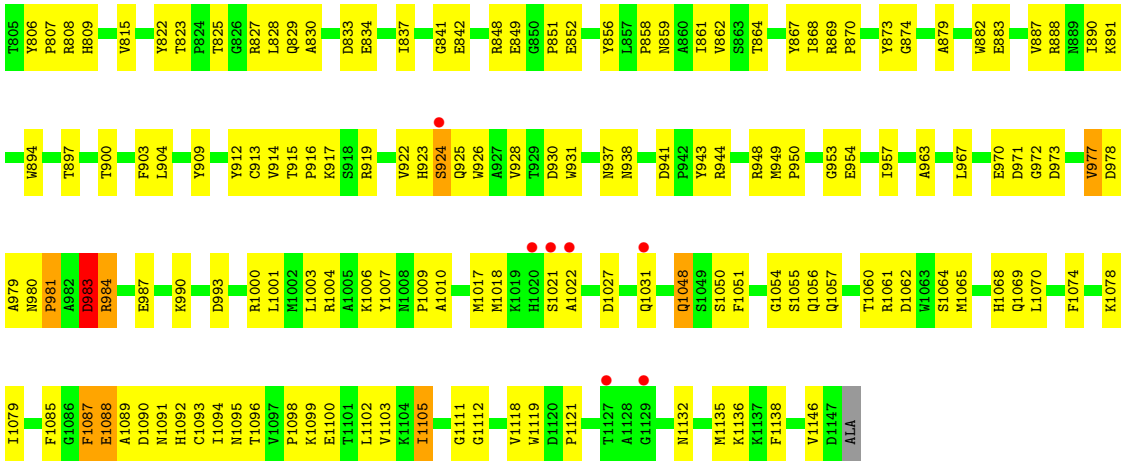
• Molecule 1: Nitrite oxidoreductase subunit B

Chain V:



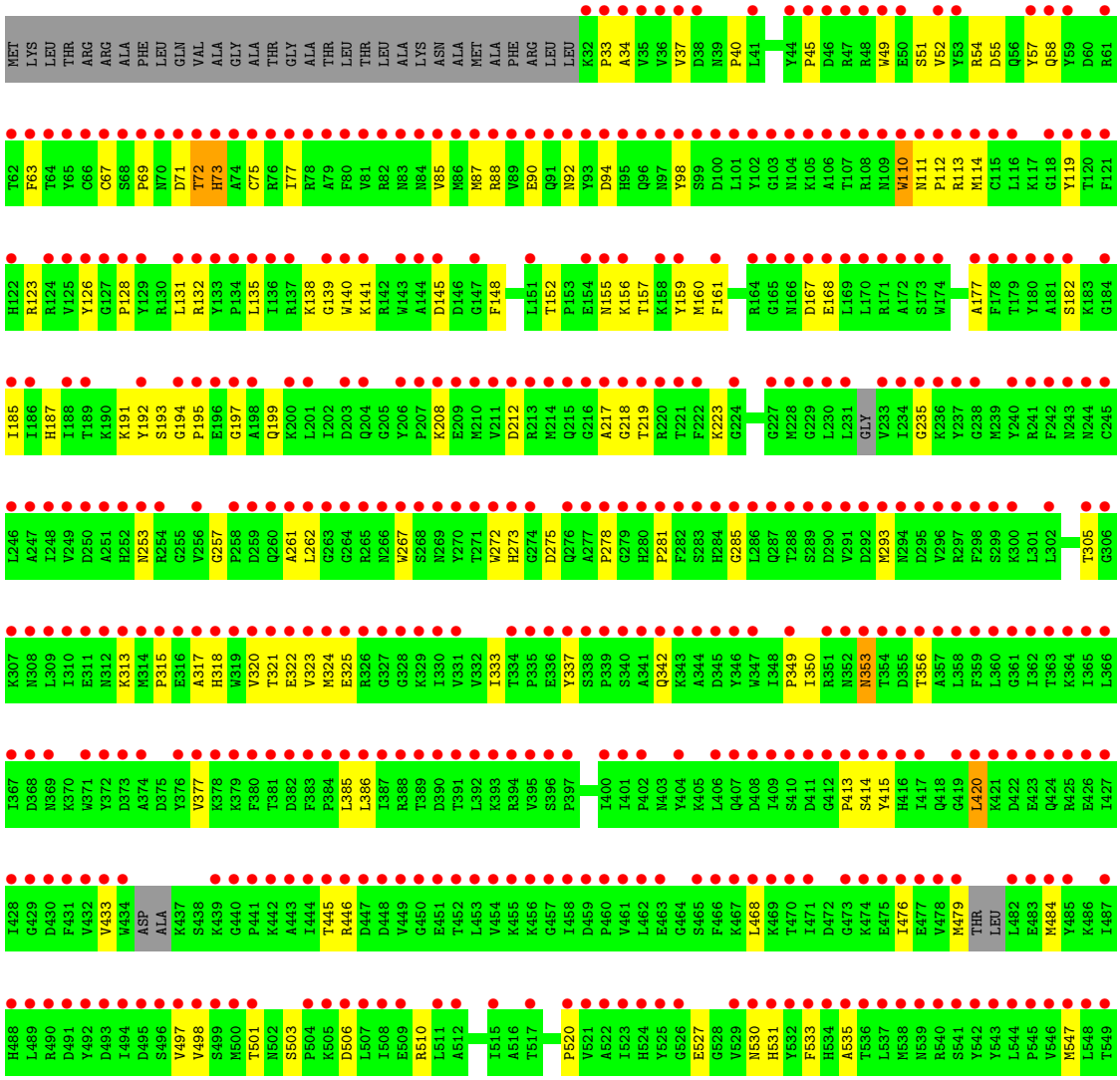
• Molecule 2: Nitrite oxidoreductase subunit A

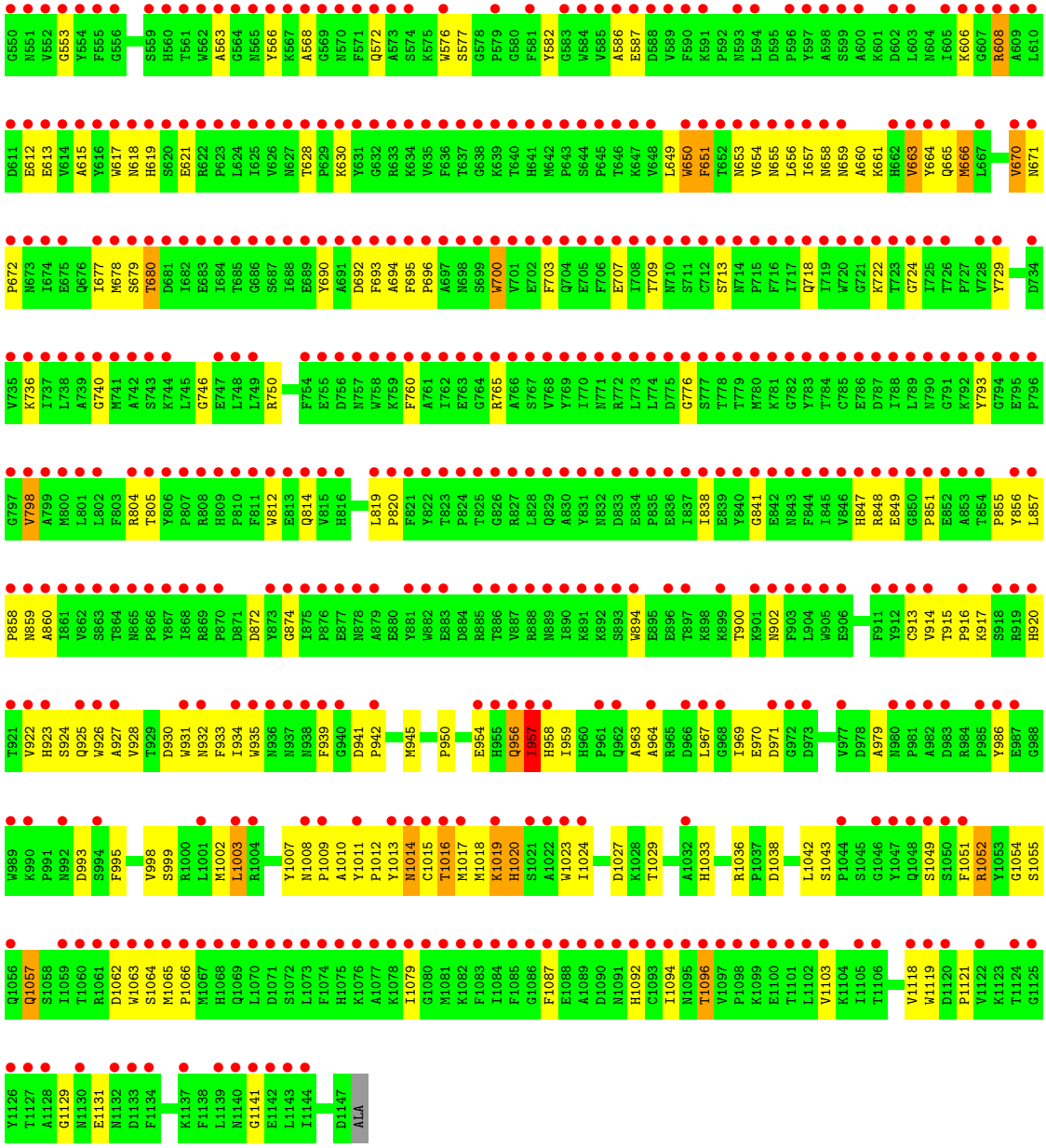
Chain B:



• Molecule 2: Nitrite oxidoreductase subunit A

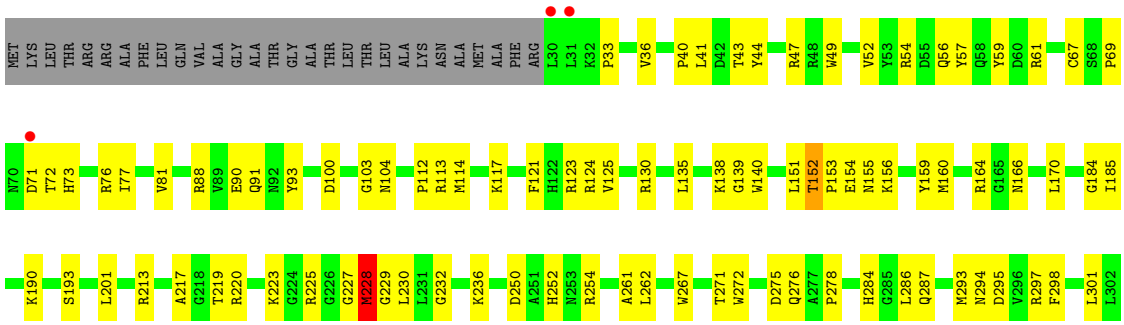
Chain E:

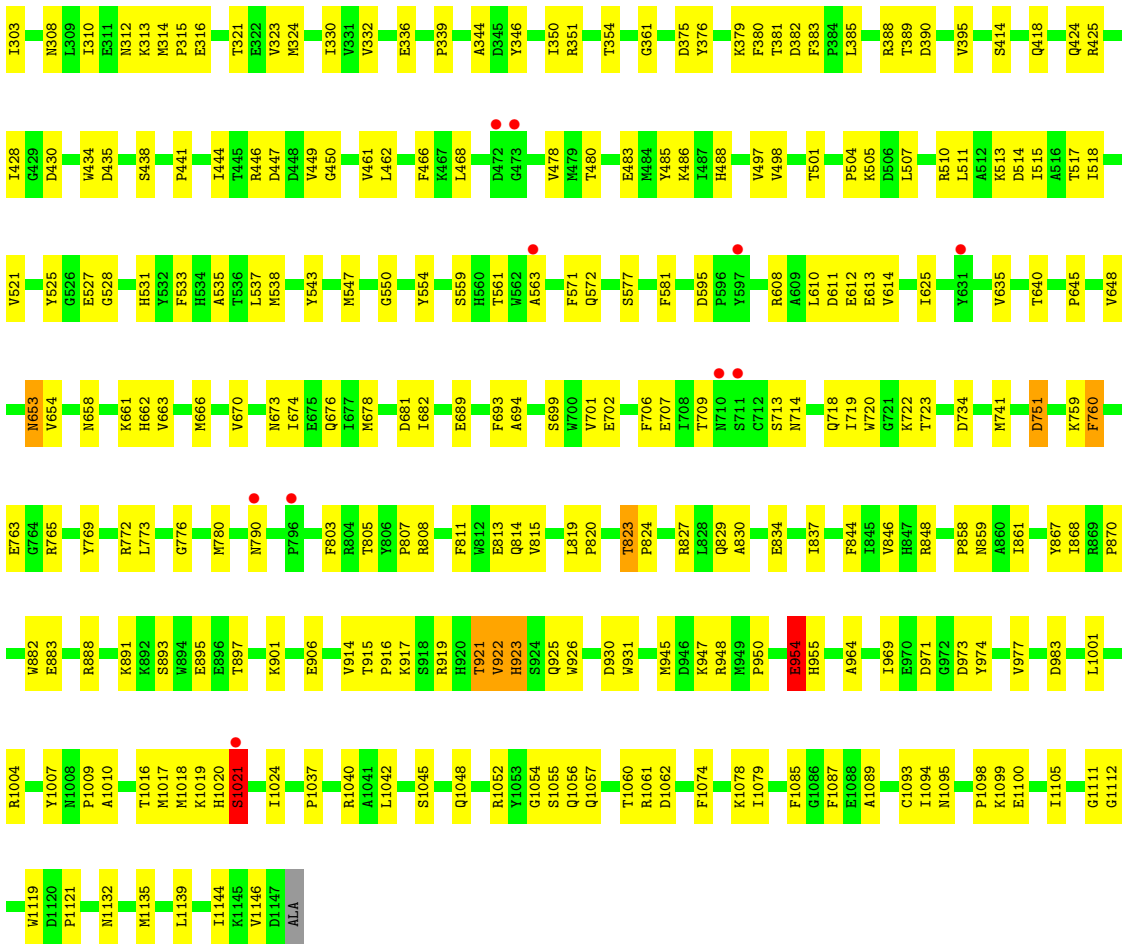




• Molecule 2: Nitrite oxidoreductase subunit A

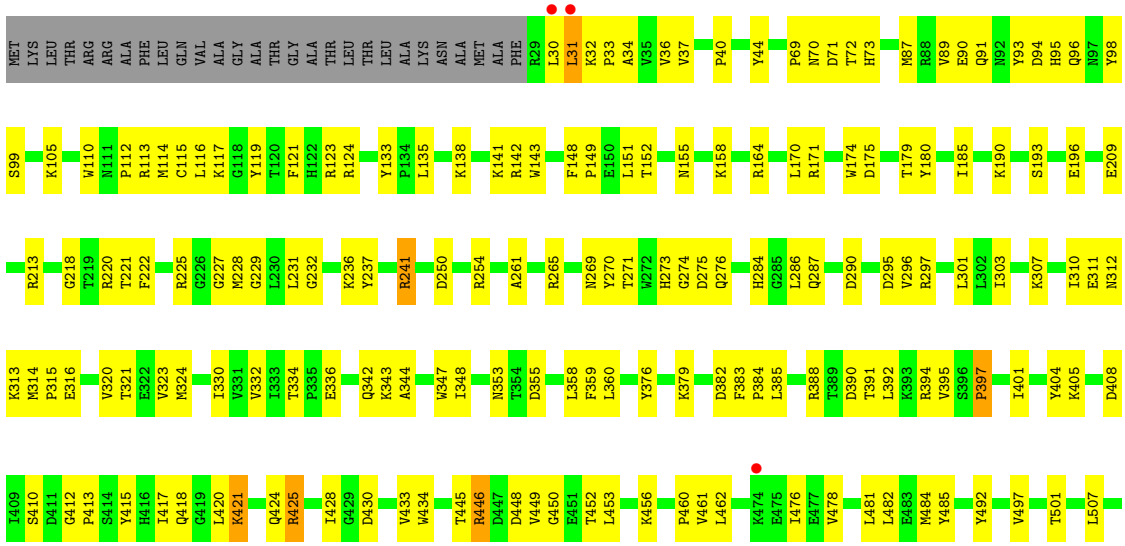
Chain H:

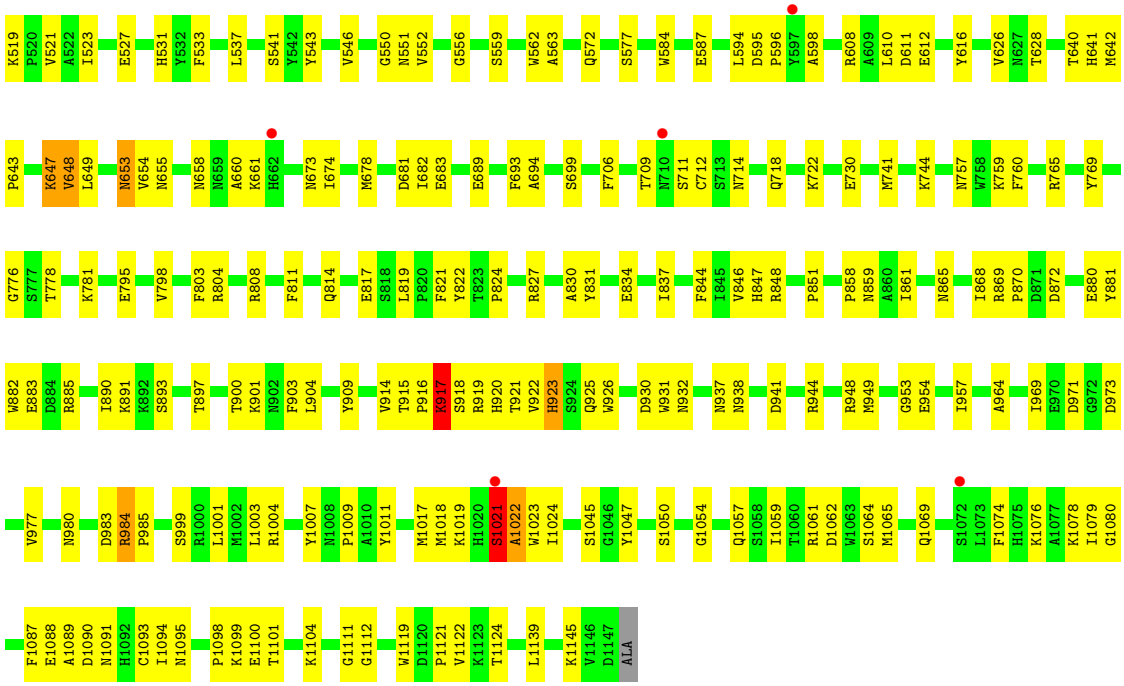




- Molecule 2: Nitrite oxidoreductase subunit A

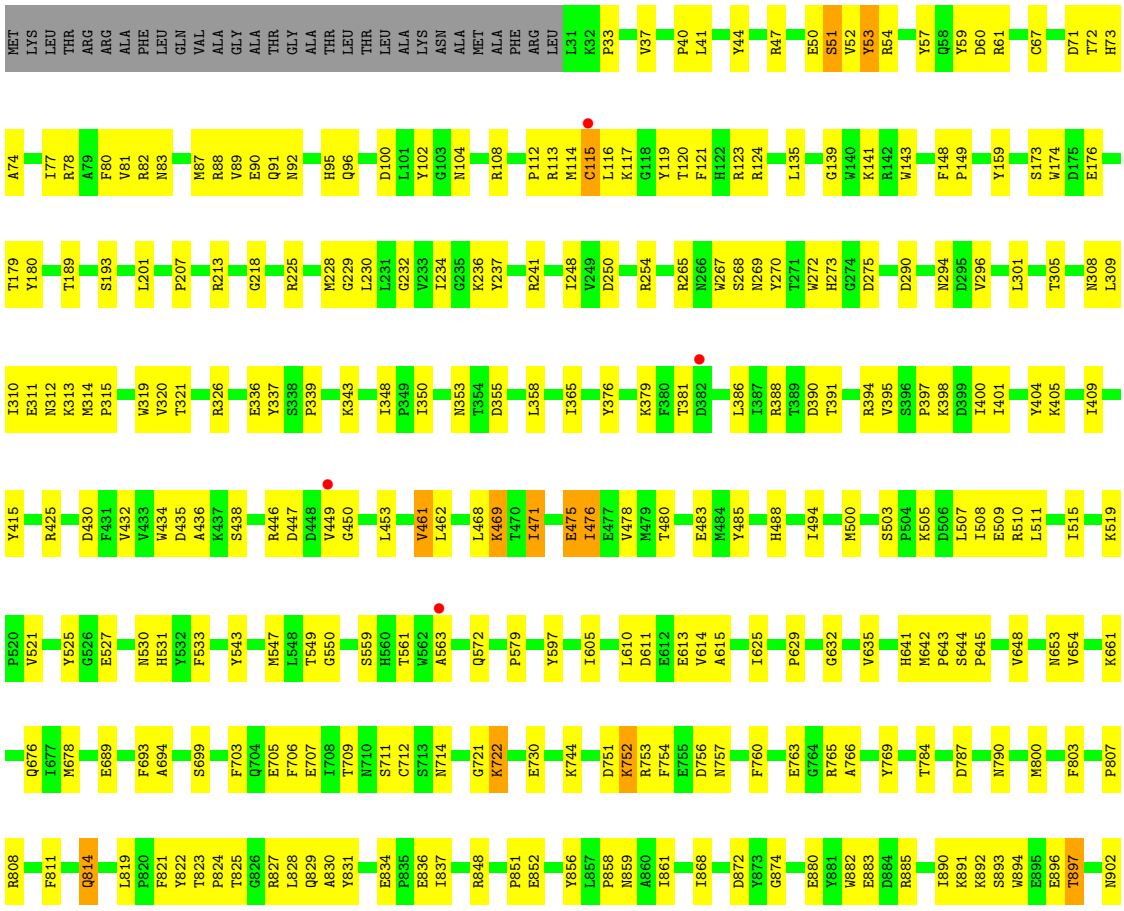
Chain K:

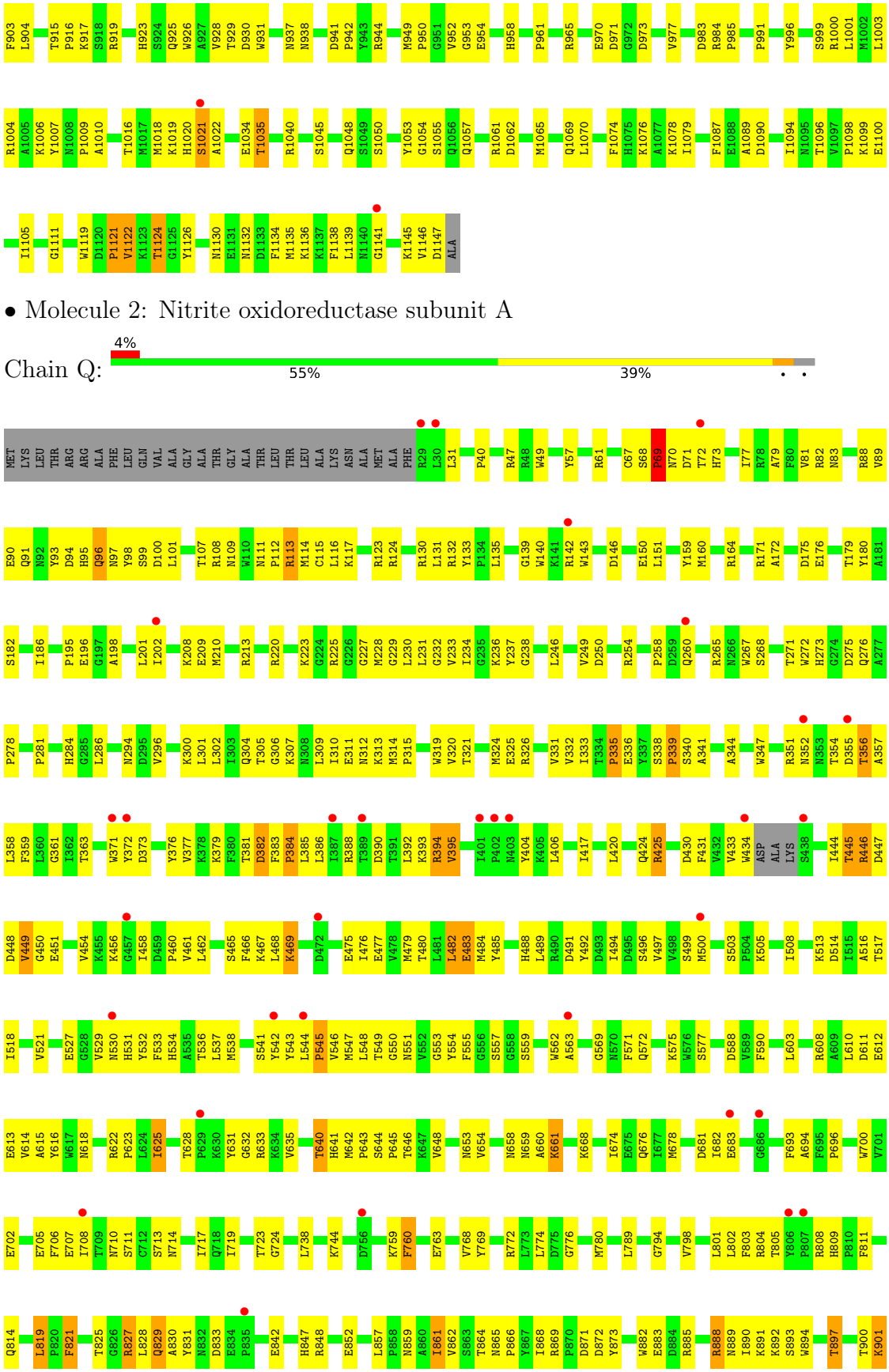




• Molecule 2: Nitrite oxidoreductase subunit A

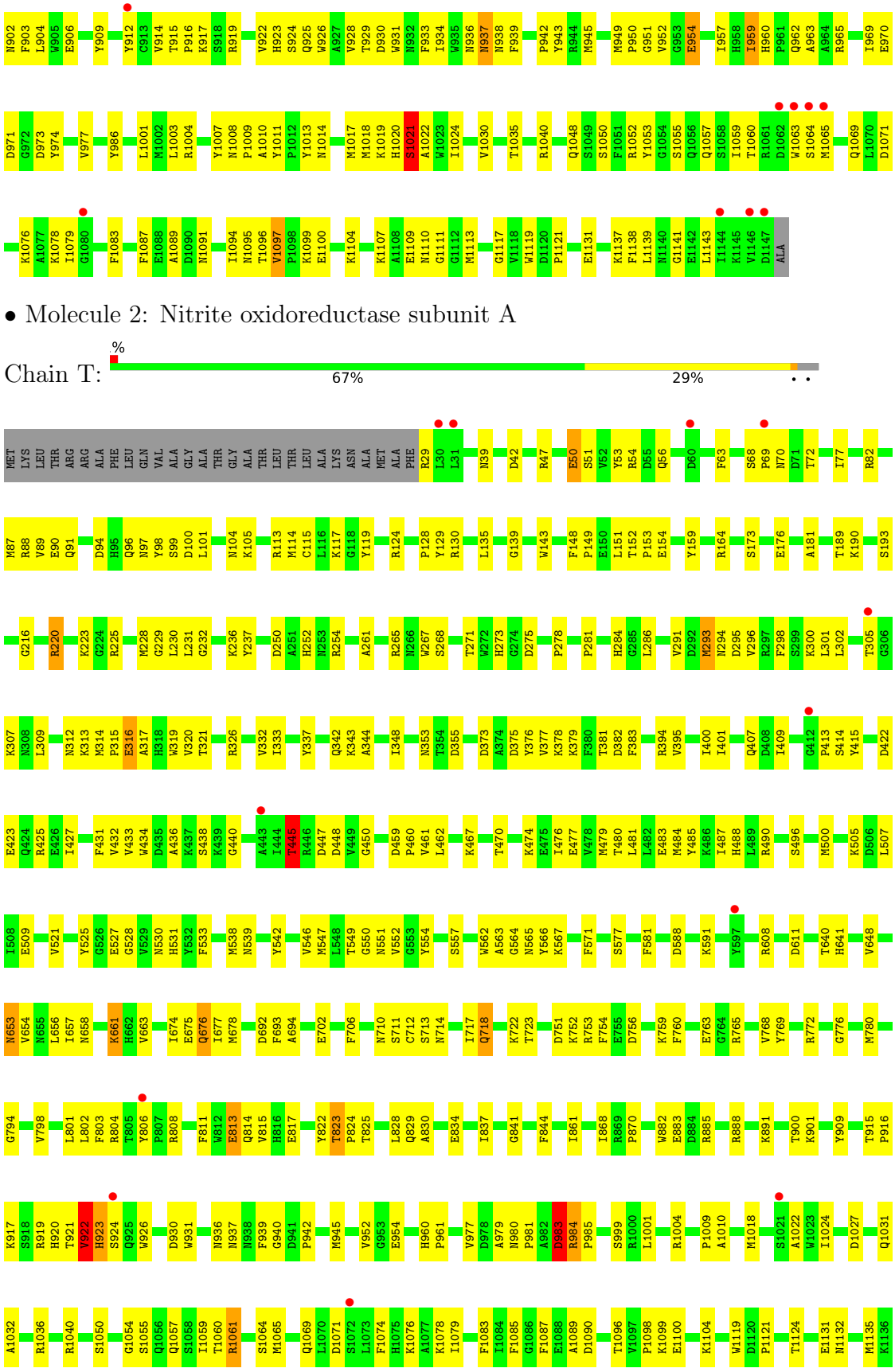
Chain N:





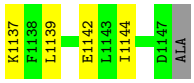
• Molecule 2: Nitrite oxidoreductase subunit A

Chain Q: 4% 55% 39%



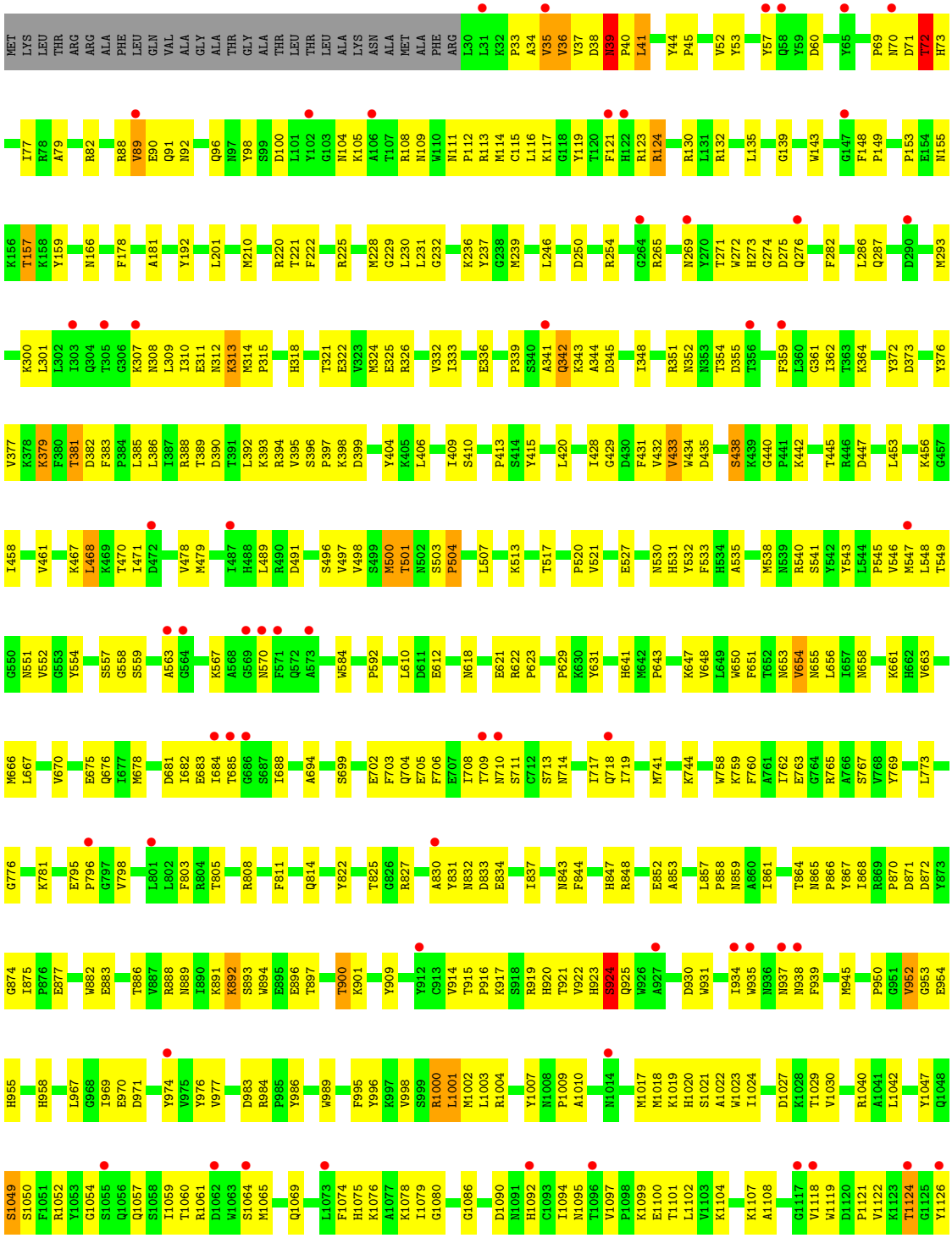
• Molecule 2: Nitrite oxidoreductase subunit A

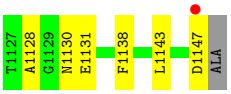
Chain T: % 67% 29% • •



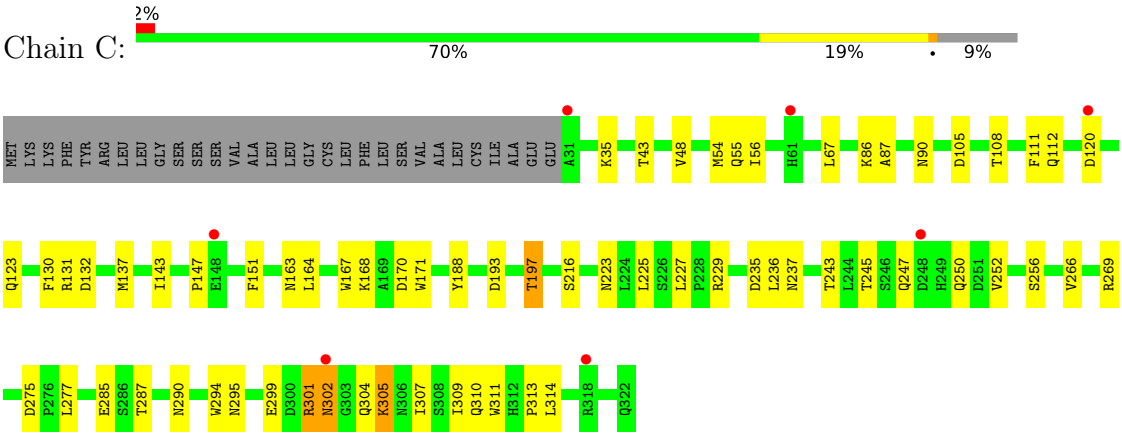
• Molecule 2: Nitrite oxidoreductase subunit A

Chain W:

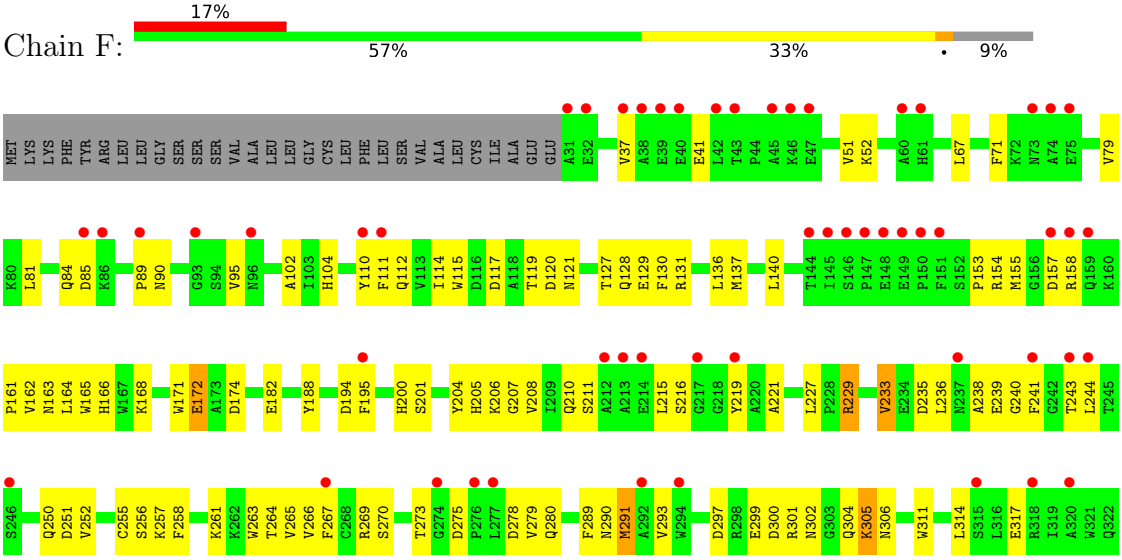




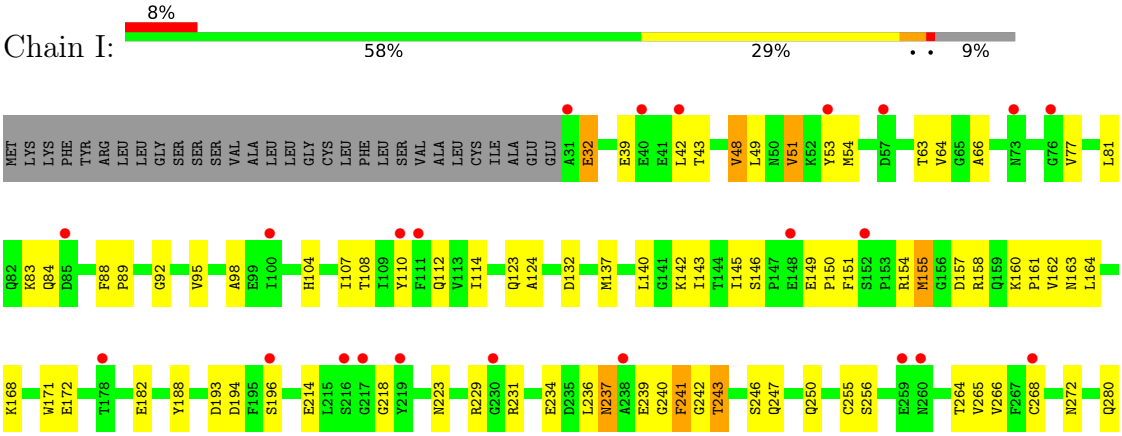
• Molecule 3: Nitrite oxidoreductase subunit C

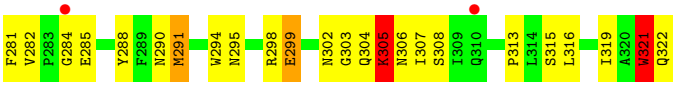


• Molecule 3: Nitrite oxidoreductase subunit C



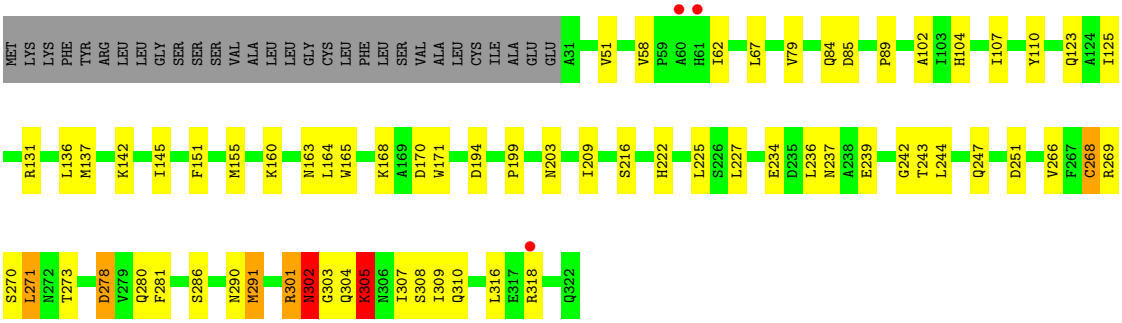
• Molecule 3: Nitrite oxidoreductase subunit C





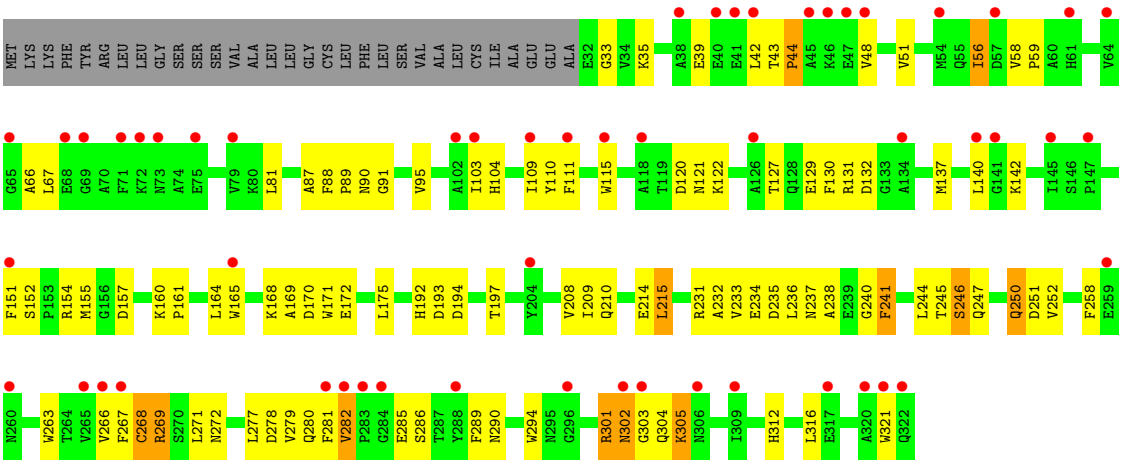
• Molecule 3: Nitrite oxidoreductase subunit C

Chain L:



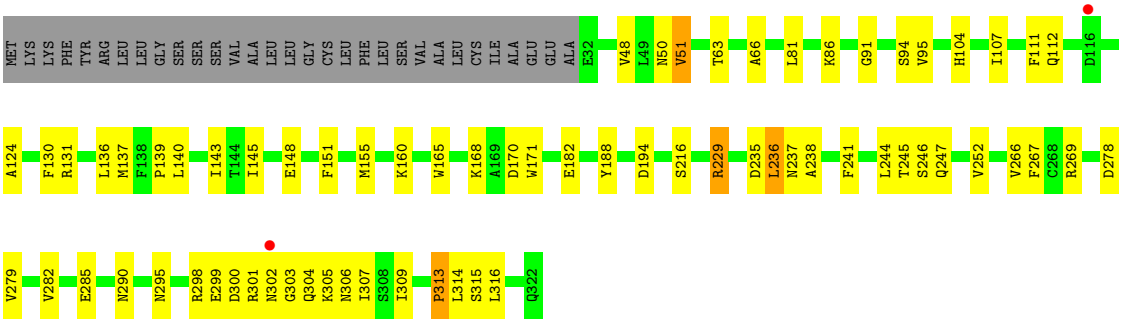
• Molecule 3: Nitrite oxidoreductase subunit C

Chain O:



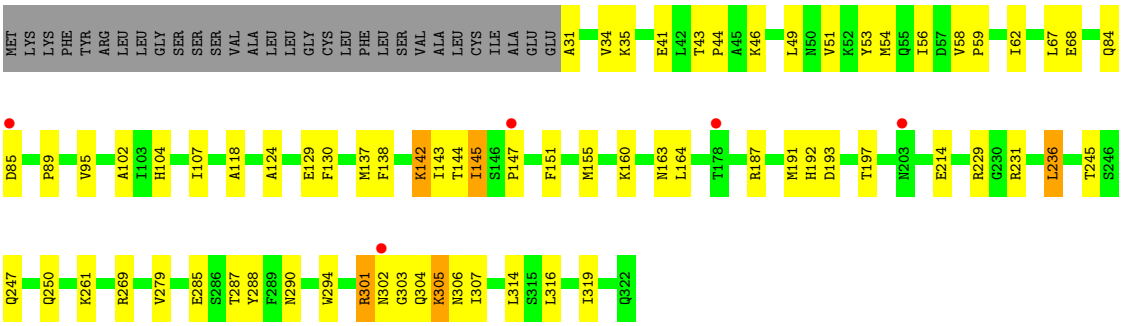
• Molecule 3: Nitrite oxidoreductase subunit C

Chain R:



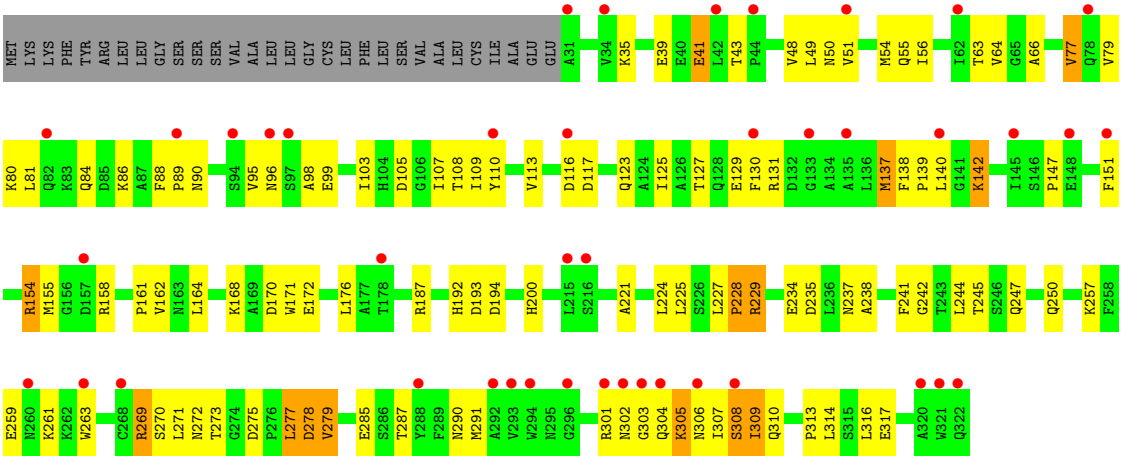
• Molecule 3: Nitrite oxidoreductase subunit C

Chain U:



- Molecule 3: Nitrite oxidoreductase subunit C

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	177.63Å 206.47Å 527.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	192.25 – 2.97 192.25 – 2.97	Depositor EDS
% Data completeness (in resolution range)	95.4 (192.25-2.97) 95.4 (192.25-2.97)	Depositor EDS
R_{merge}	0.43	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.96Å)	Xtriage
Refinement program	PHENIX v1.14rc1	Depositor
R, R_{free}	0.223 , 0.255 0.221 , 0.252	Depositor DCC
R_{free} test set	21282 reflections (3.21%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	115931	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: MO, HEM, CA, SF4, MD1, F3S

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	0.36	1/3450 (0.0%)	0.54	0/4676
1	D	0.39	2/2957 (0.1%)	0.53	1/4058 (0.0%)
1	G	0.24	0/3445	0.48	3/4670 (0.1%)
1	J	0.31	2/3462 (0.1%)	0.46	0/4690
1	M	0.32	0/3410	0.60	2/4632 (0.0%)
1	P	0.41	1/3422 (0.0%)	0.64	3/4646 (0.1%)
1	S	0.21	0/3434	0.44	0/4657
1	V	0.58	0/3339	0.90	8/4545 (0.2%)
2	B	0.47	2/9267 (0.0%)	0.66	2/12591 (0.0%)
2	E	0.52	1/7024 (0.0%)	0.89	19/9696 (0.2%)
2	H	0.41	7/9292 (0.1%)	0.62	9/12617 (0.1%)
2	K	0.47	6/9313 (0.1%)	0.62	11/12642 (0.1%)
2	N	0.42	2/9319 (0.0%)	0.62	8/12649 (0.1%)
2	Q	0.58	7/9165 (0.1%)	0.82	11/12465 (0.1%)
2	T	0.43	4/9298 (0.0%)	0.60	7/12625 (0.1%)
2	W	0.51	2/9187 (0.0%)	0.75	11/12501 (0.1%)
3	C	0.45	2/2338 (0.1%)	0.67	4/3175 (0.1%)
3	F	0.48	0/2123	0.81	0/2911
3	I	0.44	0/2272	0.81	7/3093 (0.2%)
3	L	0.57	2/2331 (0.1%)	0.67	2/3169 (0.1%)
3	O	0.54	1/2179 (0.0%)	0.86	4/2983 (0.1%)
3	R	0.50	1/2318 (0.0%)	0.61	2/3151 (0.1%)
3	U	0.44	0/2324	0.65	1/3158 (0.0%)
3	X	0.50	1/2282 (0.0%)	0.78	1/3104 (0.0%)
All	All	0.46	44/116951 (0.0%)	0.68	116/159104 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	H	0	1
2	K	0	2
2	W	0	3
All	All	0	7

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	663	VAL	C-N	23.28	1.68	1.33
2	K	148	PHE	C-O	-21.18	1.14	1.23
1	D	294	TYR	C-O	15.02	1.30	1.23
2	W	148	PHE	C-O	-12.71	1.18	1.23
2	T	981	PRO	C-O	-9.13	1.13	1.24

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	954	GLU	O-C-N	-22.56	95.87	123.17
3	I	305	LYS	CB-CA-C	12.96	137.23	110.40
2	E	663	VAL	CA-C-N	-12.86	98.64	121.14
2	E	663	VAL	C-N-CA	-12.86	98.64	121.14
2	N	1124	THR	CB-CA-C	-10.24	94.80	110.88

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	446	ARG	Sidechain
2	H	954	GLU	Mainchain
2	K	1021	SER	Mainchain
2	K	446	ARG	Sidechain
2	W	111	ASN	Peptide

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	3349	0	3216	93	0
1	D	2872	0	2267	153	0
1	G	3344	0	3208	93	0
1	J	3361	0	3242	89	0
1	M	3309	0	3136	157	0
1	P	3321	0	3149	122	0
1	S	3333	0	3198	94	0
1	V	3239	0	2948	268	0
2	B	9003	0	8576	375	0
2	E	6871	0	4598	326	0
2	H	9028	0	8644	262	0
2	K	9046	0	8683	310	0
2	N	9052	0	8682	323	0
2	Q	8902	0	8343	454	0
2	T	9034	0	8643	278	0
2	W	8920	0	8364	455	0
3	C	2281	0	2171	61	0
3	F	2068	0	1752	152	0
3	I	2216	0	2068	157	0
3	L	2274	0	2151	66	0
3	O	2124	0	1863	125	0
3	R	2261	0	2134	61	0
3	U	2267	0	2146	56	0
3	X	2225	0	2060	144	0
4	A	24	0	0	1	0
4	B	8	0	0	0	0
4	D	24	0	0	7	0
4	E	8	0	0	0	0
4	G	24	0	0	3	0
4	H	8	0	0	0	0
4	J	24	0	0	5	0
4	K	8	0	0	1	0
4	M	24	0	0	3	0
4	N	8	0	0	3	0
4	P	24	0	0	3	0
4	Q	8	0	0	3	0
4	S	24	0	0	3	0
4	T	8	0	0	3	0
4	V	24	0	0	6	0
4	W	8	0	0	2	0
5	A	7	0	0	0	0
5	D	7	0	0	3	0
5	G	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	7	0	0	0	0
5	M	7	0	0	2	0
5	P	7	0	0	0	0
5	S	7	0	0	0	0
5	V	7	0	0	5	0
6	B	94	0	43	14	0
6	E	94	0	41	19	0
6	H	94	0	42	14	0
6	K	94	0	43	18	0
6	N	94	0	43	19	0
6	Q	94	0	41	19	0
6	T	94	0	43	13	0
6	W	94	0	44	21	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
7	H	1	0	0	0	0
7	K	1	0	0	0	0
7	N	1	0	0	0	0
7	Q	1	0	0	0	0
7	T	1	0	0	0	0
7	W	1	0	0	0	0
8	C	43	0	30	8	0
8	F	43	0	30	24	0
8	I	43	0	30	29	0
8	L	43	0	30	7	0
8	O	43	0	30	10	0
8	R	43	0	30	5	0
8	U	43	0	30	4	0
8	X	43	0	30	15	0
9	C	2	0	0	0	0
9	F	2	0	0	0	0
9	I	2	0	0	0	0
9	L	2	0	0	0	0
9	O	2	0	0	0	0
9	R	2	0	0	0	0
9	U	2	0	0	0	0
9	X	2	0	0	1	0
10	A	37	0	0	0	0
10	B	72	0	0	7	0
10	C	35	0	0	1	0
10	D	6	0	0	0	0
10	E	13	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	F	8	0	0	0	0
10	G	25	0	0	1	0
10	H	83	0	0	2	0
10	I	20	0	0	1	0
10	J	28	0	0	2	0
10	K	74	0	0	3	0
10	L	30	0	0	0	0
10	M	10	0	0	0	0
10	N	76	0	0	5	0
10	O	17	0	0	3	0
10	P	16	0	0	4	0
10	Q	43	0	0	3	0
10	R	22	0	0	1	0
10	S	20	0	0	1	0
10	T	62	0	0	4	0
10	U	25	0	0	3	0
10	V	12	0	0	1	0
10	W	41	0	0	3	0
10	X	24	0	0	3	0
All	All	115931	0	105822	4322	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 20.

The worst 5 of 4322 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)
2:W:939:PHE:CE2	2:W:1004:ARG:CD	1.78	1.66
1:V:16:PRO:CG	1:V:128:TRP:CE2	1.81	1.62
2:W:939:PHE:CE2	2:W:1004:ARG:HD2	1.10	1.59
1:V:16:PRO:HG3	1:V:128:TRP:CZ2	0.98	1.50
1:V:241:ARG:HH12	1:V:257:ARG:CG	1.20	1.50

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	407/410 (99%)	403 (99%)	4 (1%)	0	100	100
1	D	406/410 (99%)	388 (96%)	18 (4%)	0	100	100
1	G	407/410 (99%)	399 (98%)	8 (2%)	0	100	100
1	J	407/410 (99%)	403 (99%)	4 (1%)	0	100	100
1	M	407/410 (99%)	401 (98%)	6 (2%)	0	100	100
1	P	407/410 (99%)	400 (98%)	7 (2%)	0	100	100
1	S	407/410 (99%)	400 (98%)	7 (2%)	0	100	100
1	V	407/410 (99%)	395 (97%)	12 (3%)	0	100	100
2	B	1119/1148 (98%)	1078 (96%)	41 (4%)	0	100	100
2	E	1104/1148 (96%)	1034 (94%)	68 (6%)	2 (0%)	43	73
2	H	1117/1148 (97%)	1073 (96%)	43 (4%)	1 (0%)	48	78
2	K	1118/1148 (97%)	1075 (96%)	43 (4%)	0	100	100
2	N	1118/1148 (97%)	1075 (96%)	43 (4%)	0	100	100
2	Q	1113/1148 (97%)	1071 (96%)	39 (4%)	3 (0%)	36	67
2	T	1117/1148 (97%)	1079 (97%)	38 (3%)	0	100	100
2	W	1117/1148 (97%)	1072 (96%)	44 (4%)	1 (0%)	48	78
3	C	291/322 (90%)	282 (97%)	9 (3%)	0	100	100
3	F	290/322 (90%)	278 (96%)	12 (4%)	0	100	100
3	I	290/322 (90%)	279 (96%)	11 (4%)	0	100	100
3	L	291/322 (90%)	288 (99%)	3 (1%)	0	100	100
3	O	289/322 (90%)	280 (97%)	9 (3%)	0	100	100
3	R	289/322 (90%)	279 (96%)	10 (4%)	0	100	100
3	U	290/322 (90%)	284 (98%)	6 (2%)	0	100	100
3	X	290/322 (90%)	279 (96%)	11 (4%)	0	100	100
All	All	14498/15040 (96%)	13995 (96%)	496 (3%)	7 (0%)	100	100

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	520	PRO
2	H	1021	SER
2	Q	69	PRO
2	Q	113	ARG
2	Q	1021	SER

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	359/365 (98%)	355 (99%)	4 (1%)	65	82
1	D	229/365 (63%)	228 (100%)	1 (0%)	84	90
1	G	356/365 (98%)	355 (100%)	1 (0%)	86	91
1	J	362/365 (99%)	360 (99%)	2 (1%)	78	88
1	M	348/365 (95%)	342 (98%)	6 (2%)	53	77
1	P	350/365 (96%)	340 (97%)	10 (3%)	37	68
1	S	355/365 (97%)	355 (100%)	0	100	100
1	V	324/365 (89%)	300 (93%)	24 (7%)	13	40
2	B	943/991 (95%)	914 (97%)	29 (3%)	35	66
2	E	373/991 (38%)	357 (96%)	16 (4%)	26	58
2	H	952/991 (96%)	943 (99%)	9 (1%)	70	85
2	K	956/991 (96%)	941 (98%)	15 (2%)	55	78
2	N	959/991 (97%)	945 (98%)	14 (2%)	57	79
2	Q	913/991 (92%)	879 (96%)	34 (4%)	30	62
2	T	953/991 (96%)	934 (98%)	19 (2%)	48	75
2	W	918/991 (93%)	884 (96%)	34 (4%)	30	62
3	C	238/265 (90%)	233 (98%)	5 (2%)	47	74
3	F	175/265 (66%)	168 (96%)	7 (4%)	28	60
3	I	220/265 (83%)	209 (95%)	11 (5%)	22	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	236/265 (89%)	228 (97%)	8 (3%)	32	64
3	O	196/265 (74%)	180 (92%)	16 (8%)	10	35
3	R	235/265 (89%)	228 (97%)	7 (3%)	36	67
3	U	235/265 (89%)	227 (97%)	8 (3%)	32	64
3	X	223/265 (84%)	205 (92%)	18 (8%)	11	36
All	All	11408/12968 (88%)	11110 (97%)	298 (3%)	40	70

5 of 298 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	146	GLU
3	X	142	LYS
1	V	241	ARG
2	W	438	SER
2	K	765	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	962	GLN
2	N	1057	GLN
1	V	176	ASN
3	L	90	ASN
1	M	296	GLN

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 88 ligands modelled in this entry, 24 are monoatomic - leaving 64 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	MD1	E	5801	6,7	43,51,51	5.52	27 (62%)	53,78,78	1.93	18 (33%)
4	SF4	V	503	1	0,12,12	-	-	-		
5	F3S	A	504	1	0,9,9	-	-	-		
4	SF4	P	501	1	0,12,12	-	-	-		
6	MD1	E	5802	6,7	43,51,51	5.83	26 (60%)	53,78,78	1.99	15 (28%)
4	SF4	A	501	1	0,12,12	-	-	-		
6	MD1	T	5802	7	43,51,51	5.81	26 (60%)	53,78,78	1.96	18 (33%)
4	SF4	S	502	1	0,12,12	-	-	-		
4	SF4	J	502	1	0,12,12	-	-	-		
4	SF4	E	5804	2	0,12,12	-	-	-		
6	MD1	W	5801	7	43,51,51	5.69	26 (60%)	53,78,78	1.89	14 (26%)
4	SF4	D	503	1	0,12,12	-	-	-		
6	MD1	N	5801	7	43,51,51	5.69	26 (60%)	53,78,78	1.90	16 (30%)
4	SF4	S	503	1	0,12,12	-	-	-		
5	F3S	V	504	1	0,9,9	-	-	-		
4	SF4	M	502	1	0,12,12	-	-	-		
6	MD1	W	5802	7	43,51,51	5.80	26 (60%)	53,78,78	1.97	17 (32%)
6	MD1	Q	5801	7	43,51,51	5.60	26 (60%)	53,78,78	1.97	16 (30%)
4	SF4	Q	5804	2	0,12,12	-	-	-		
6	MD1	B	5801	7	43,51,51	5.69	27 (62%)	53,78,78	1.88	16 (30%)
6	MD1	K	5801	7	43,51,51	5.70	26 (60%)	53,78,78	1.88	15 (28%)
4	SF4	V	501	1	0,12,12	-	-	-		
4	SF4	G	502	1	0,12,12	-	-	-		
4	SF4	J	503	1	0,12,12	-	-	-		
4	SF4	B	5804	2	0,12,12	-	-	-		
4	SF4	D	501	1	0,12,12	-	-	-		
4	SF4	K	5804	2	0,12,12	-	-	-		
4	SF4	G	503	1	0,12,12	-	-	-		
4	SF4	P	502	1	0,12,12	-	-	-		
5	F3S	D	504	1	0,9,9	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	HEM	I	401	3	50,50,50	2.33	22 (44%)	66,82,82	1.86	22 (33%)
8	HEM	U	401	3	50,50,50	1.49	8 (16%)	66,82,82	1.25	7 (10%)
8	HEM	X	401	3	50,50,50	1.57	7 (14%)	66,82,82	1.35	7 (10%)
5	F3S	S	504	1	0,9,9	-	-	-		
6	MD1	T	5801	7	43,51,51	5.72	26 (60%)	53,78,78	1.87	14 (26%)
5	F3S	J	504	1	0,9,9	-	-	-		
8	HEM	F	401	3	50,50,50	1.54	5 (10%)	66,82,82	1.36	11 (16%)
6	MD1	H	5802	7	43,51,51	5.77	26 (60%)	53,78,78	1.94	18 (33%)
4	SF4	A	503	1	0,12,12	-	-	-		
8	HEM	L	401	3	50,50,50	1.55	8 (16%)	66,82,82	1.34	7 (10%)
4	SF4	S	501	1	0,12,12	-	-	-		
4	SF4	A	502	1	0,12,12	-	-	-		
4	SF4	T	5804	2	0,12,12	-	-	-		
6	MD1	N	5802	7	43,51,51	5.79	26 (60%)	53,78,78	1.95	18 (33%)
6	MD1	B	5802	7	43,51,51	5.78	26 (60%)	53,78,78	1.97	18 (33%)
6	MD1	Q	5802	7	43,51,51	5.78	26 (60%)	53,78,78	1.99	18 (33%)
4	SF4	P	503	1	0,12,12	-	-	-		
6	MD1	K	5802	7	43,51,51	5.79	26 (60%)	53,78,78	1.95	19 (35%)
6	MD1	H	5801	7	43,51,51	5.72	26 (60%)	53,78,78	1.89	15 (28%)
5	F3S	G	504	1	0,9,9	-	-	-		
5	F3S	P	504	1	0,9,9	-	-	-		
8	HEM	R	401	3	50,50,50	1.60	8 (16%)	66,82,82	1.27	7 (10%)
5	F3S	M	504	1	0,9,9	-	-	-		
4	SF4	J	501	1	0,12,12	-	-	-		
4	SF4	H	5804	2	0,12,12	-	-	-		
4	SF4	N	5804	2	0,12,12	-	-	-		
4	SF4	V	502	1	0,12,12	-	-	-		
4	SF4	D	502	1	0,12,12	-	-	-		
4	SF4	M	503	1	0,12,12	-	-	-		
8	HEM	C	401	3	50,50,50	1.82	5 (10%)	66,82,82	1.39	8 (12%)
4	SF4	M	501	1	0,12,12	-	-	-		
4	SF4	W	5804	2	0,12,12	-	-	-		
8	HEM	O	401	3	50,50,50	1.62	7 (14%)	66,82,82	1.25	6 (9%)
4	SF4	G	501	1	0,12,12	-	-	-		

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
6	MD1	E	5801	6,7	1/1/10/12	9/22/59/59	0/5/5/5
4	SF4	V	503	1	-	-	0/6/5/5
5	F3S	A	504	1	-	-	0/3/3/3
4	SF4	P	501	1	-	-	0/6/5/5
6	MD1	E	5802	6,7	-	5/22/59/59	0/5/5/5
4	SF4	A	501	1	-	-	0/6/5/5
6	MD1	T	5802	7	-	4/22/59/59	0/5/5/5
4	SF4	S	502	1	-	-	0/6/5/5
4	SF4	J	502	1	-	-	0/6/5/5
4	SF4	E	5804	2	-	-	0/6/5/5
6	MD1	W	5801	7	-	11/22/59/59	0/5/5/5
4	SF4	D	503	1	-	-	0/6/5/5
6	MD1	N	5801	7	-	12/22/59/59	0/5/5/5
4	SF4	S	503	1	-	-	0/6/5/5
5	F3S	V	504	1	-	-	0/3/3/3
6	MD1	W	5802	7	-	8/22/59/59	0/5/5/5
4	SF4	M	502	1	-	-	0/6/5/5
6	MD1	Q	5801	7	-	11/22/59/59	0/5/5/5
4	SF4	Q	5804	2	-	-	0/6/5/5
6	MD1	B	5801	7	-	11/22/59/59	0/5/5/5
6	MD1	K	5801	7	-	11/22/59/59	0/5/5/5
4	SF4	V	501	1	-	-	0/6/5/5
4	SF4	G	502	1	-	-	0/6/5/5
4	SF4	B	5804	2	-	-	0/6/5/5
4	SF4	J	503	1	-	-	0/6/5/5
4	SF4	D	501	1	-	-	0/6/5/5
4	SF4	K	5804	2	-	-	0/6/5/5
4	SF4	G	503	1	-	-	0/6/5/5
4	SF4	P	502	1	-	-	0/6/5/5
5	F3S	D	504	1	-	-	0/3/3/3
8	HEM	I	401	3	-	7/14/54/54	-
8	HEM	U	401	3	-	6/14/54/54	-
8	HEM	X	401	3	-	4/14/54/54	-
5	F3S	S	504	1	-	-	0/3/3/3
6	MD1	T	5801	7	-	11/22/59/59	0/5/5/5
5	F3S	J	504	1	-	-	0/3/3/3
8	HEM	F	401	3	-	6/14/54/54	-
6	MD1	H	5802	7	-	5/22/59/59	0/5/5/5
4	SF4	A	503	1	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HEM	L	401	3	-	3/14/54/54	-
4	SF4	S	501	1	-	-	0/6/5/5
6	MD1	N	5802	7	-	5/22/59/59	0/5/5/5
4	SF4	A	502	1	-	-	0/6/5/5
6	MD1	Q	5802	7	-	9/22/59/59	0/5/5/5
6	MD1	B	5802	7	-	5/22/59/59	0/5/5/5
4	SF4	T	5804	2	-	-	0/6/5/5
4	SF4	P	503	1	-	-	0/6/5/5
6	MD1	K	5802	7	-	5/22/59/59	0/5/5/5
6	MD1	H	5801	7	-	12/22/59/59	0/5/5/5
5	F3S	G	504	1	-	-	0/3/3/3
8	HEM	R	401	3	-	6/14/54/54	-
5	F3S	P	504	1	-	-	0/3/3/3
5	F3S	M	504	1	-	-	0/3/3/3
4	SF4	J	501	1	-	-	0/6/5/5
4	SF4	H	5804	2	-	-	0/6/5/5
4	SF4	N	5804	2	-	-	0/6/5/5
4	SF4	V	502	1	-	-	0/6/5/5
4	SF4	D	502	1	-	-	0/6/5/5
4	SF4	M	503	1	-	-	0/6/5/5
8	HEM	C	401	3	-	6/14/54/54	-
4	SF4	M	501	1	-	-	0/6/5/5
4	SF4	W	5804	2	-	-	0/6/5/5
8	HEM	O	401	3	-	4/14/54/54	-
4	SF4	G	501	1	-	-	0/6/5/5

The worst 5 of 488 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	5802	MD1	C7-N8	25.57	1.61	1.28
6	T	5802	MD1	C7-N8	25.30	1.61	1.28
6	K	5802	MD1	C7-N8	25.27	1.61	1.28
6	W	5802	MD1	C7-N8	25.15	1.61	1.28
6	N	5802	MD1	C7-N8	25.13	1.61	1.28

The worst 5 of 340 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	5802	MD1	C5-C4-N3	-5.28	119.90	128.46
6	Q	5801	MD1	C5-C4-N3	-5.17	120.07	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	W	5802	MD1	C5-C4-N3	-5.13	120.13	128.46
6	N	5802	MD1	C5-C4-N3	-5.12	120.15	128.46
6	T	5802	MD1	C5-C4-N3	-5.11	120.18	128.46

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	E	5801	MD1	C14

5 of 176 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	5801	MD1	C10-O3A-PB-O3B
6	B	5801	MD1	O3A-C10-C11-O11
6	B	5801	MD1	O3A-C10-C11-C12
6	B	5801	MD1	C3'-C4'-C5'-O5'
6	E	5801	MD1	O3A-C10-C11-O11

There are no ring outliers.

48 monomers are involved in 292 short contacts:

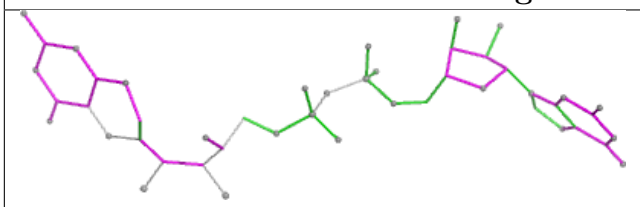
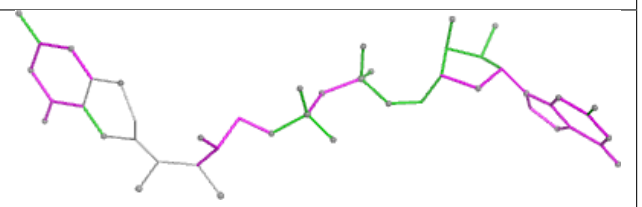
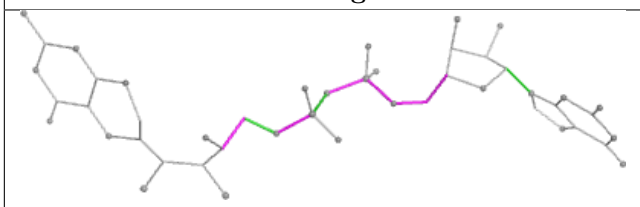
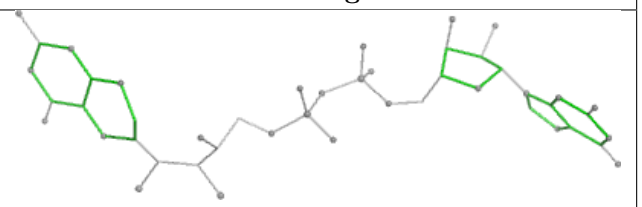
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	5801	MD1	14	0
4	V	503	SF4	3	0
6	E	5802	MD1	5	0
6	T	5802	MD1	5	0
6	W	5801	MD1	13	0
4	D	503	SF4	1	0
6	N	5801	MD1	10	0
4	S	503	SF4	2	0
5	V	504	F3S	5	0
6	W	5802	MD1	8	0
6	Q	5801	MD1	12	0
4	Q	5804	SF4	3	0
6	B	5801	MD1	8	0
6	K	5801	MD1	11	0
4	V	501	SF4	2	0
4	J	503	SF4	4	0
4	D	501	SF4	4	0
4	K	5804	SF4	1	0
4	G	503	SF4	2	0
5	D	504	F3S	3	0

Continued on next page...

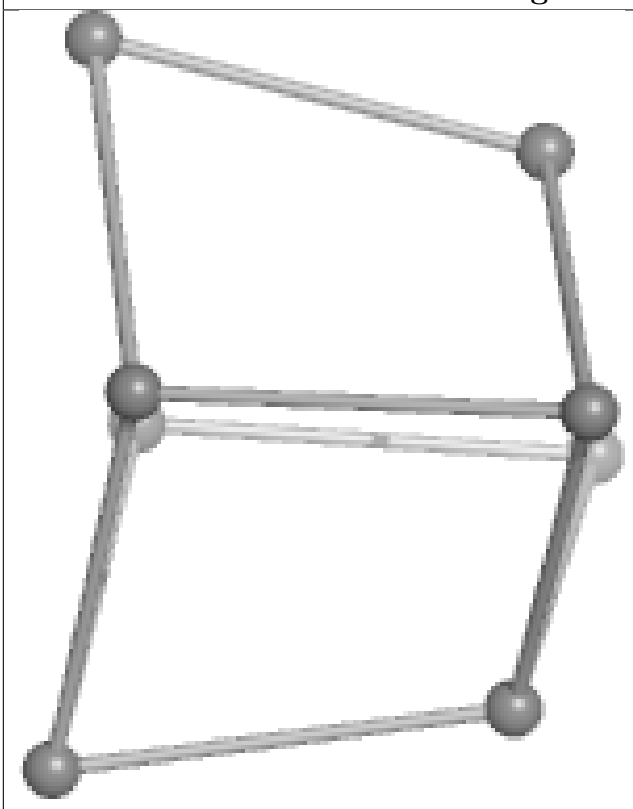
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	401	HEM	29	0
8	U	401	HEM	4	0
8	X	401	HEM	15	0
6	T	5801	MD1	8	0
8	F	401	HEM	24	0
6	H	5802	MD1	8	0
4	A	503	SF4	1	0
8	L	401	HEM	7	0
4	S	501	SF4	1	0
4	T	5804	SF4	3	0
6	N	5802	MD1	9	0
6	B	5802	MD1	6	0
6	Q	5802	MD1	7	0
4	P	503	SF4	3	0
6	K	5802	MD1	7	0
6	H	5801	MD1	6	0
8	R	401	HEM	5	0
5	M	504	F3S	2	0
4	J	501	SF4	1	0
4	N	5804	SF4	3	0
4	V	502	SF4	1	0
4	D	502	SF4	2	0
4	M	503	SF4	2	0
8	C	401	HEM	8	0
4	M	501	SF4	1	0
4	W	5804	SF4	2	0
8	O	401	HEM	10	0
4	G	501	SF4	1	0

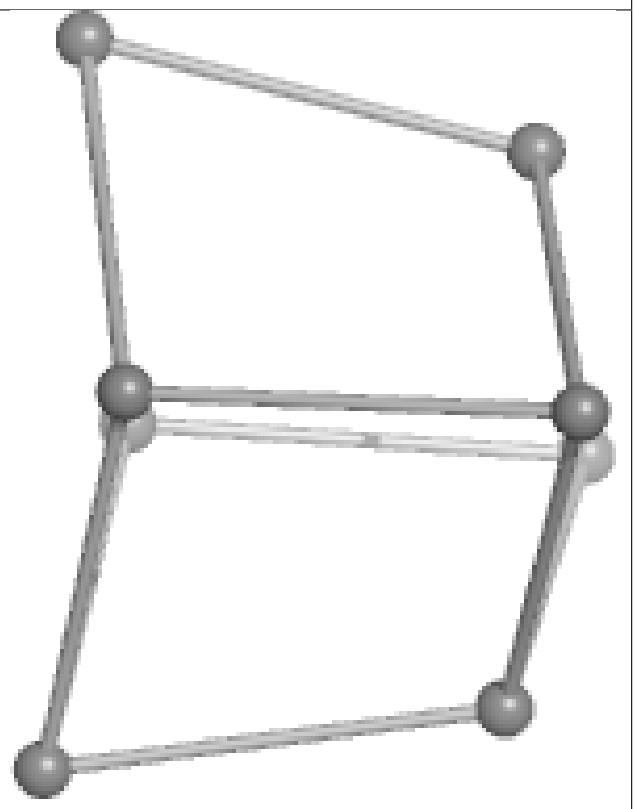
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 MD1 E 5801	
 Bond lengths	 Bond angles
 Torsions	 Rings

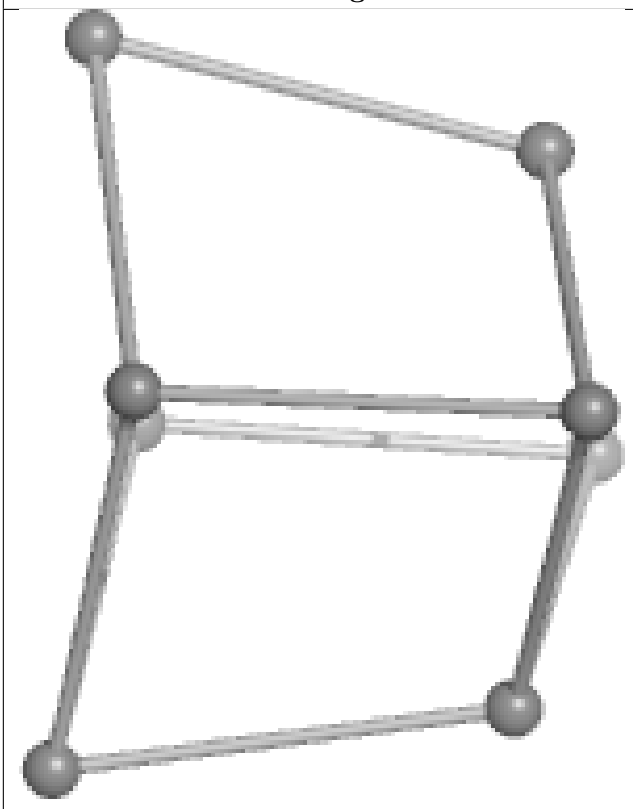
Ligand SF4 V 503



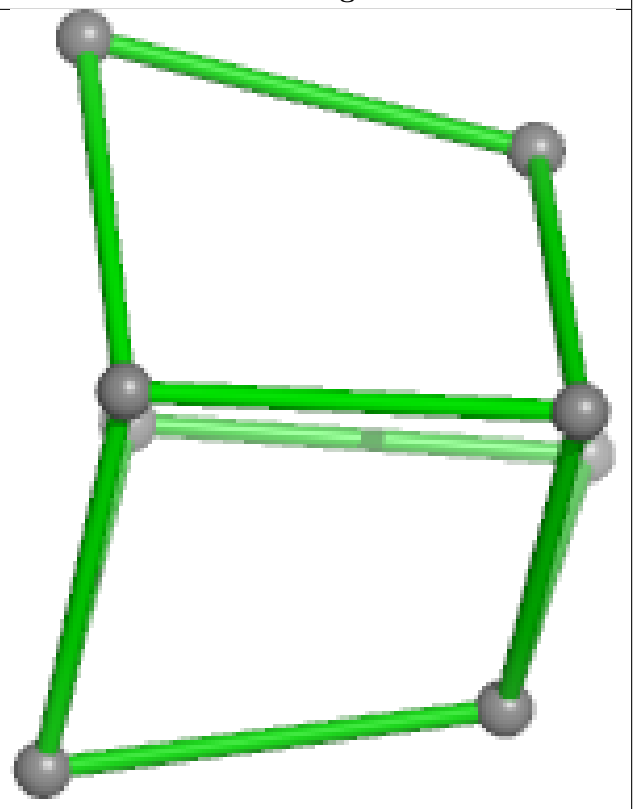
Bond lengths



Bond angles

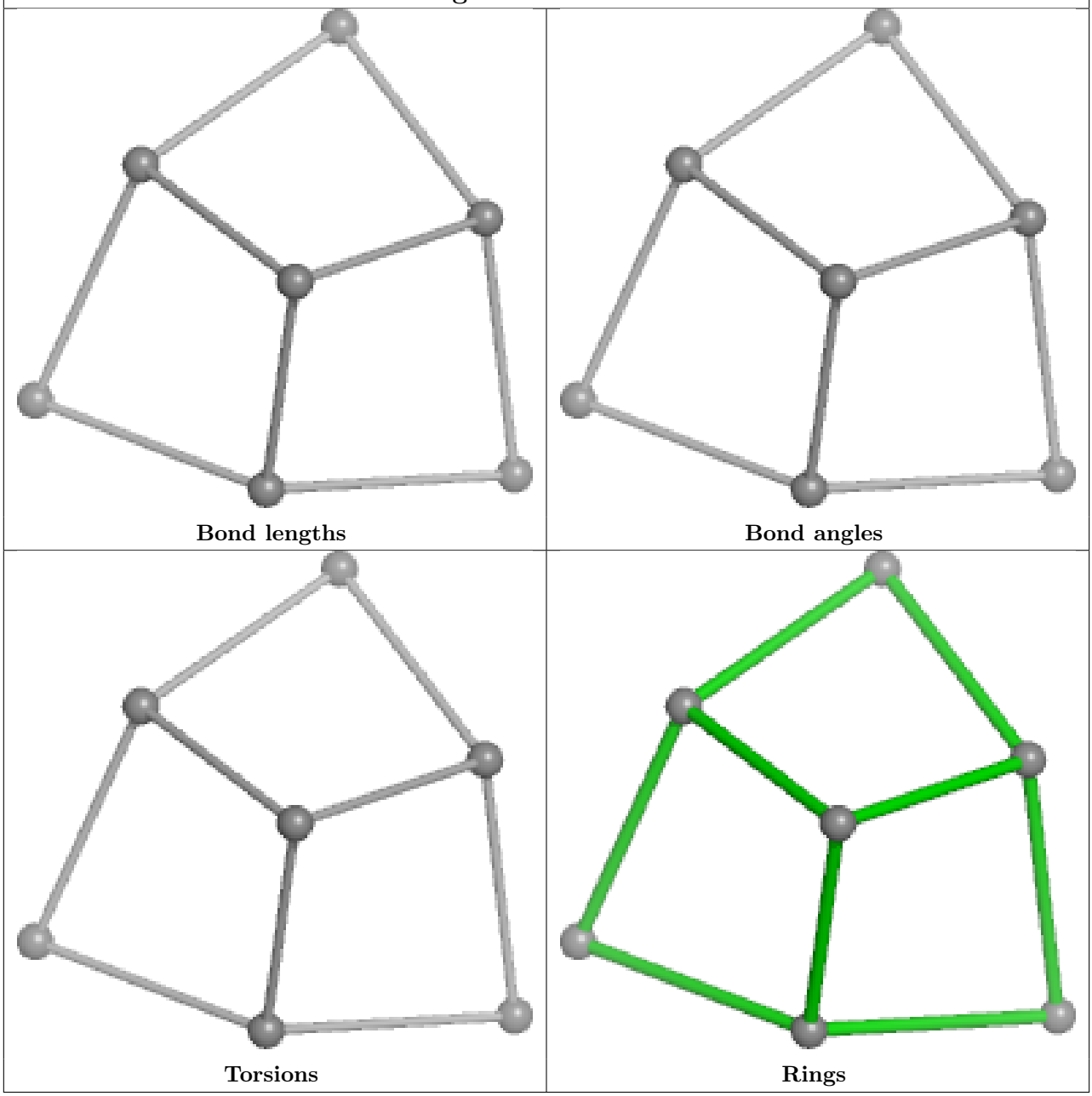


Torsions

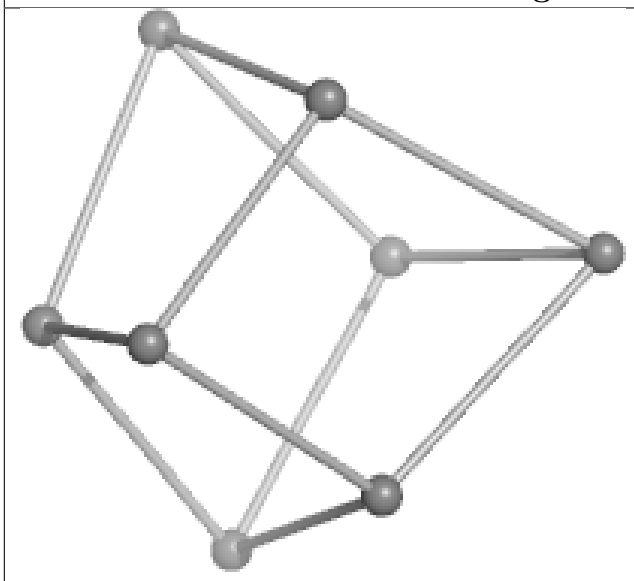


Rings

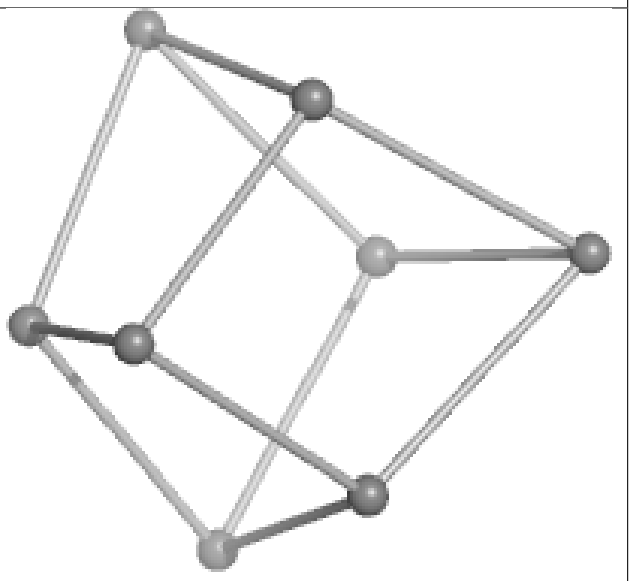
Ligand F3S A 504



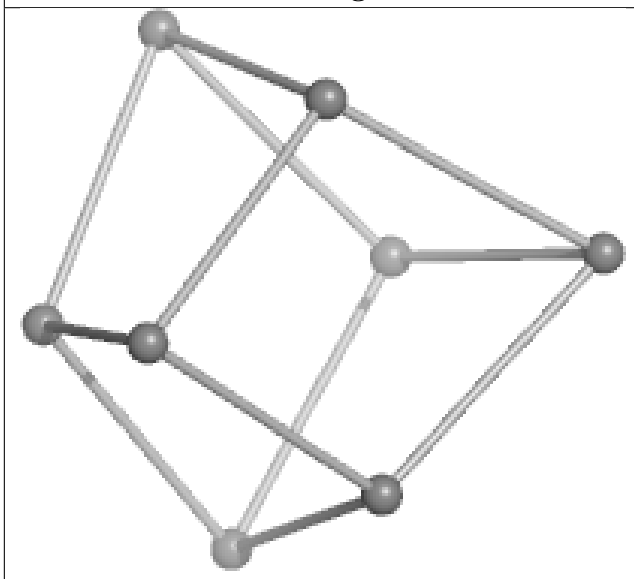
Ligand SF4 P 501



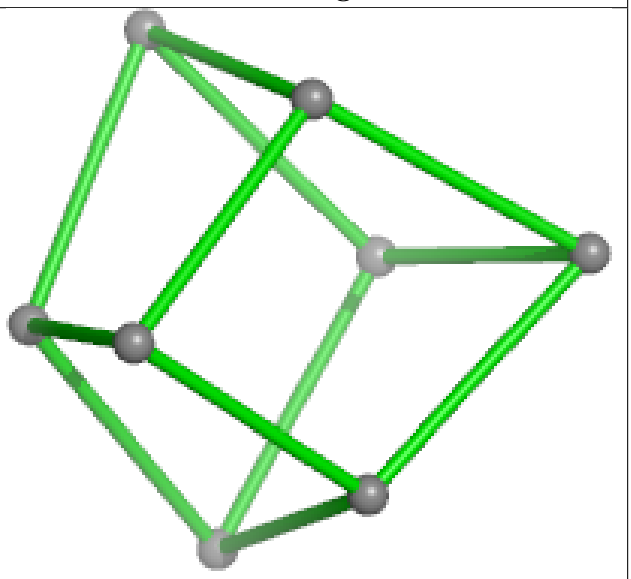
Bond lengths



Bond angles

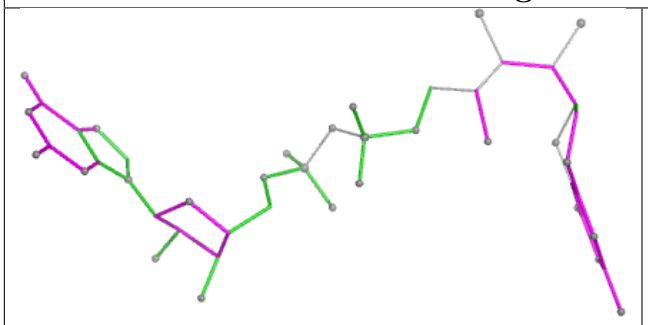


Torsions

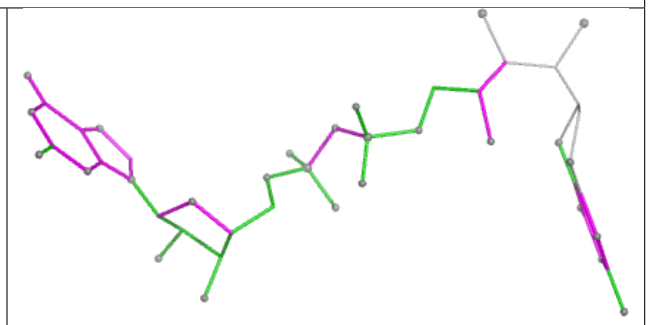


Rings

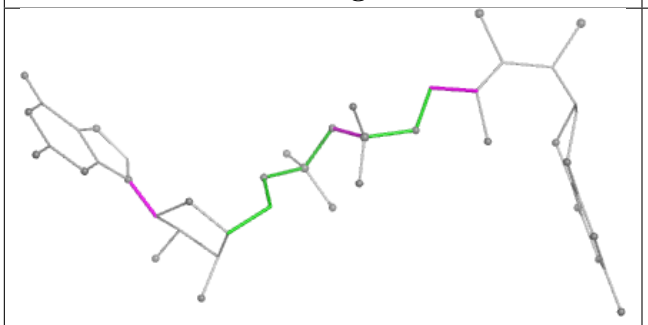
Ligand MD1 E 5802



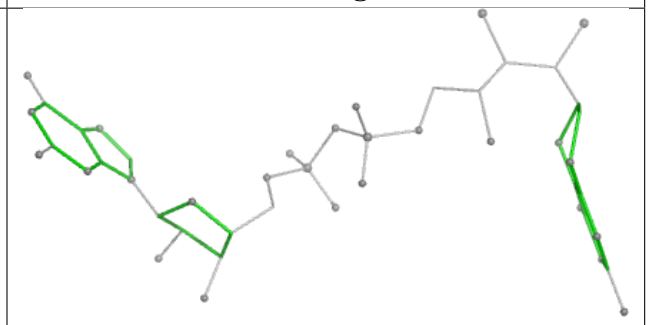
Bond lengths



Bond angles

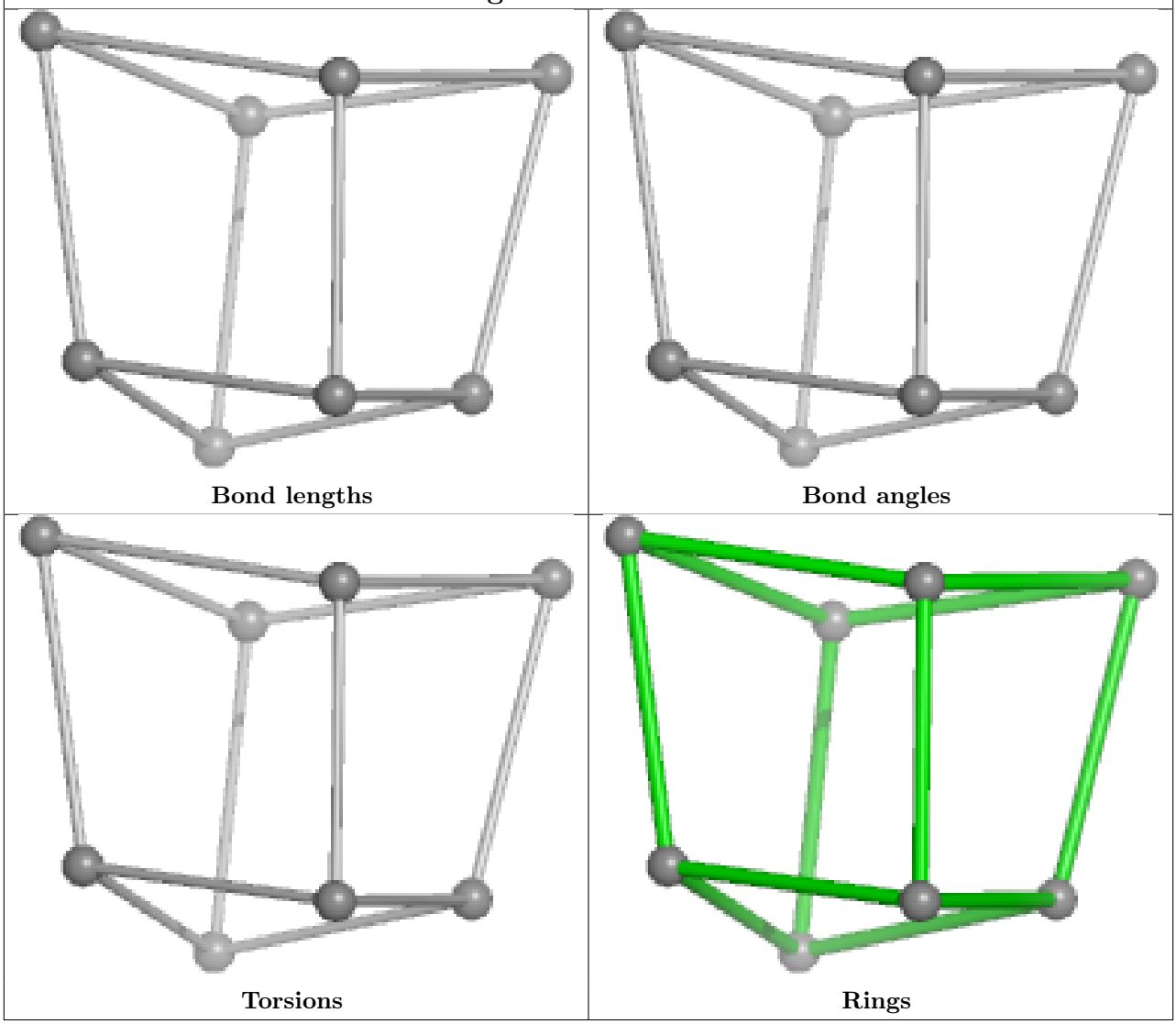


Torsions

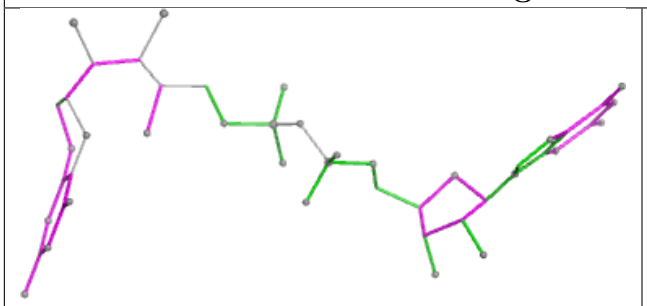


Rings

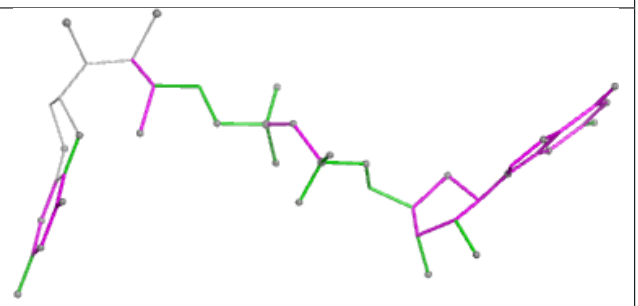
Ligand SF4 A 501



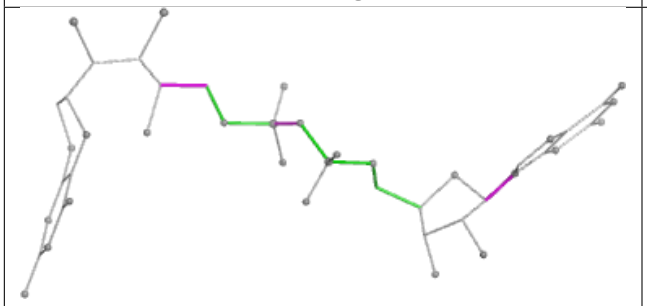
Ligand MD1 T 5802



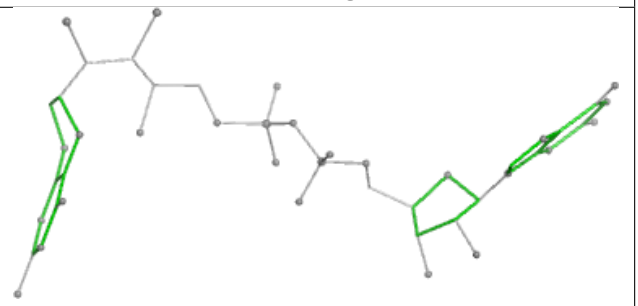
Bond lengths



Bond angles

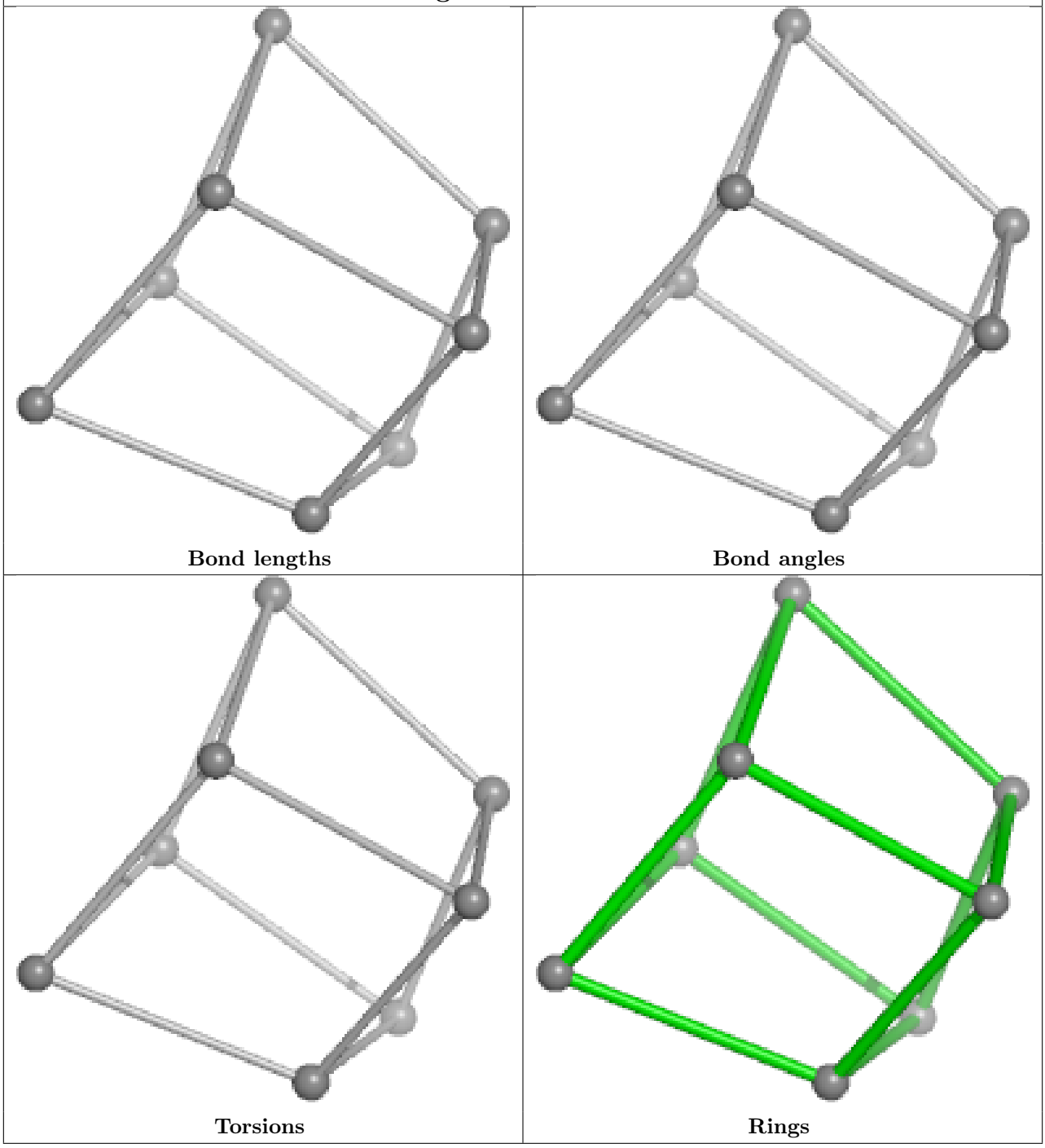


Torsions

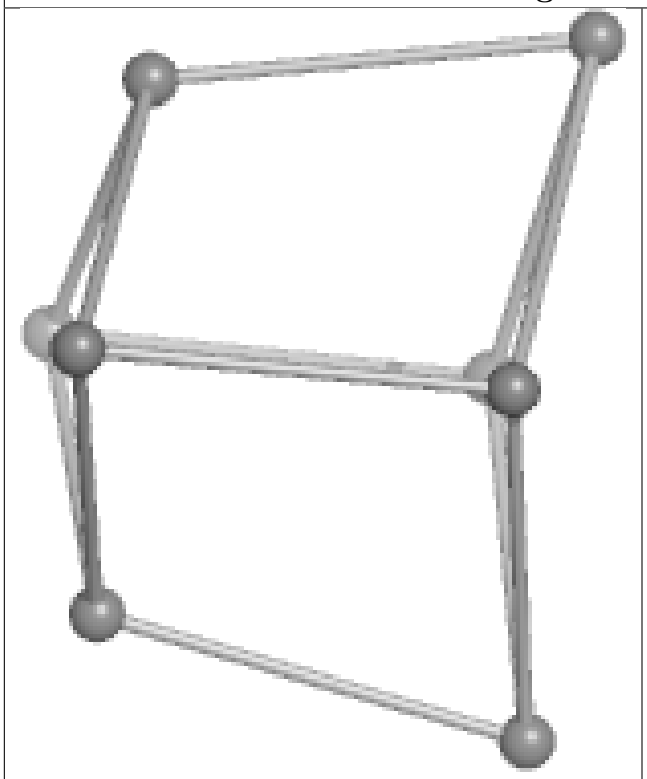


Rings

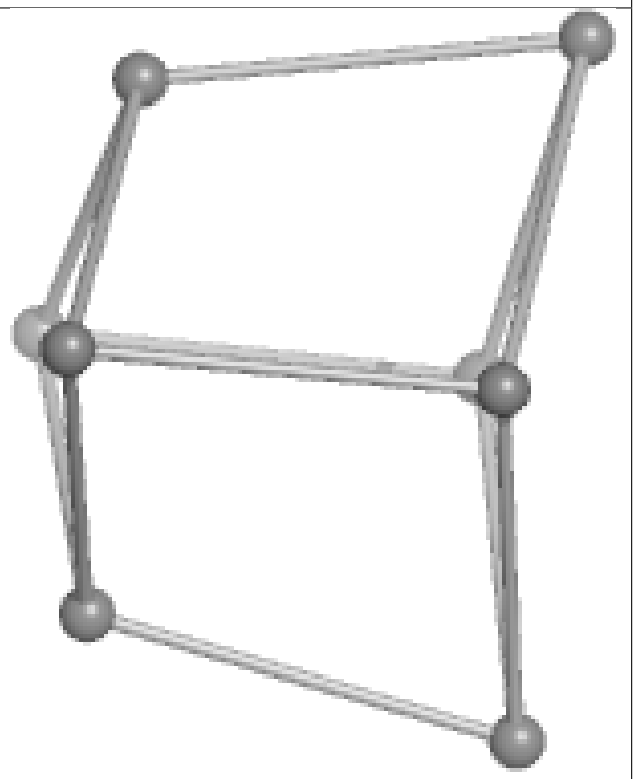
Ligand SF4 S 502



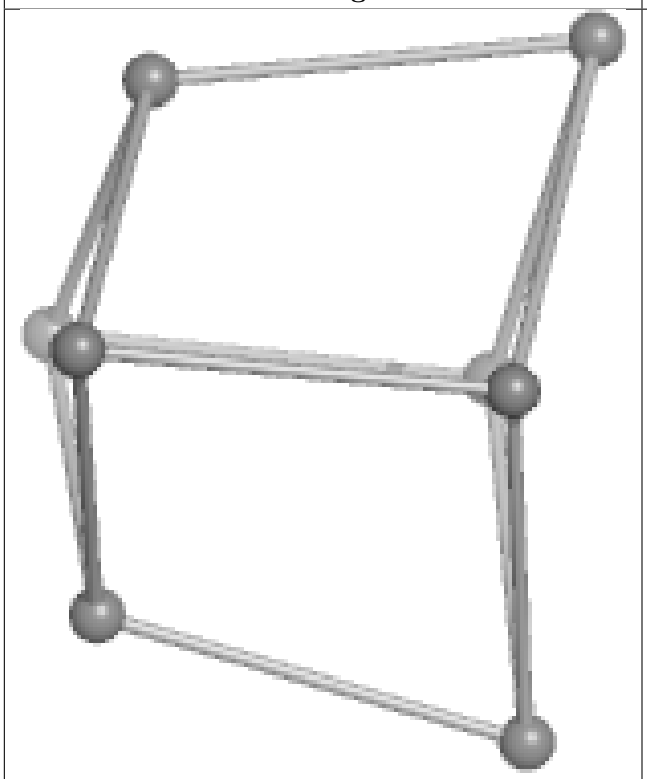
Ligand SF4 J 502



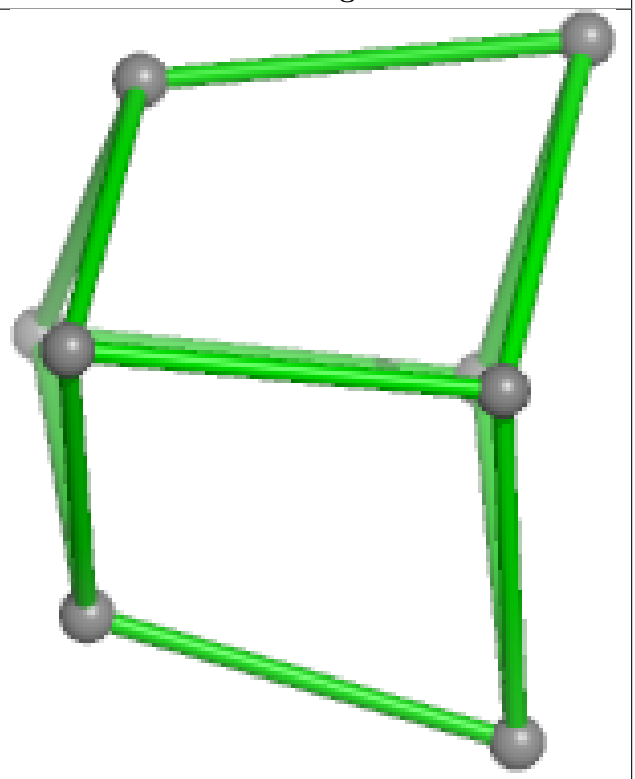
Bond lengths



Bond angles

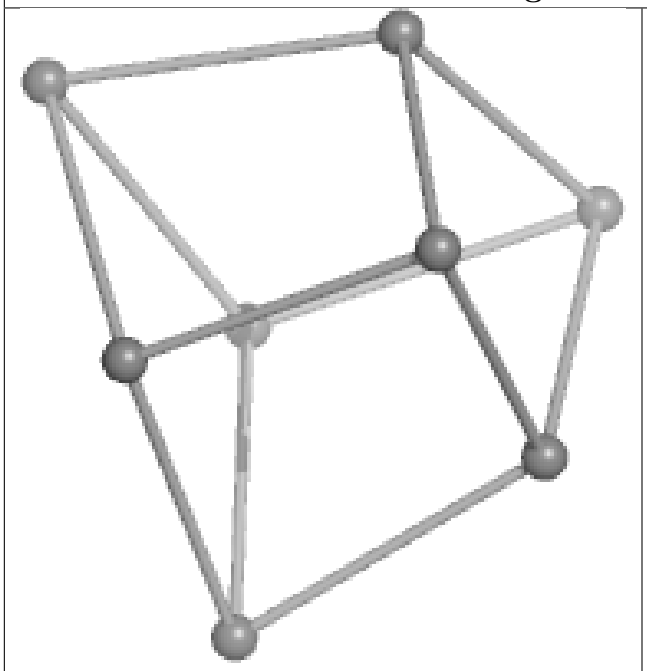


Torsions

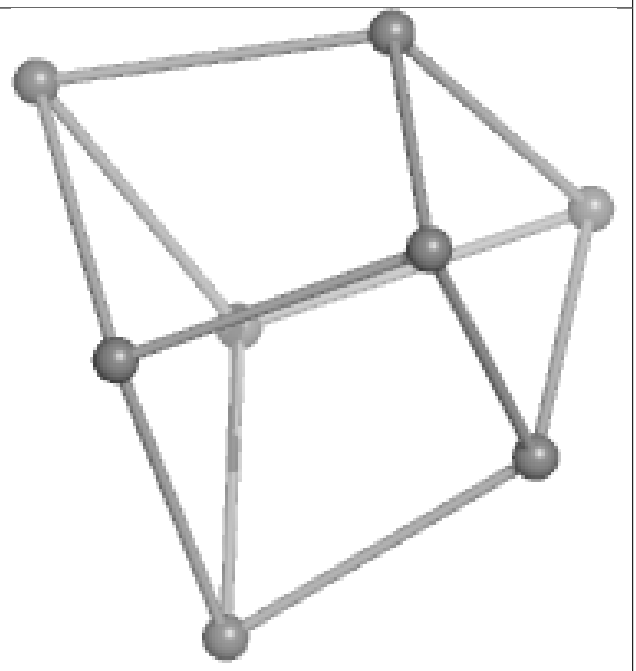


Rings

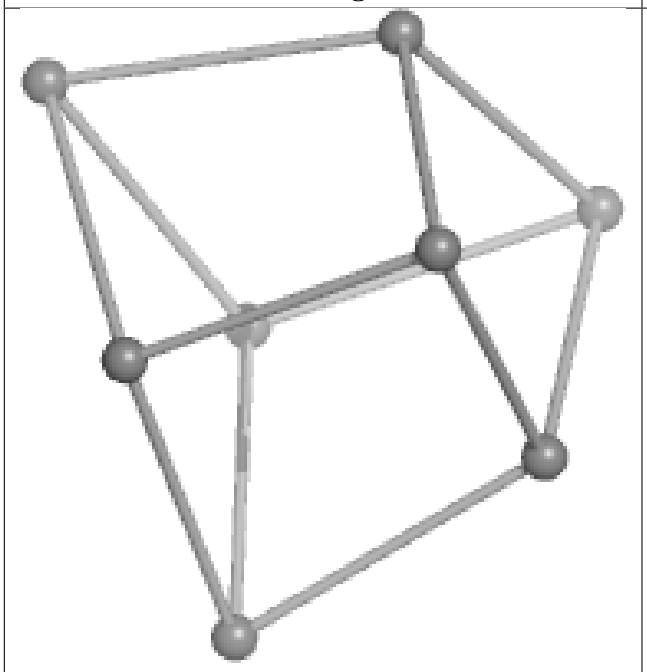
Ligand SF4 E 5804



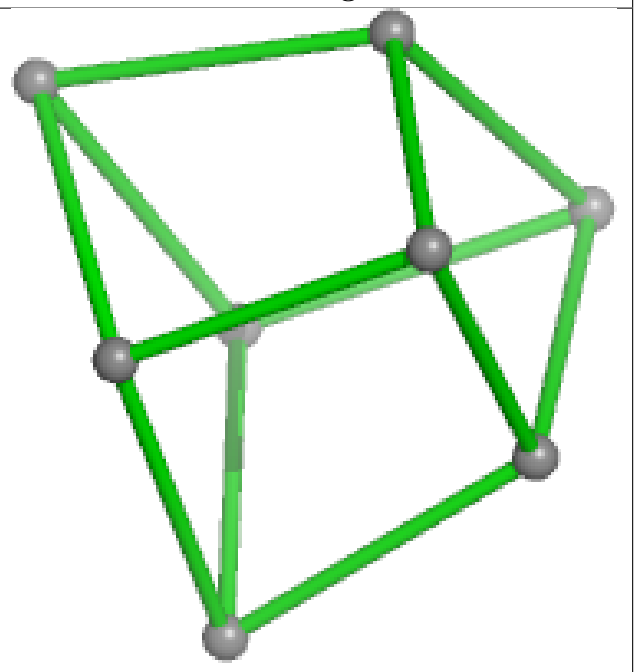
Bond lengths



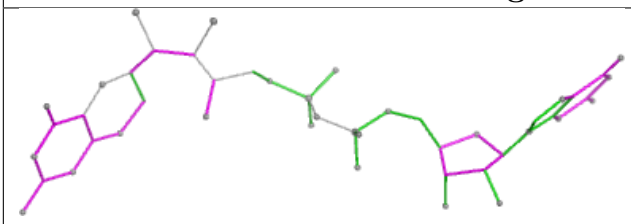
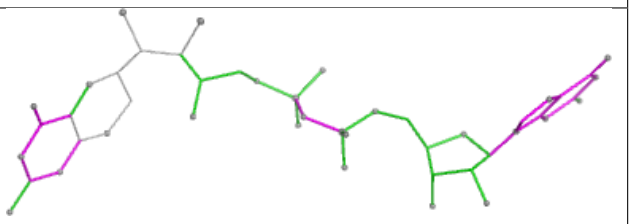
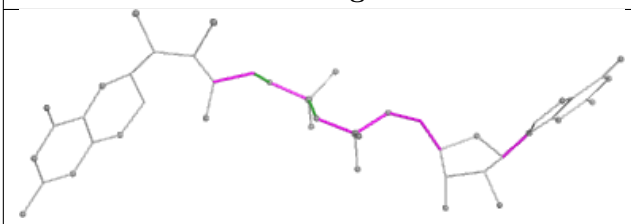
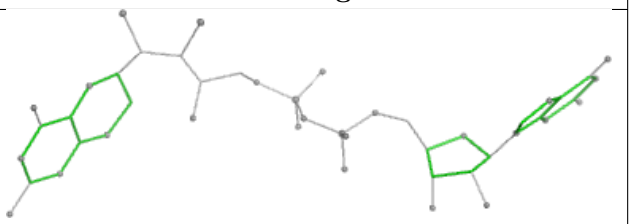
Bond angles



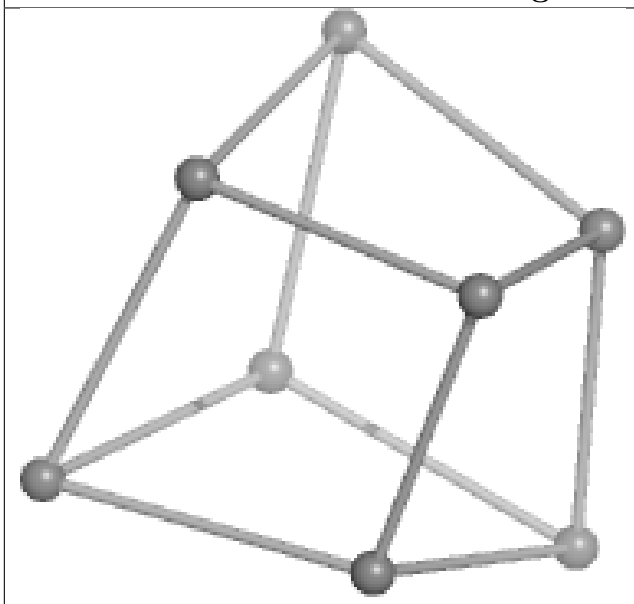
Torsions



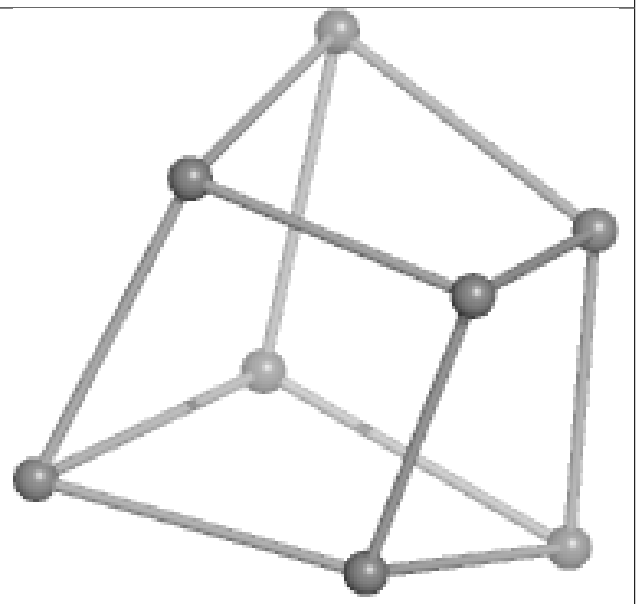
Rings

Ligand MD1 W 5801	
 Bond lengths	 Bond angles
 Torsions	 Rings

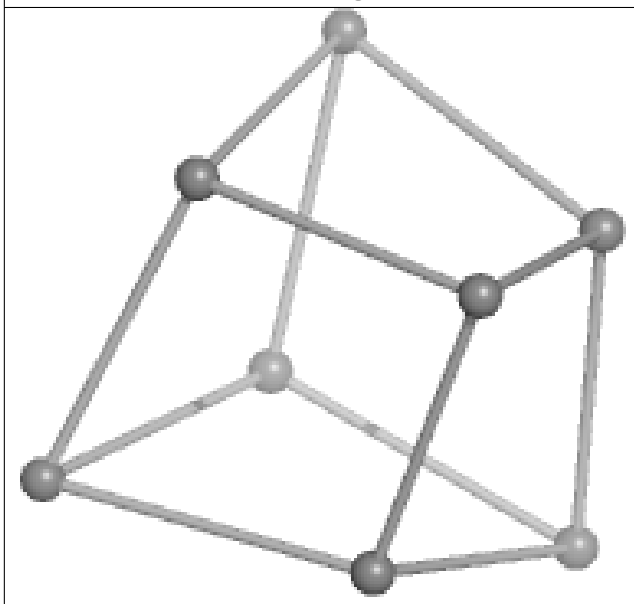
Ligand SF4 D 503



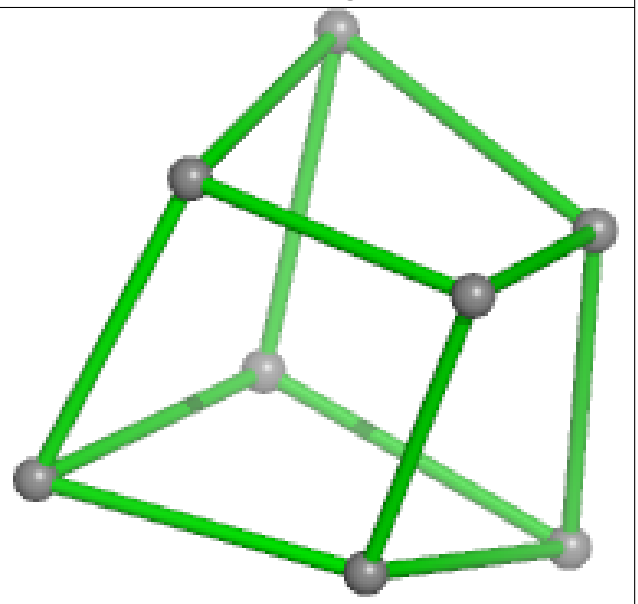
Bond lengths



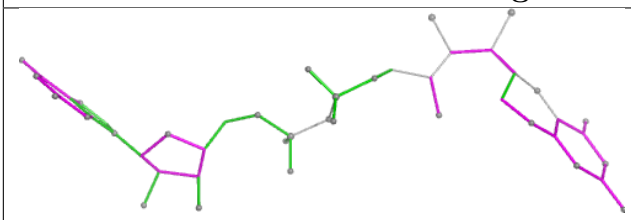
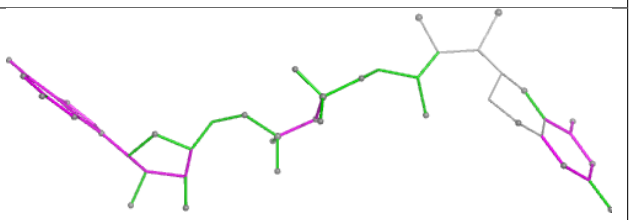
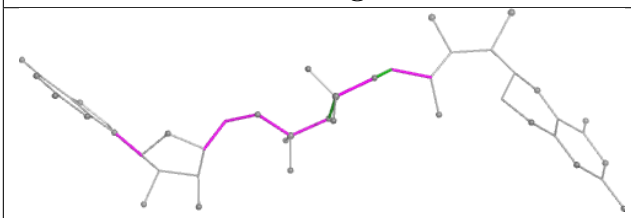
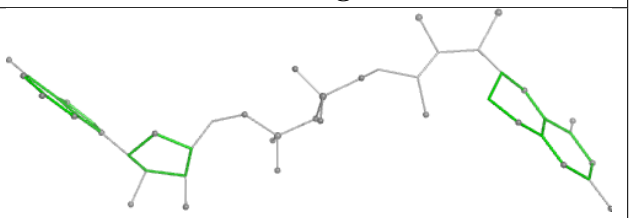
Bond angles



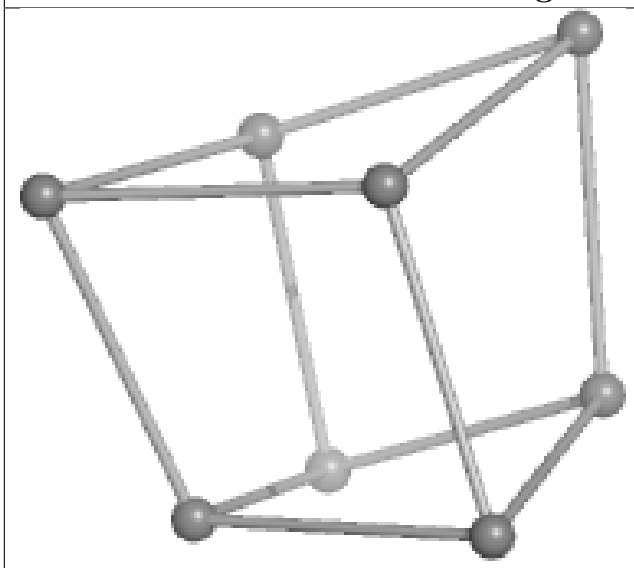
Torsions



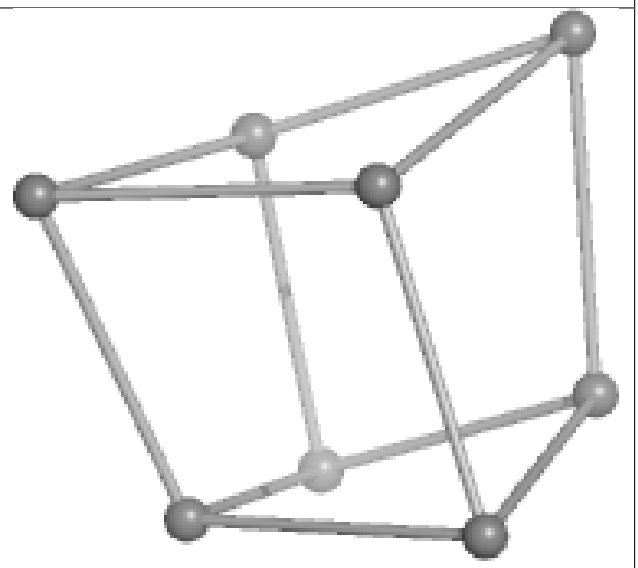
Rings

Ligand MD1 N 5801	
 Bond lengths	 Bond angles
 Torsions	 Rings

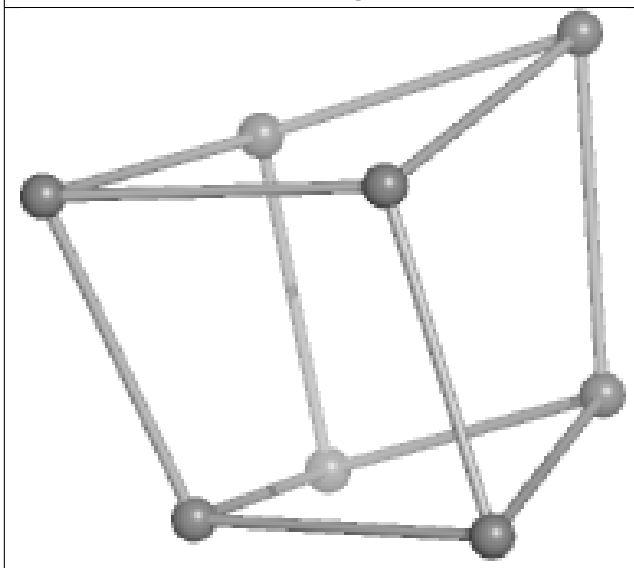
Ligand SF4 S 503



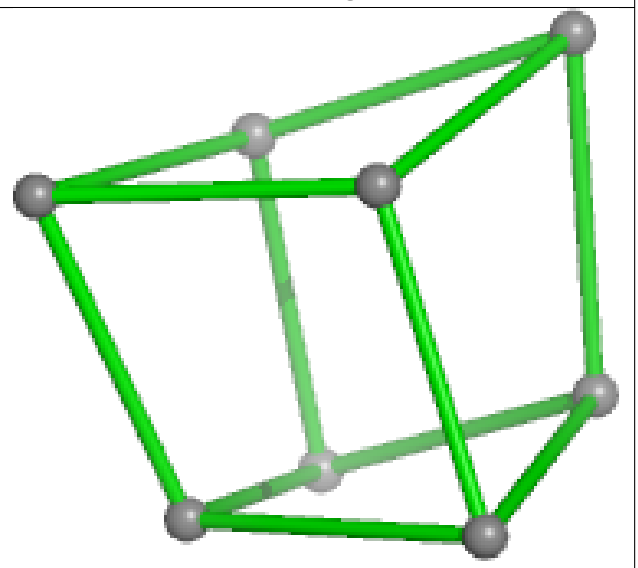
Bond lengths



Bond angles

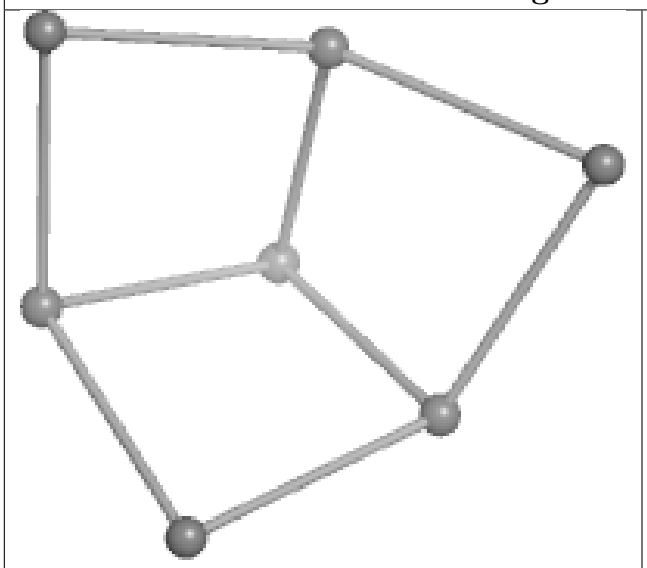


Torsions

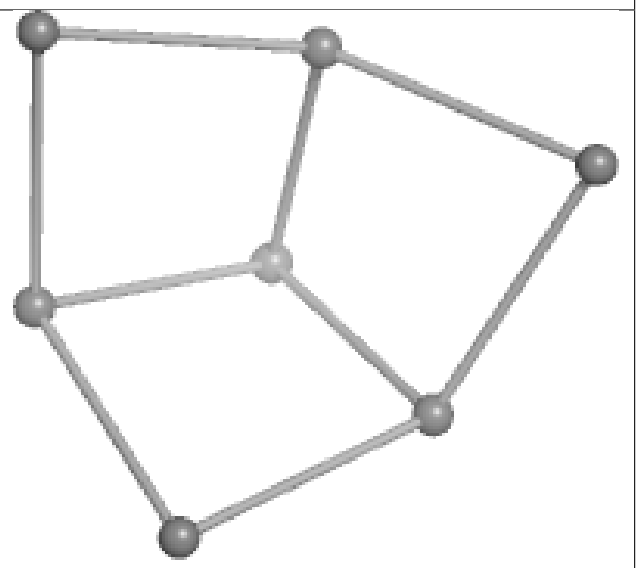


Rings

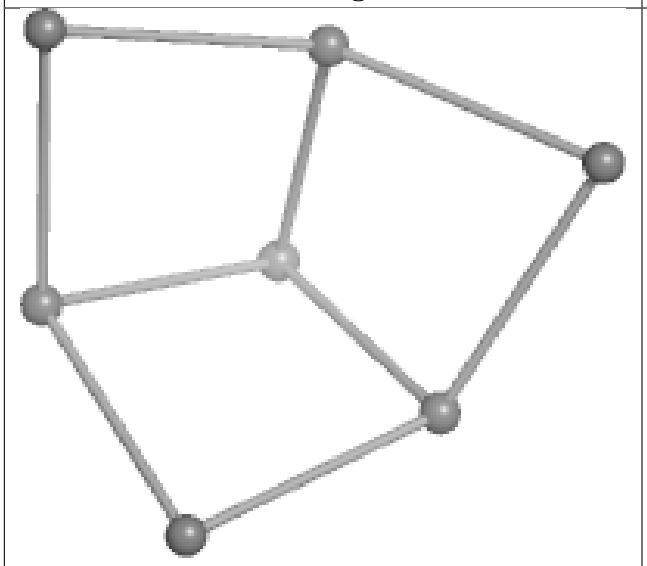
Ligand F3S V 504



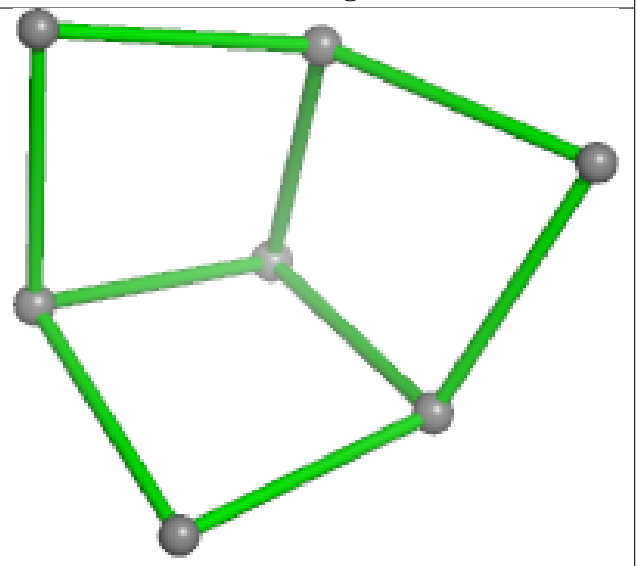
Bond lengths



Bond angles

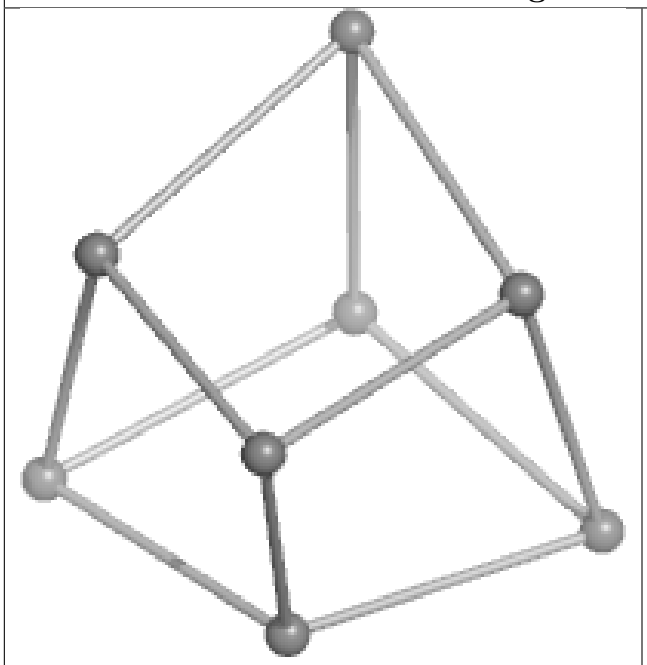


Torsions

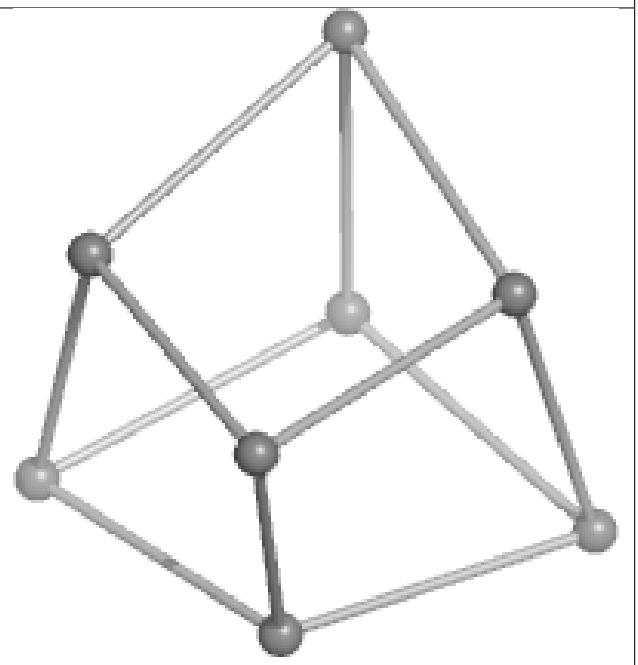


Rings

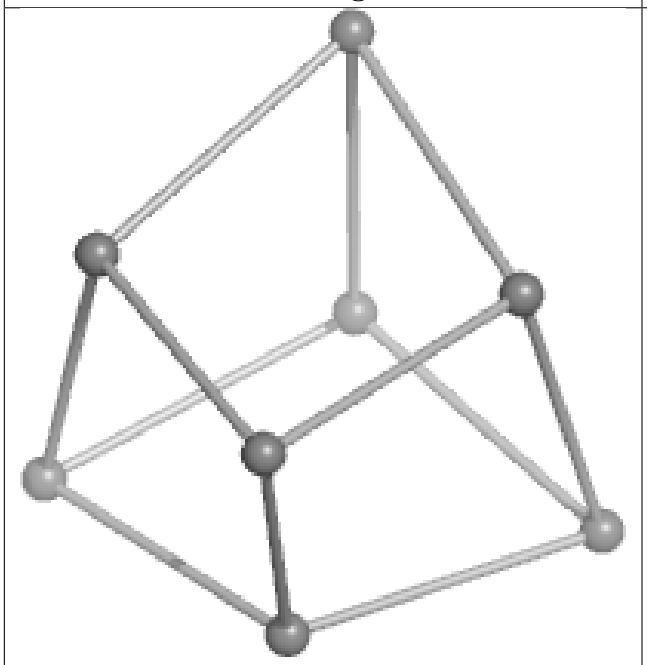
Ligand SF4 M 502



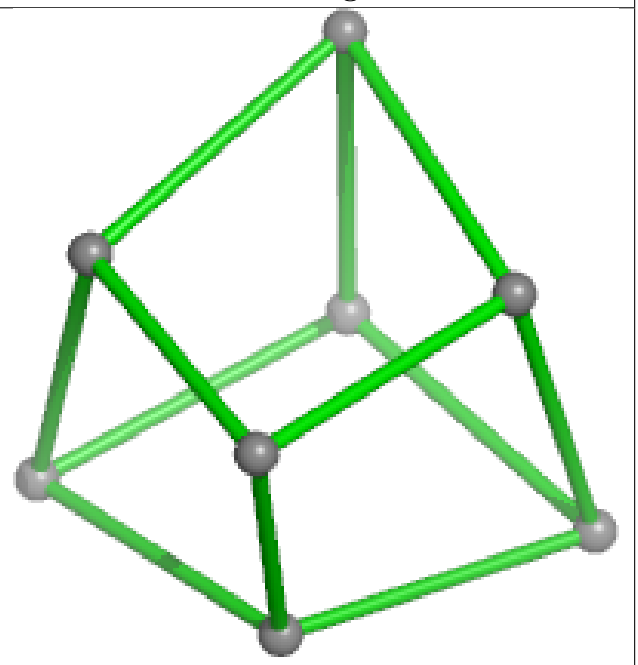
Bond lengths



Bond angles

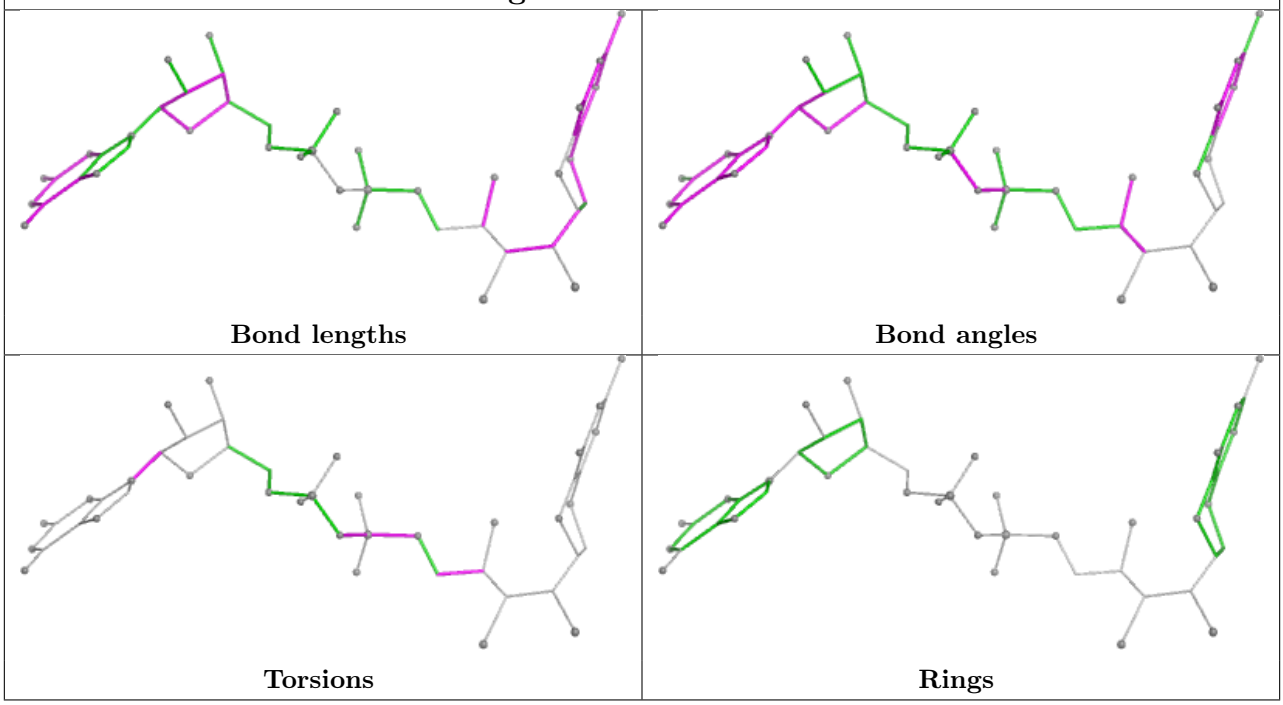


Torsions

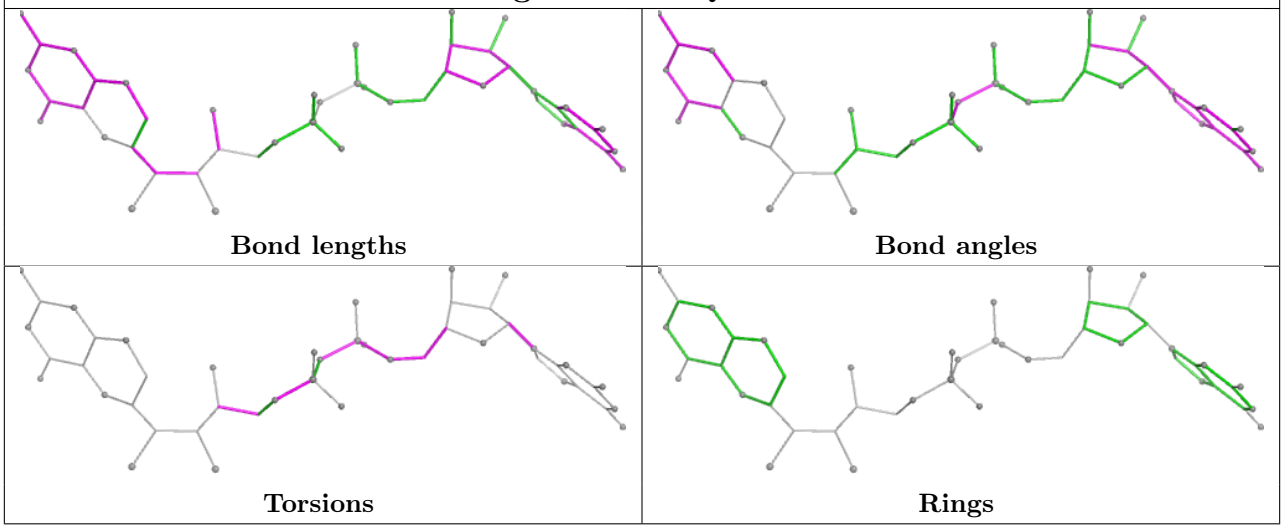


Rings

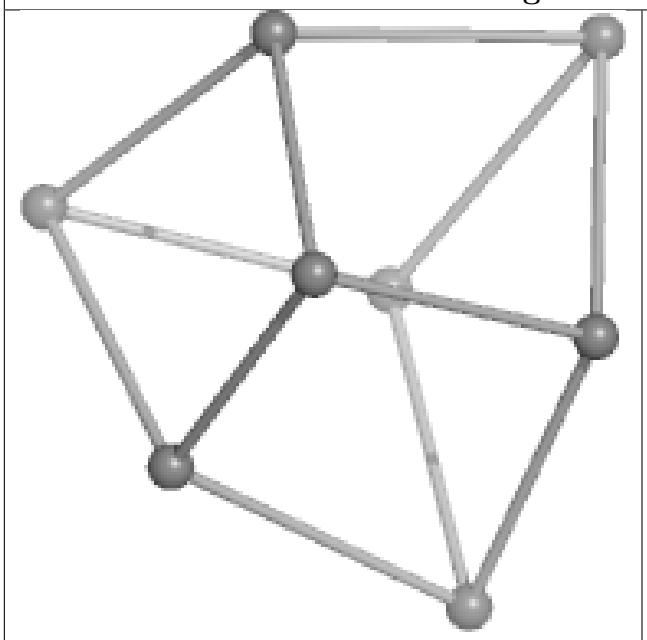
Ligand MD1 W 5802



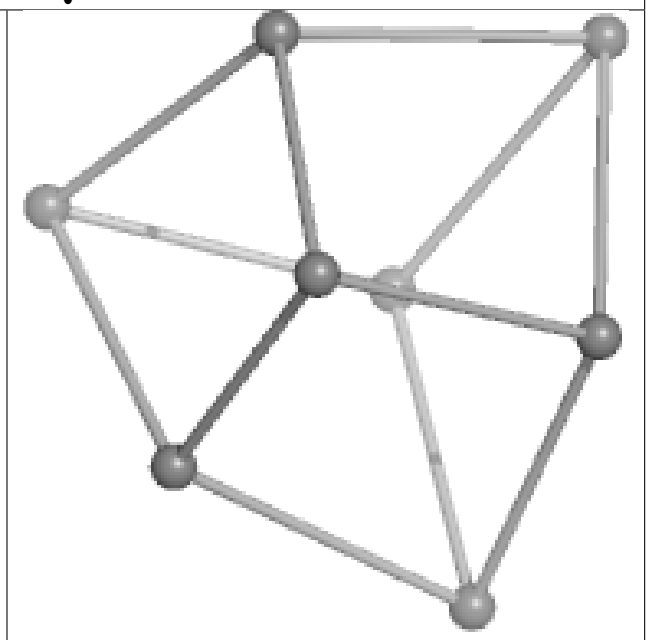
Ligand MD1 Q 5801



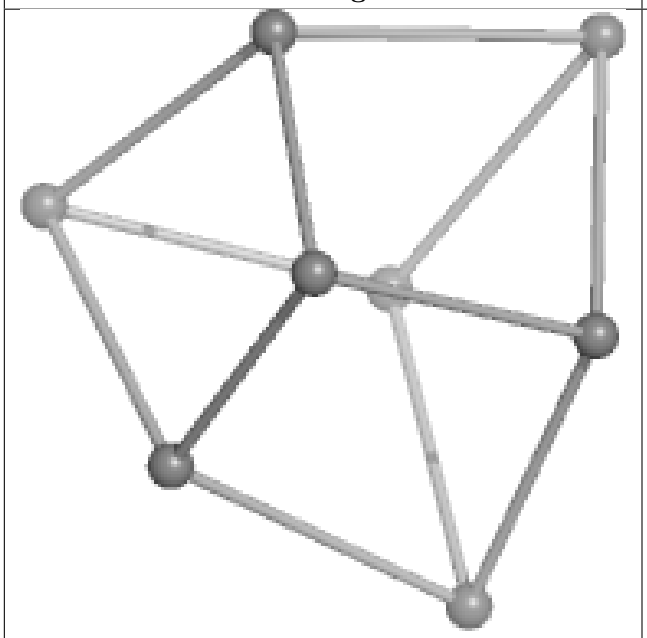
Ligand SF4 Q 5804



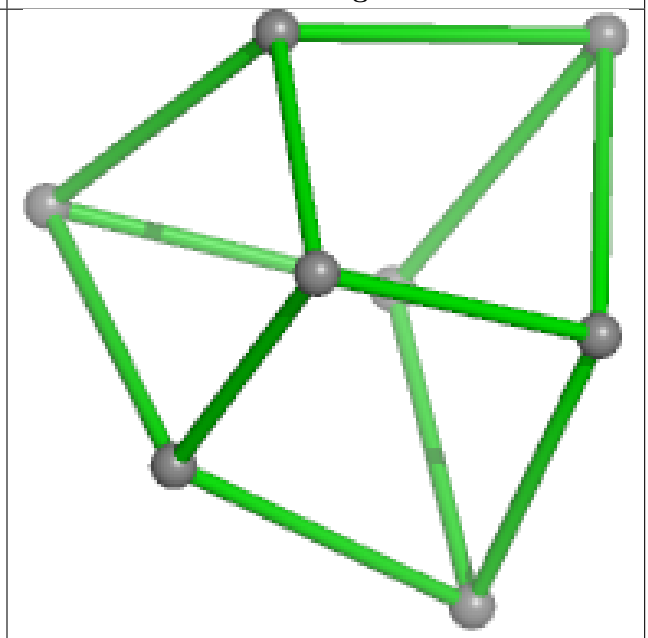
Bond lengths



Bond angles

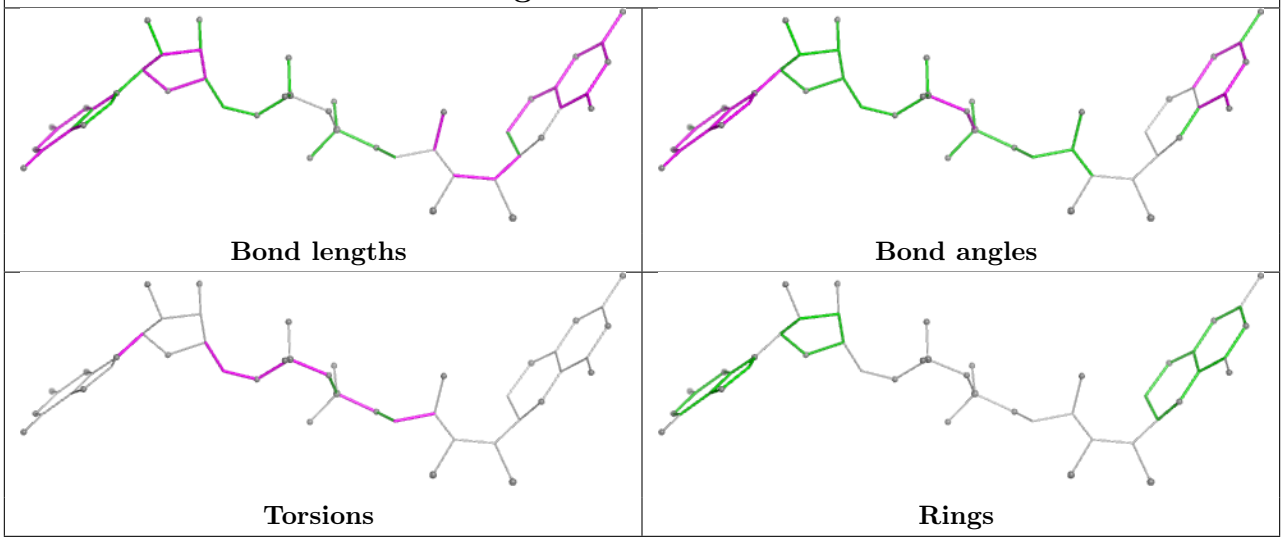


Torsions

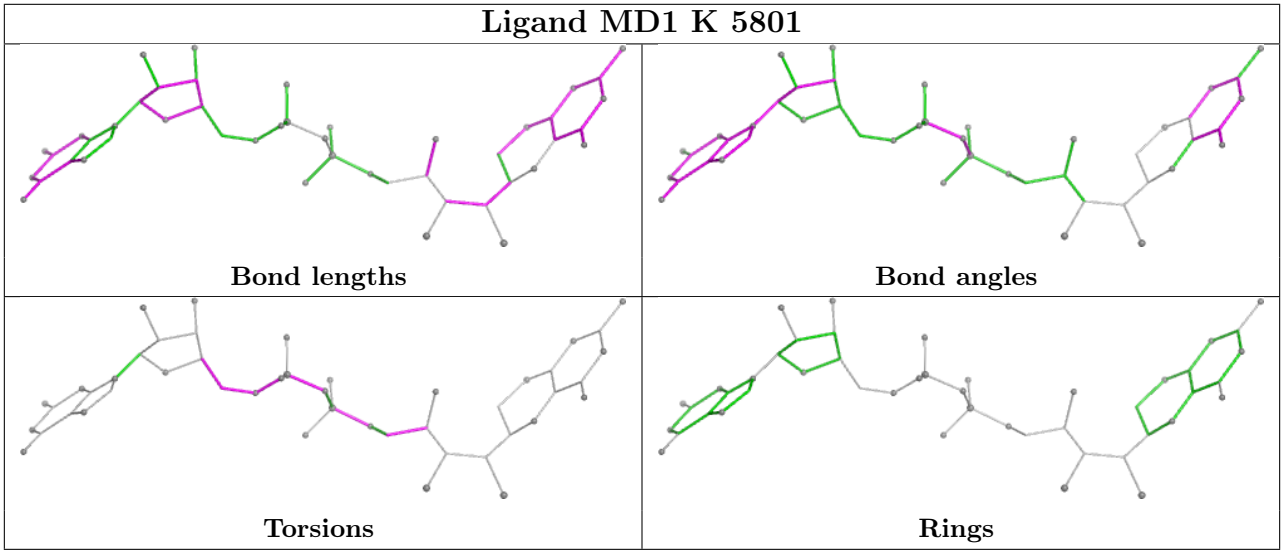


Rings

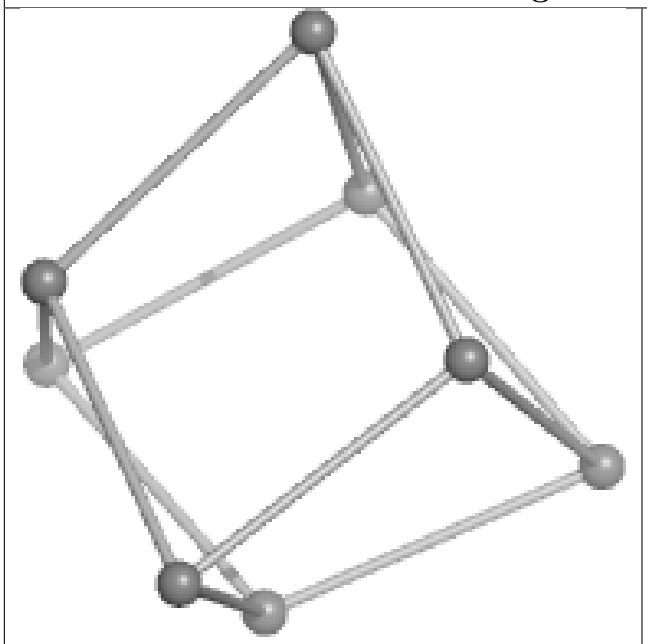
Ligand MD1 B 5801



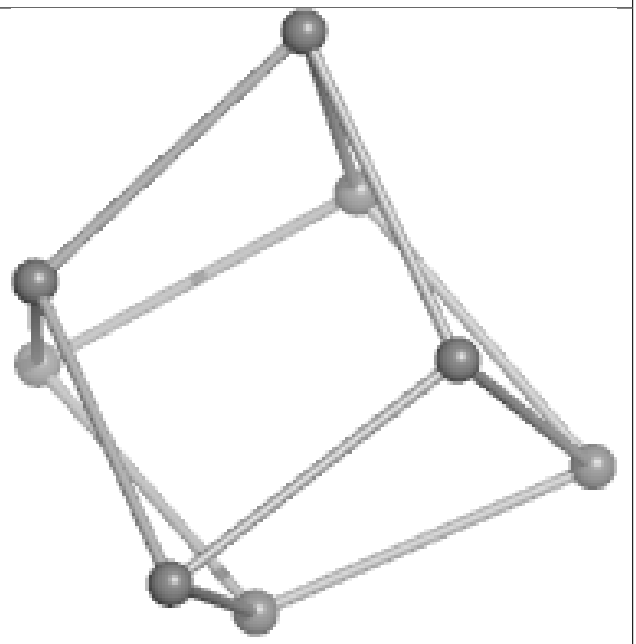
Ligand MD1 K 5801



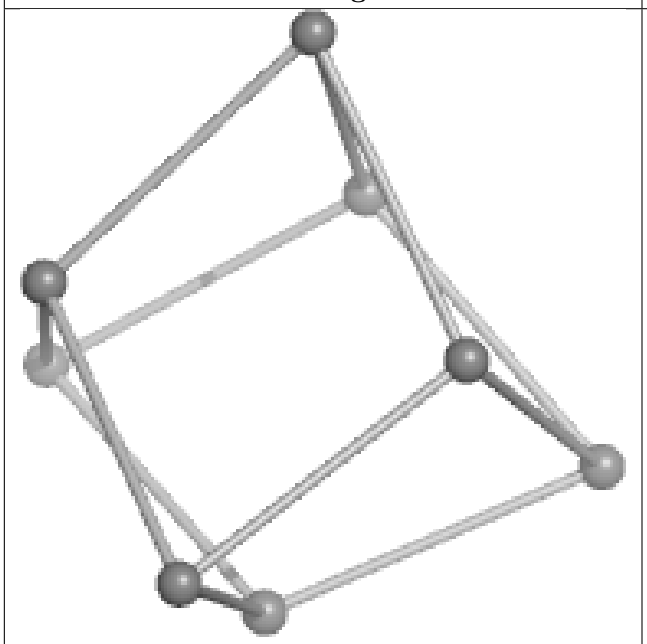
Ligand SF4 V 501



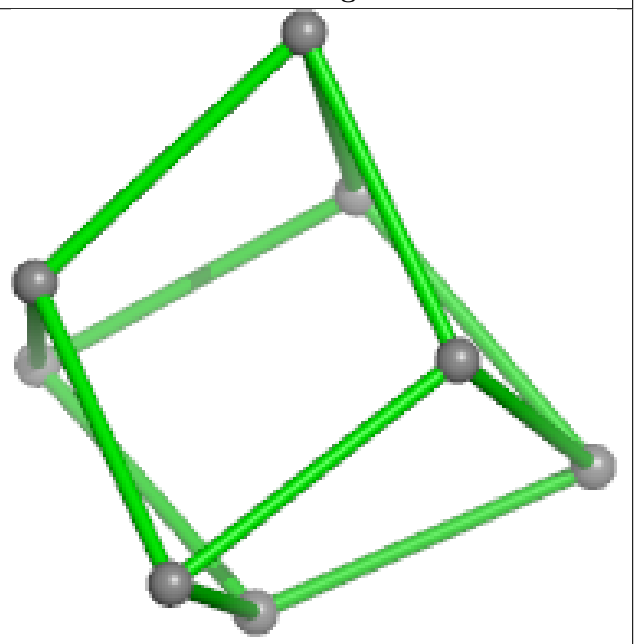
Bond lengths



Bond angles

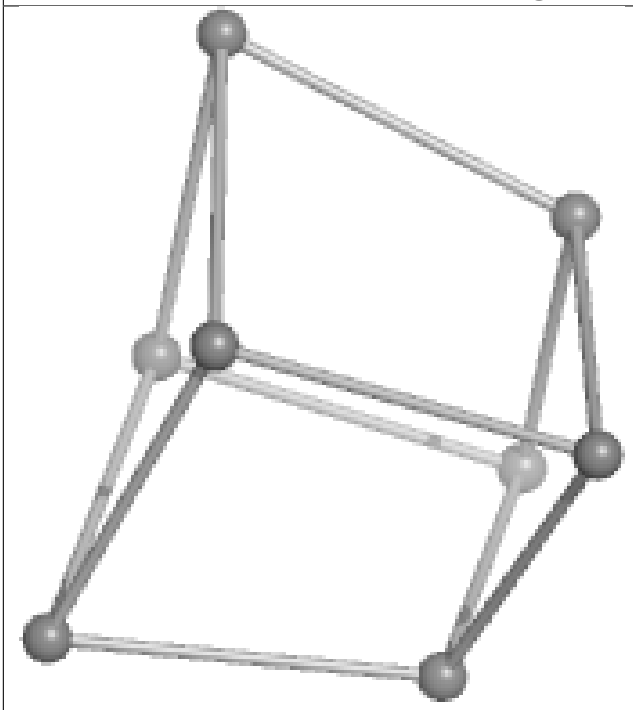


Torsions

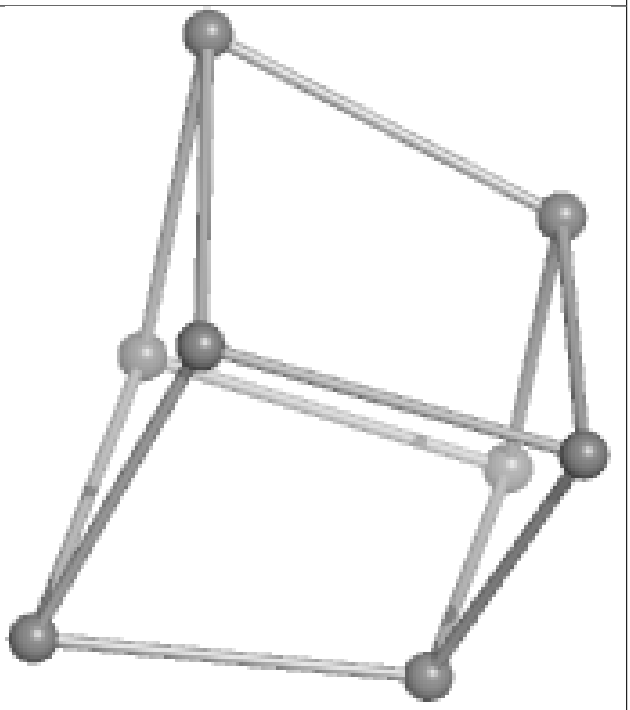


Rings

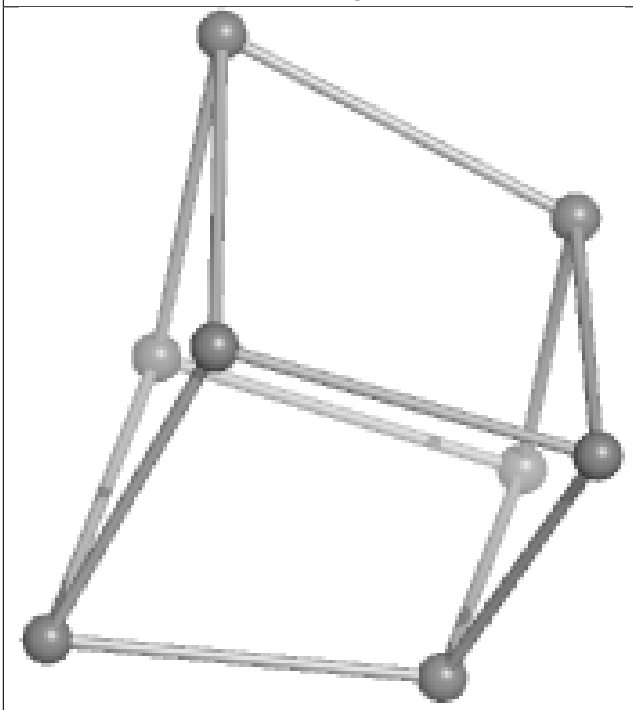
Ligand SF4 G 502



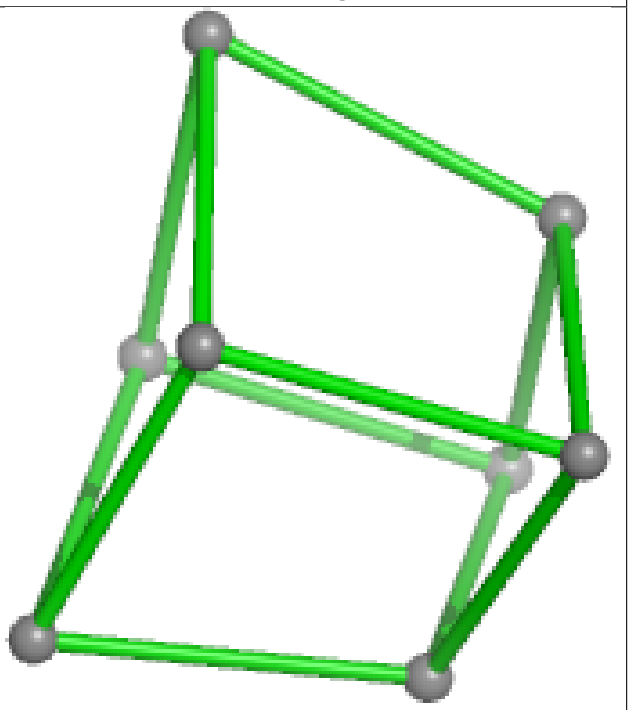
Bond lengths



Bond angles

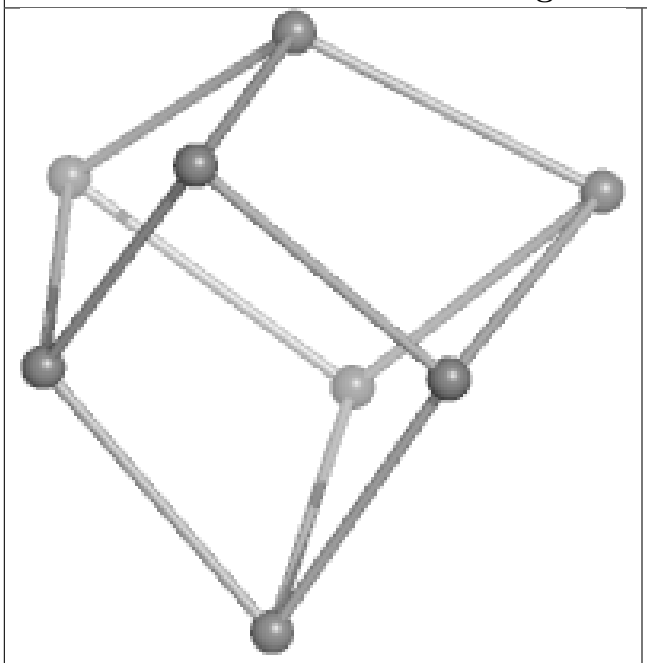


Torsions

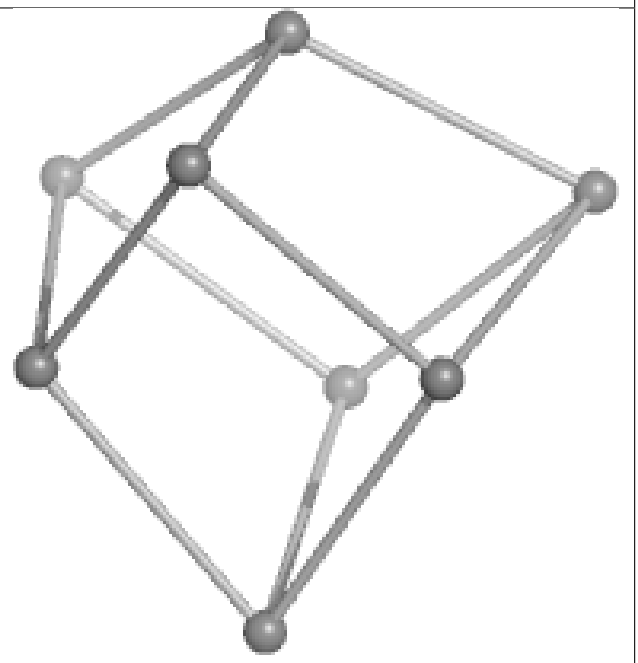


Rings

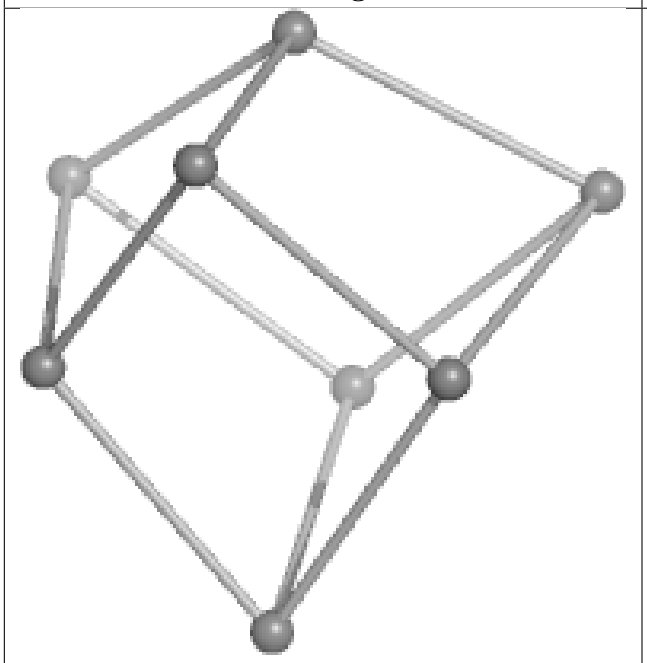
Ligand SF4 J 503



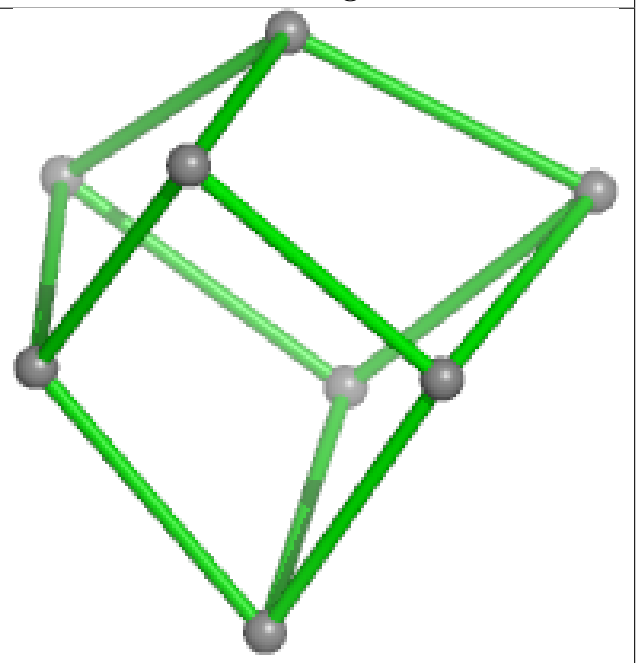
Bond lengths



Bond angles

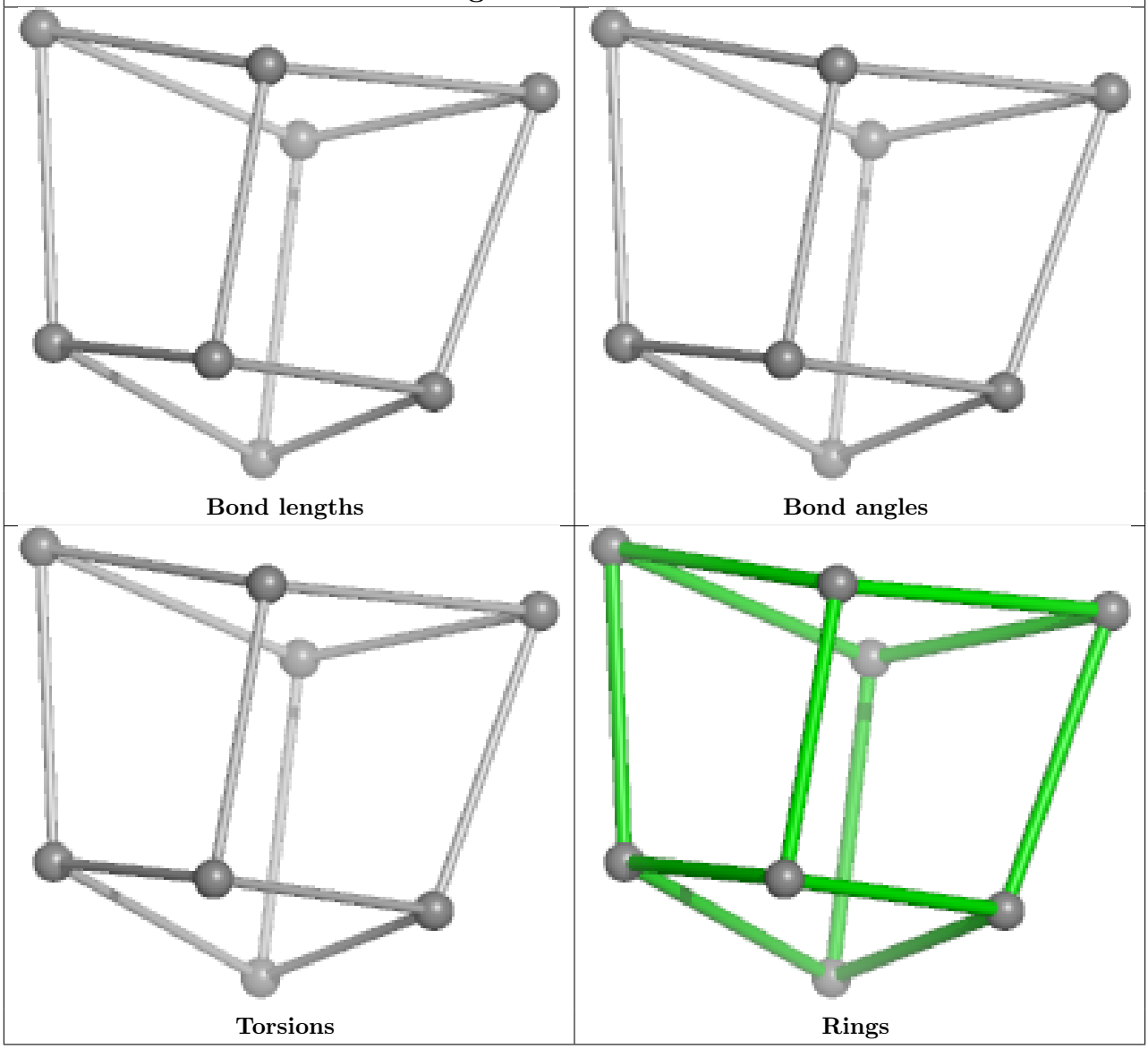


Torsions

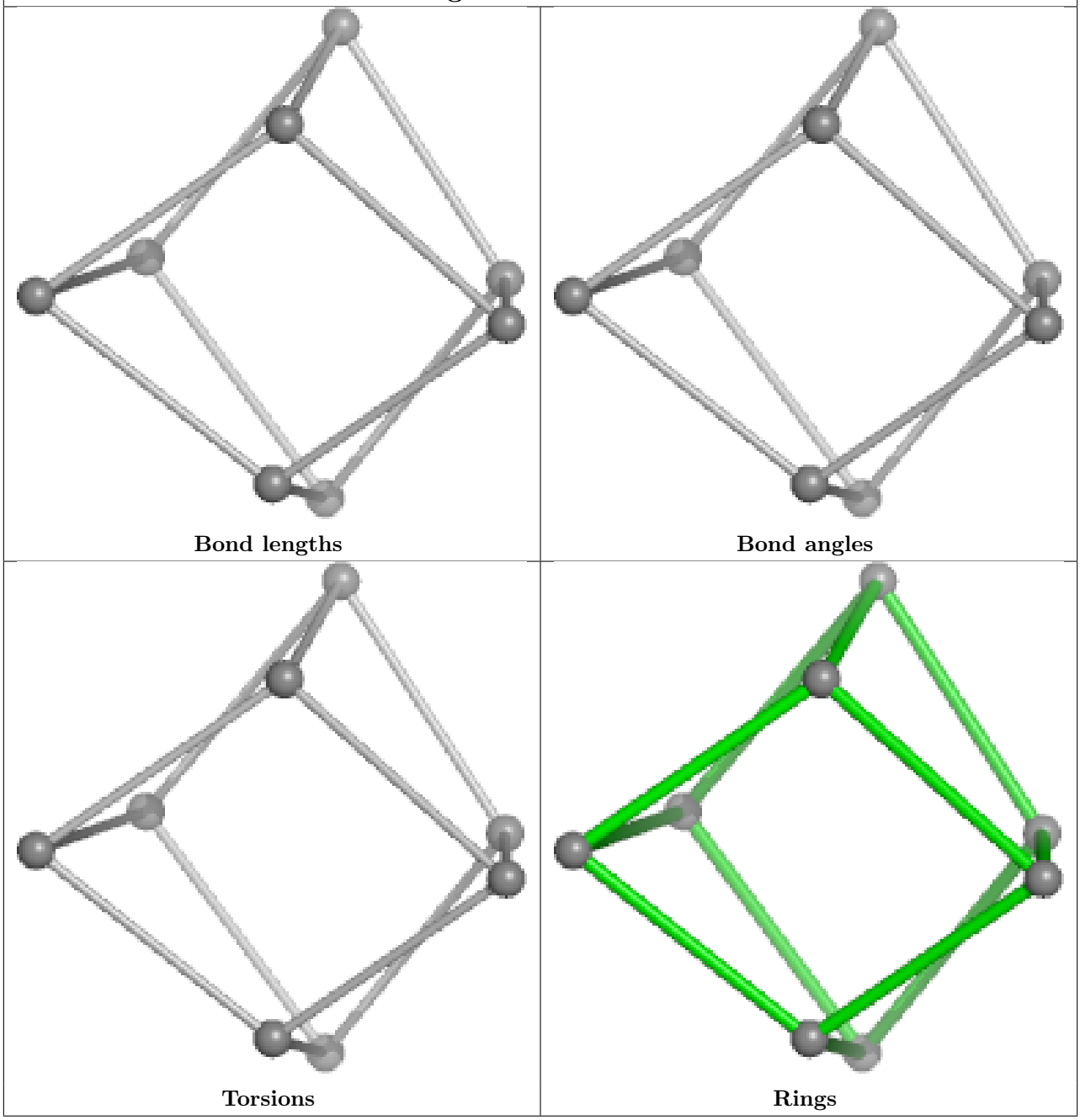


Rings

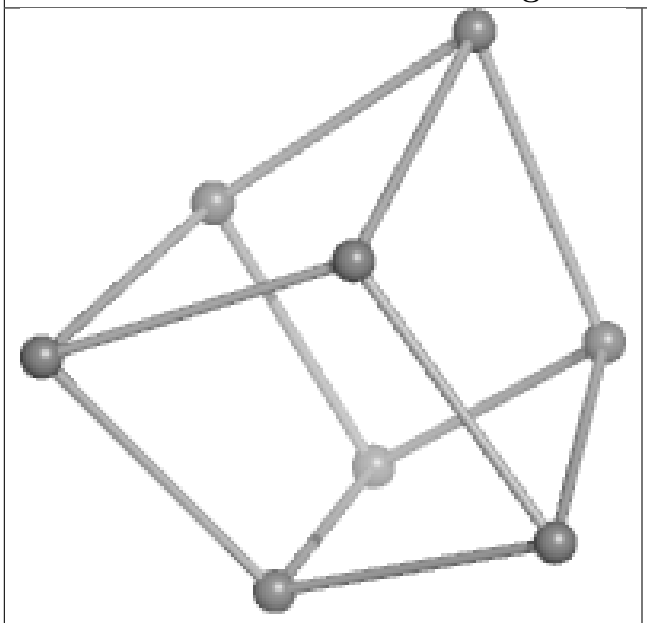
Ligand SF4 B 5804



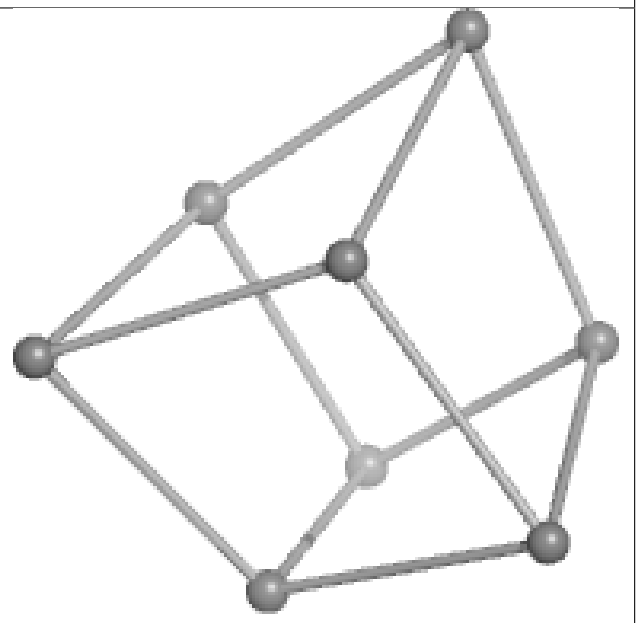
Ligand SF4 D 501



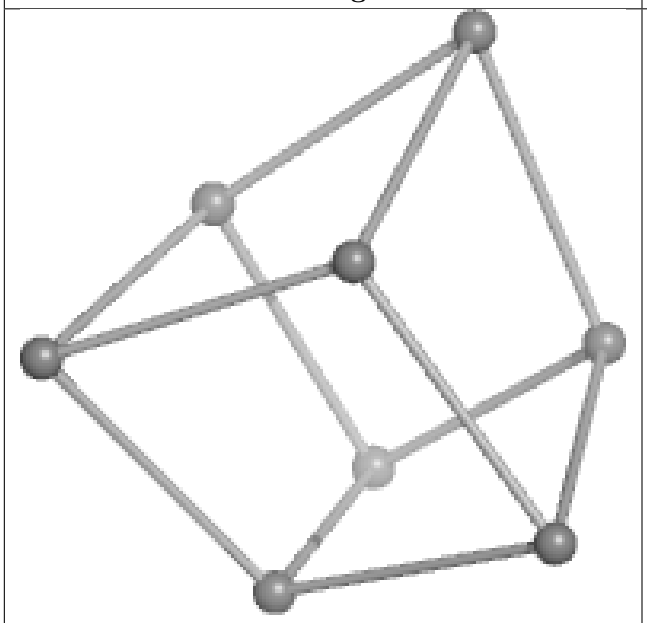
Ligand SF4 K 5804



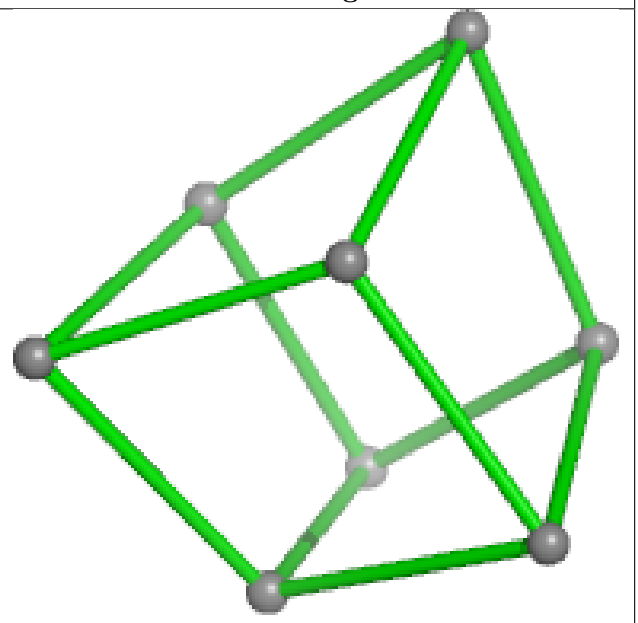
Bond lengths



Bond angles

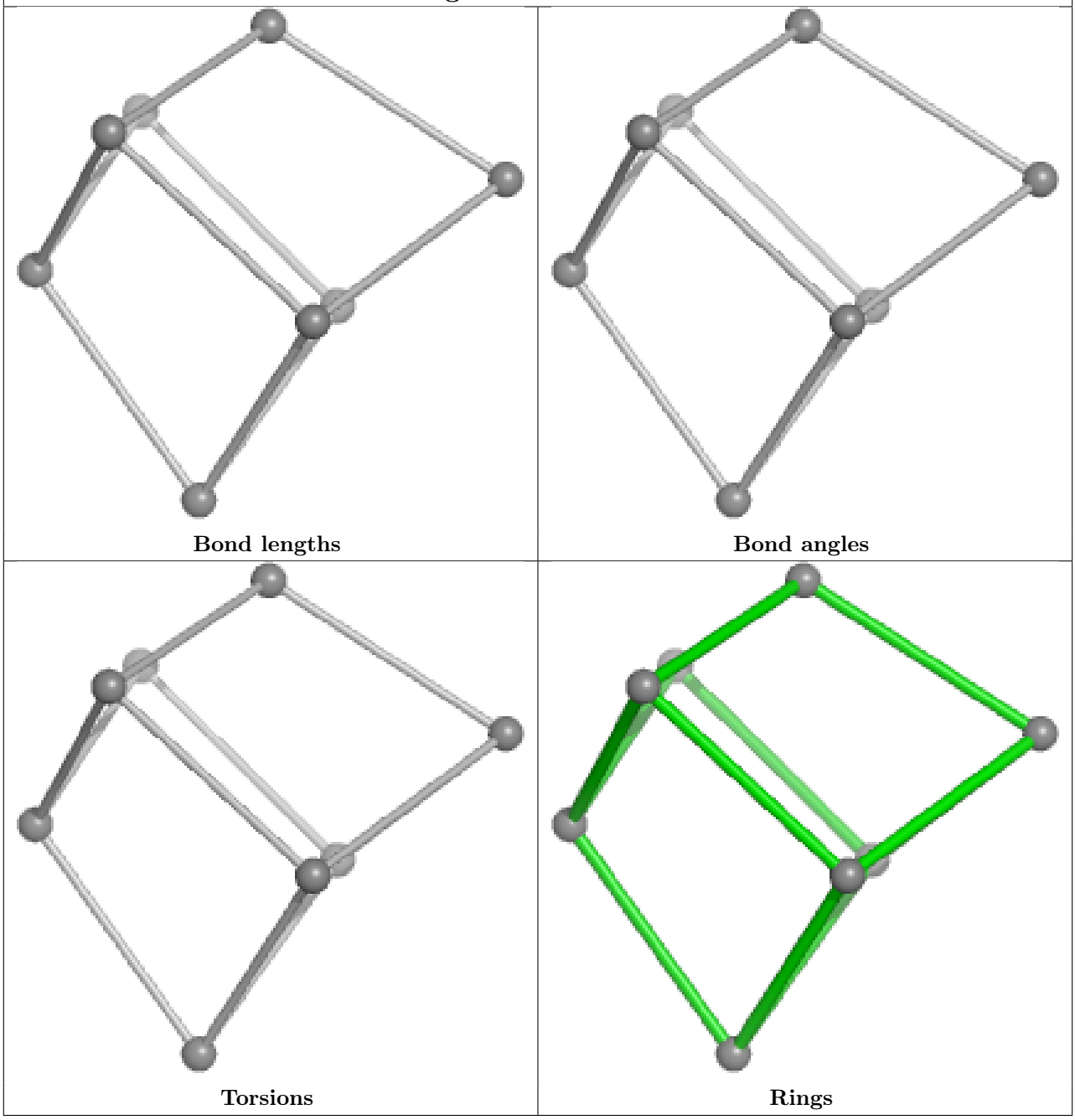


Torsions

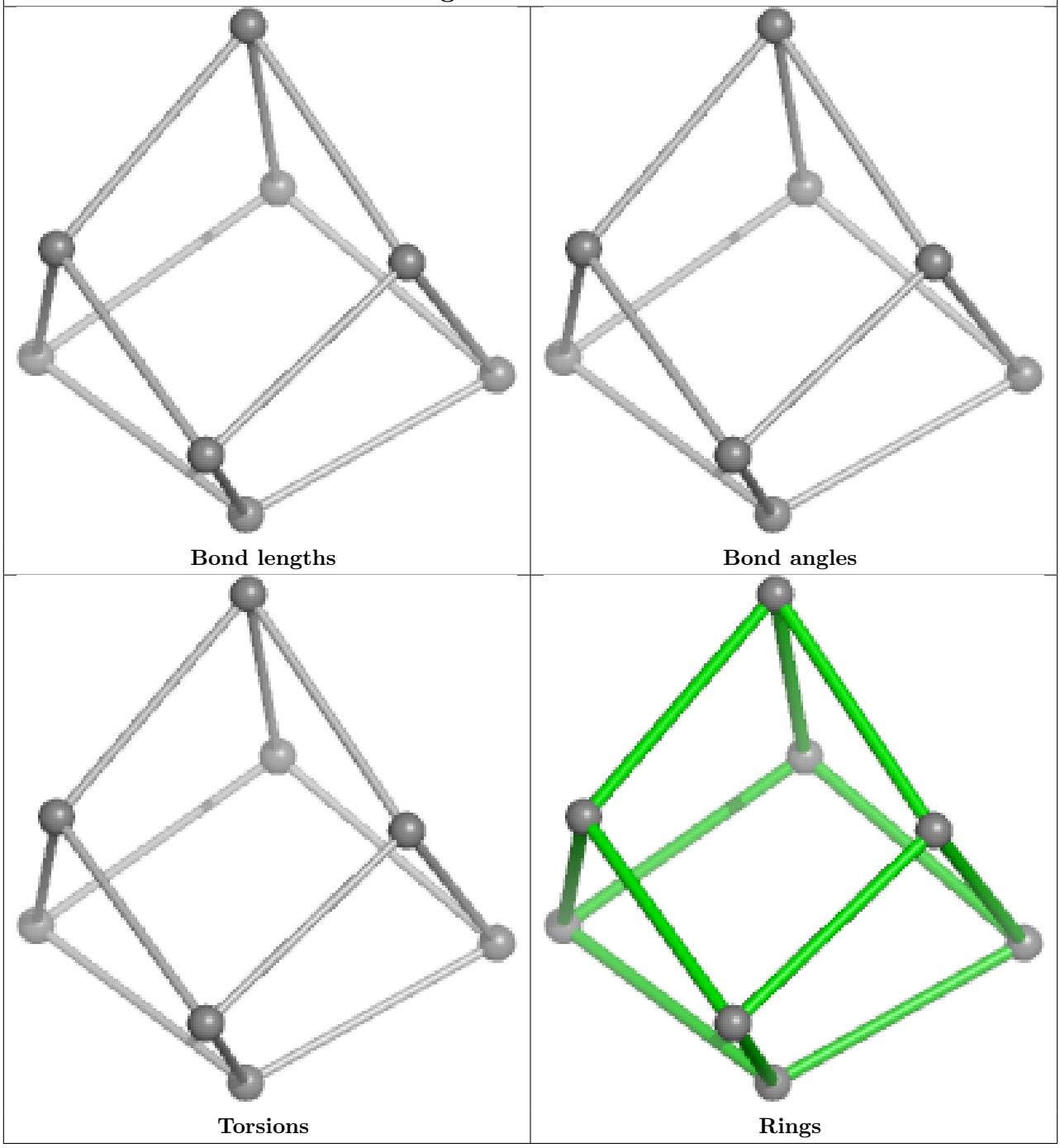


Rings

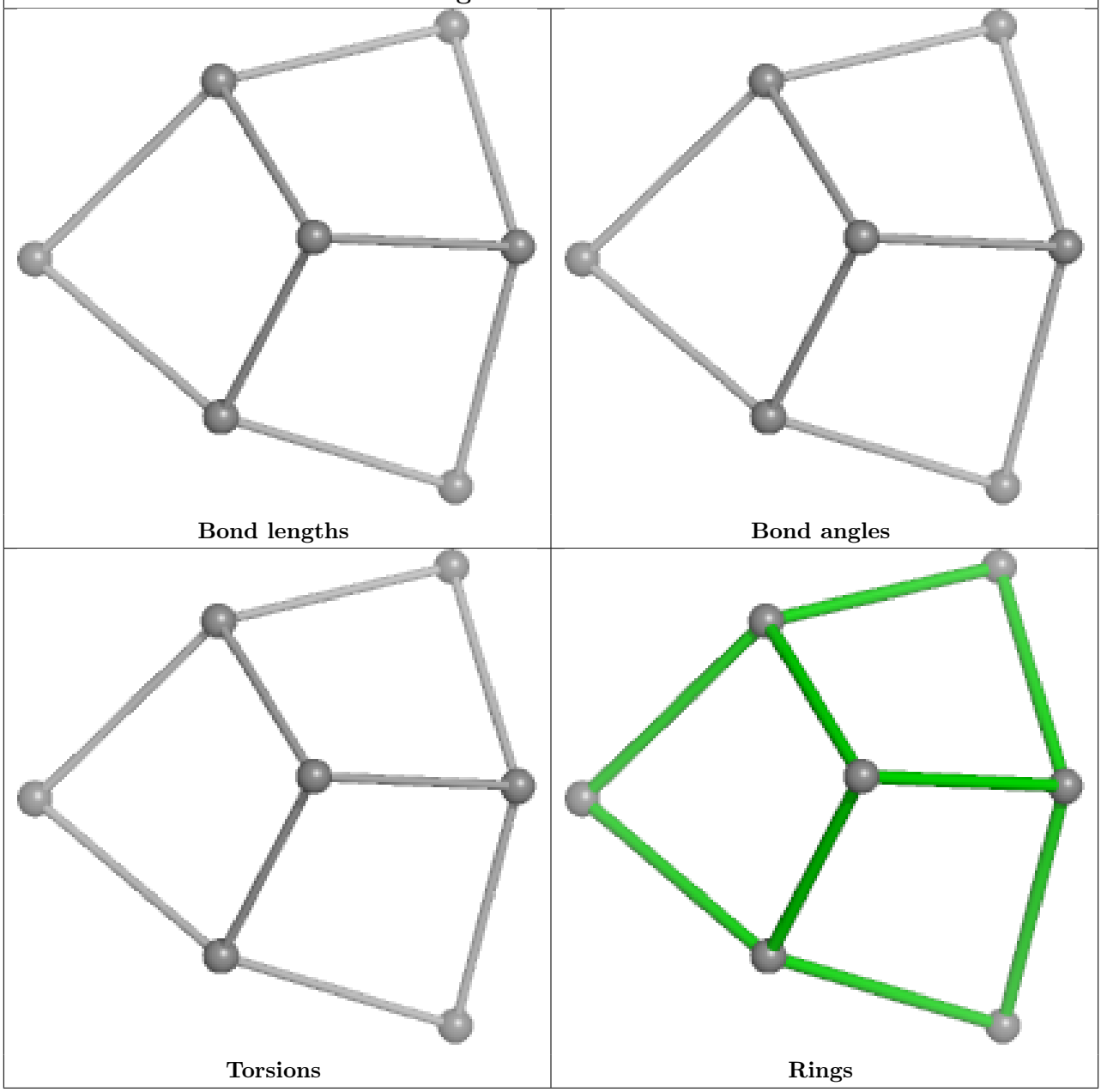
Ligand SF4 G 503



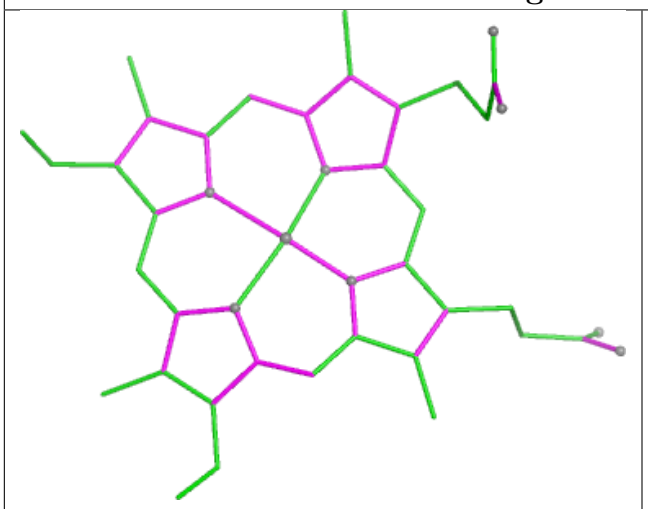
Ligand SF4 P 502



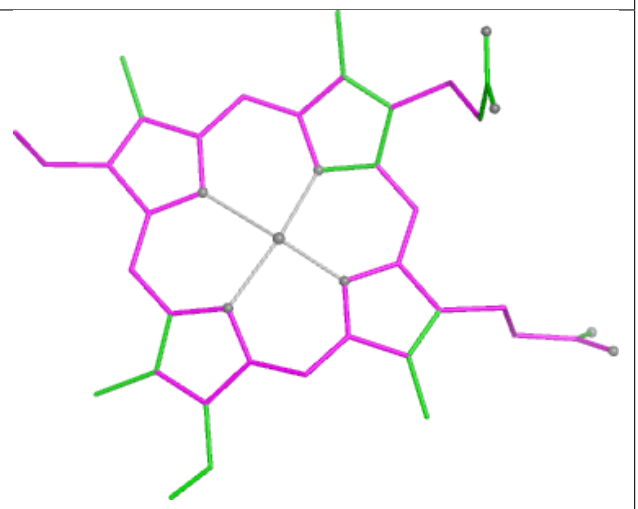
Ligand F3S D 504



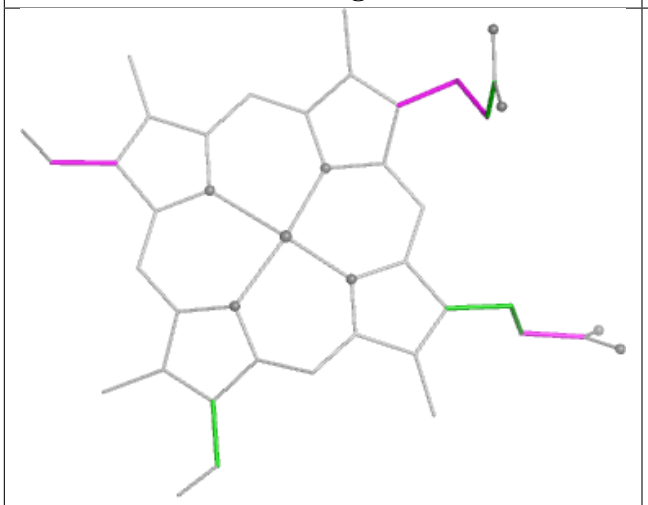
Ligand HEM I 401



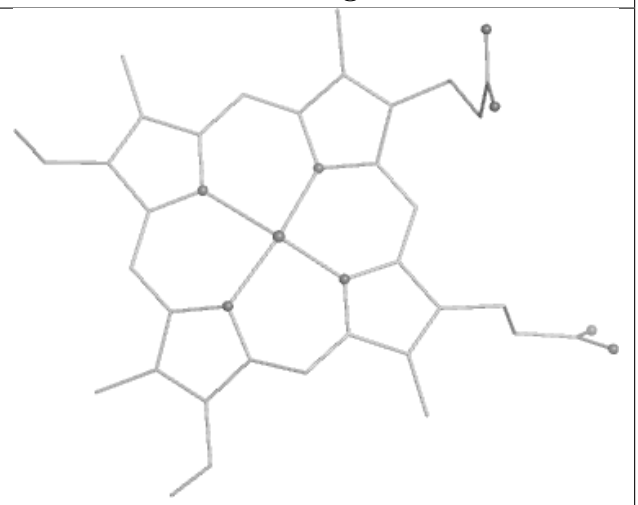
Bond lengths



Bond angles

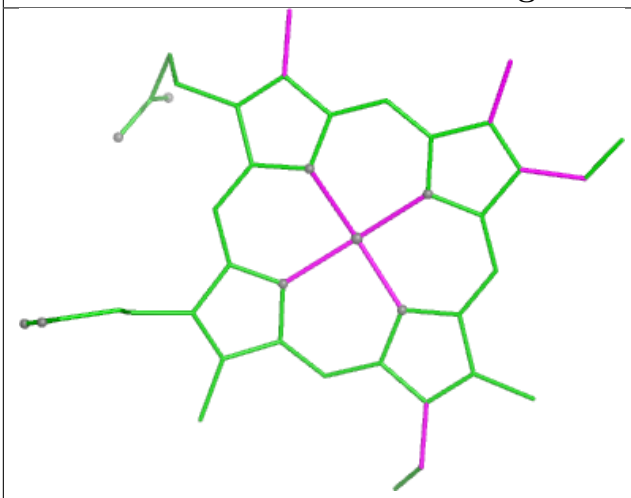


Torsions

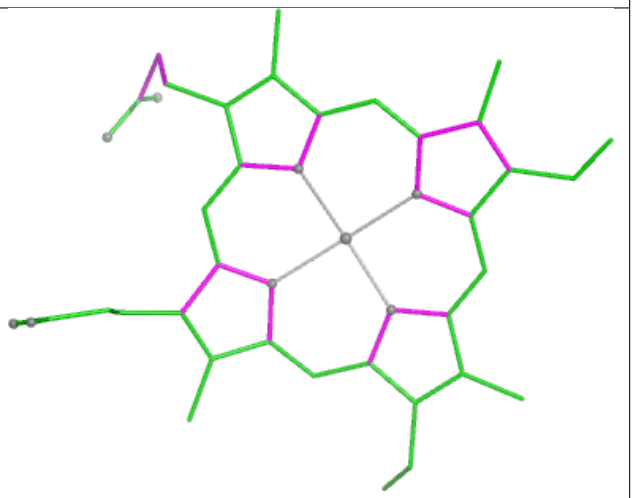


Rings

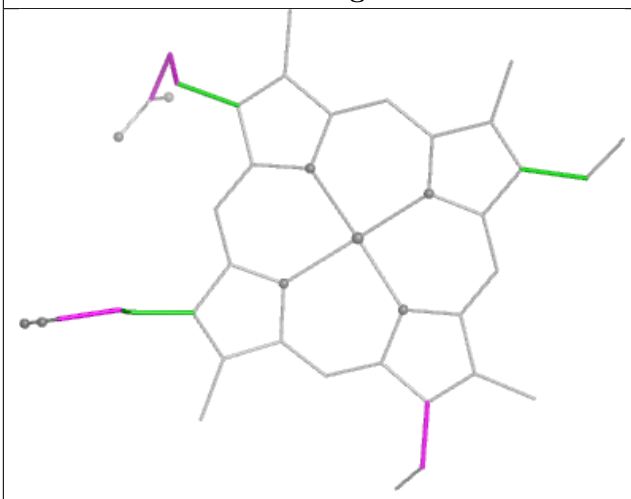
Ligand HEM U 401



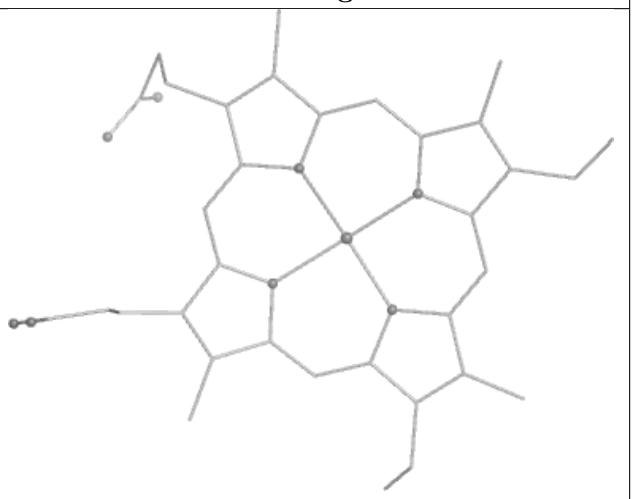
Bond lengths



Bond angles

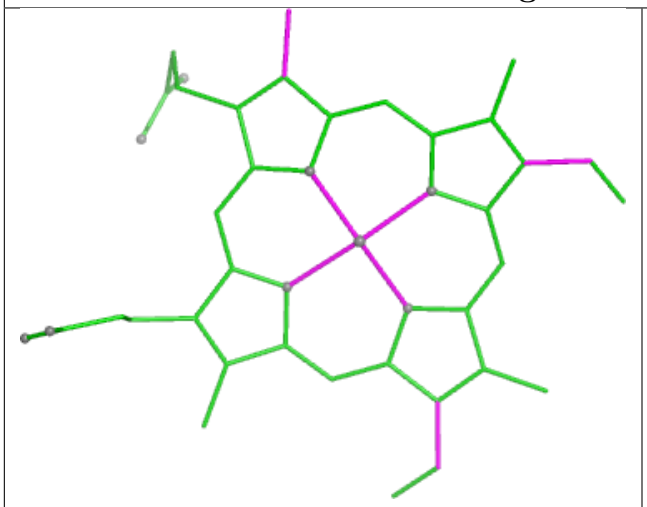


Torsions

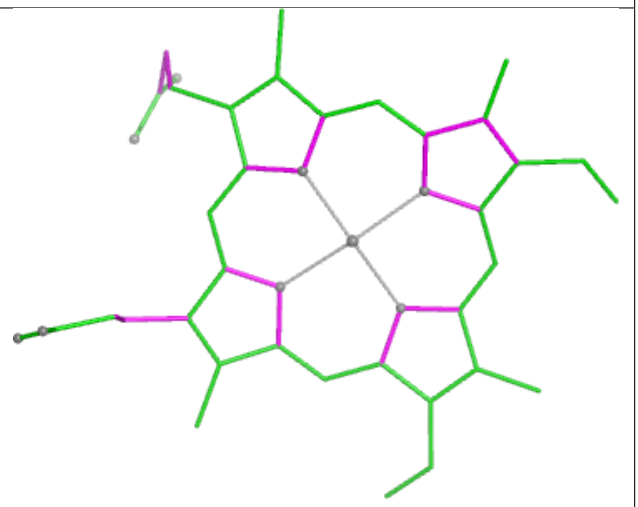


Rings

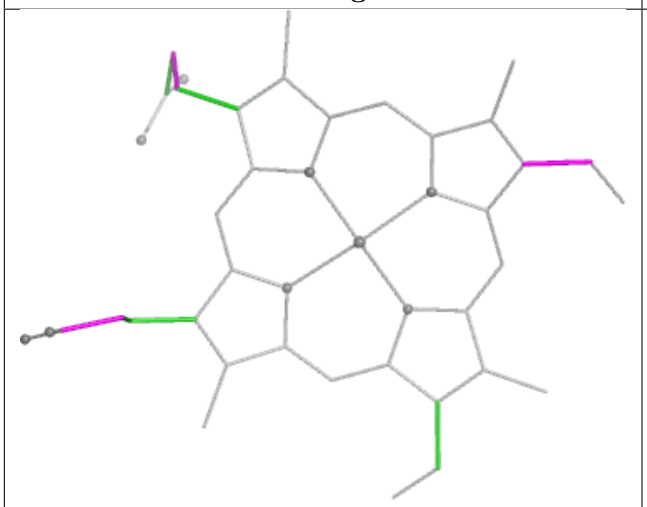
Ligand HEM X 401



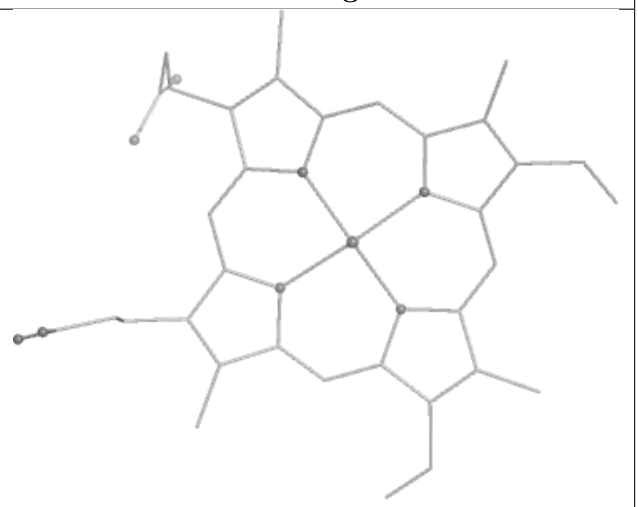
Bond lengths



Bond angles

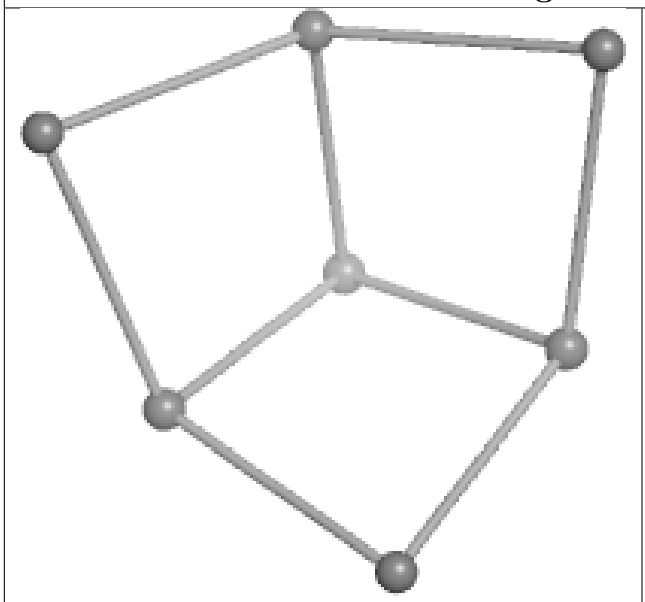


Torsions

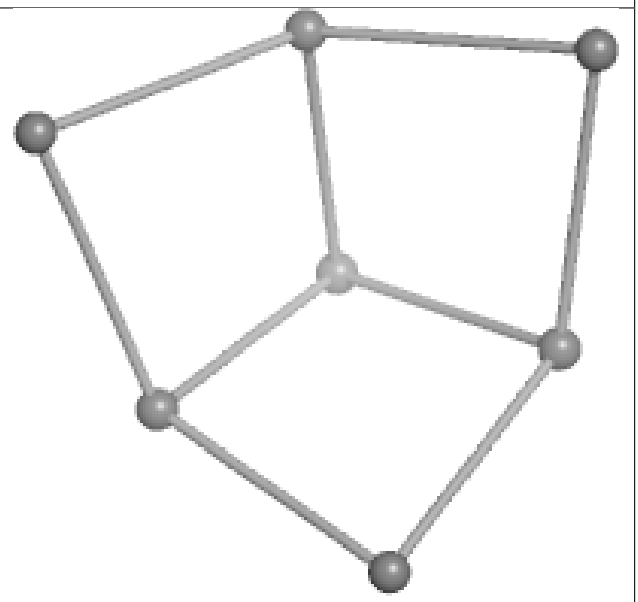


Rings

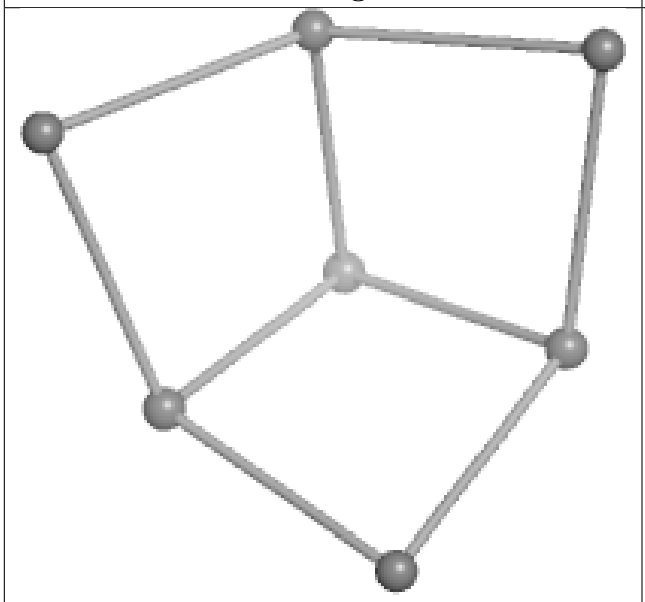
Ligand F3S S 504



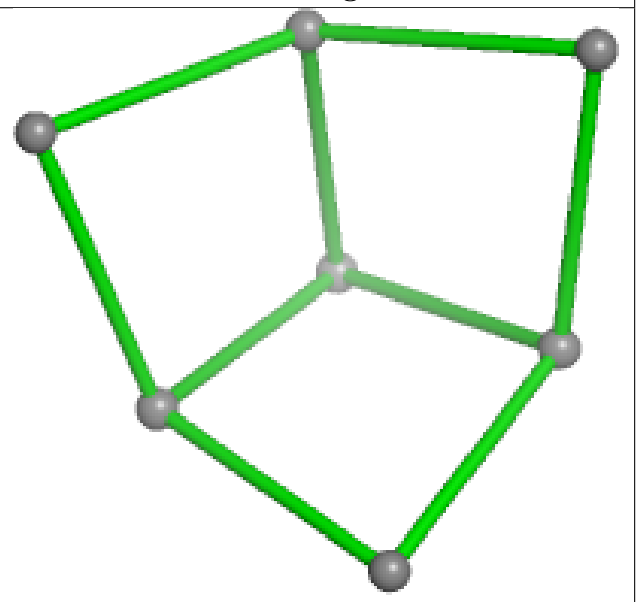
Bond lengths



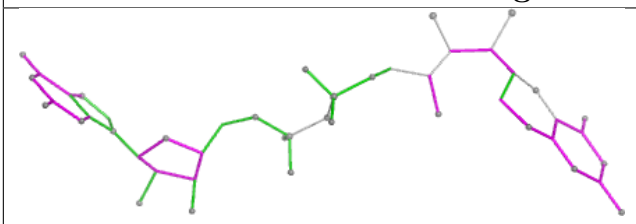
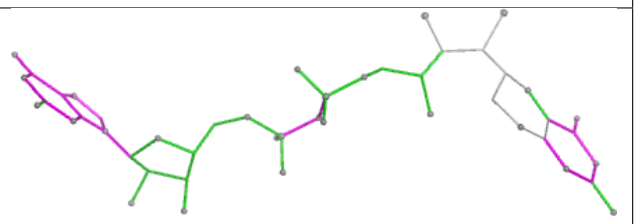
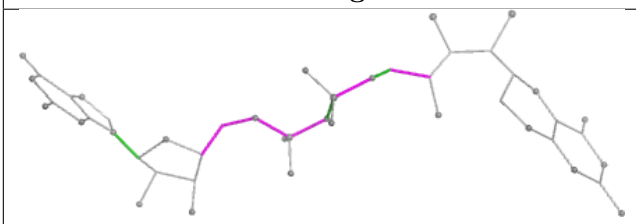
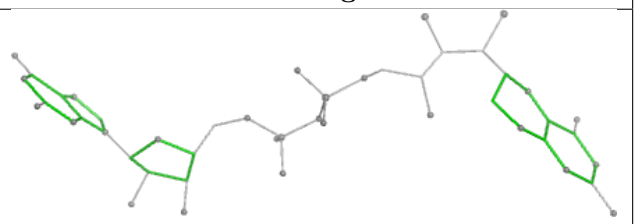
Bond angles



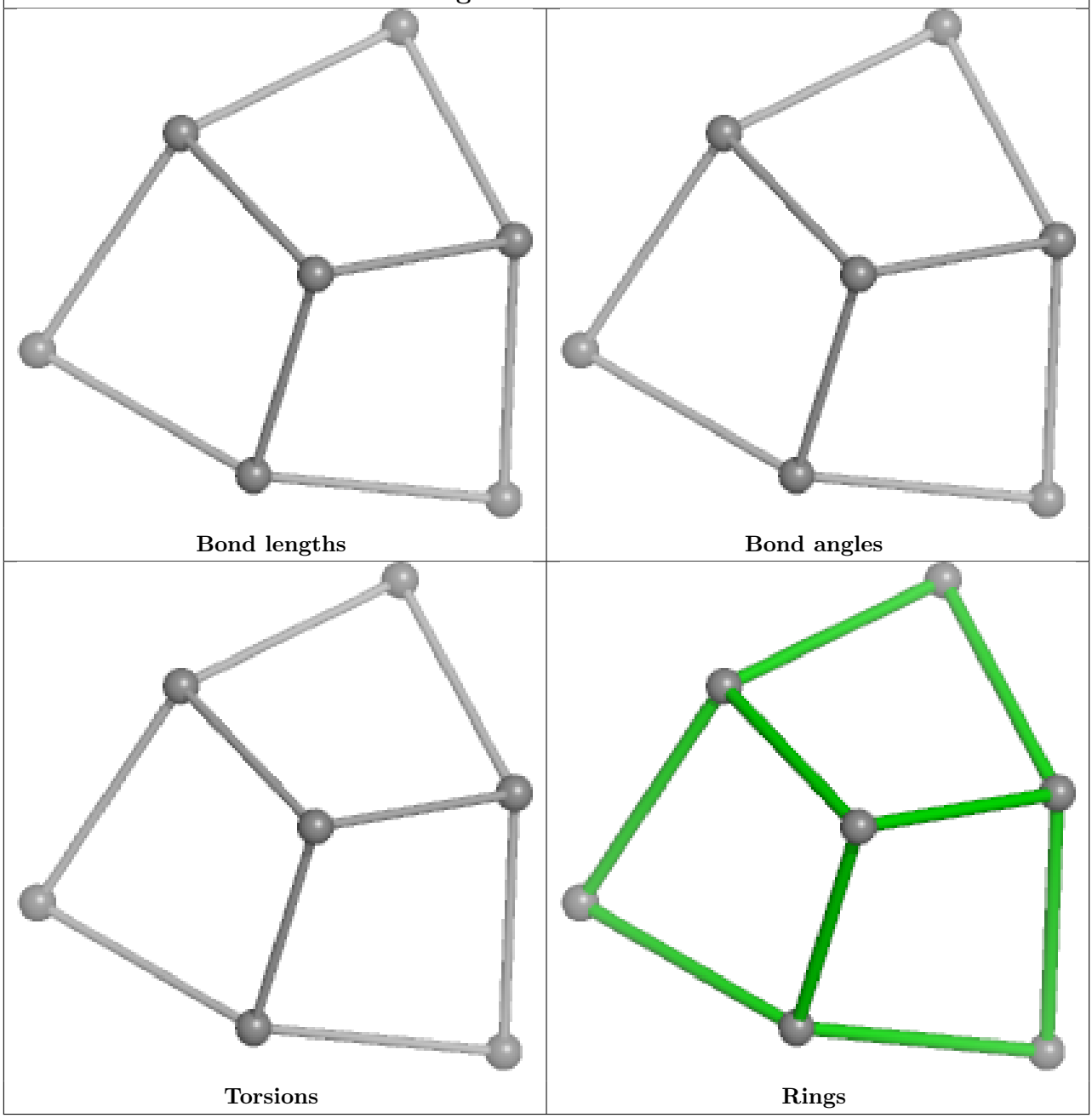
Torsions



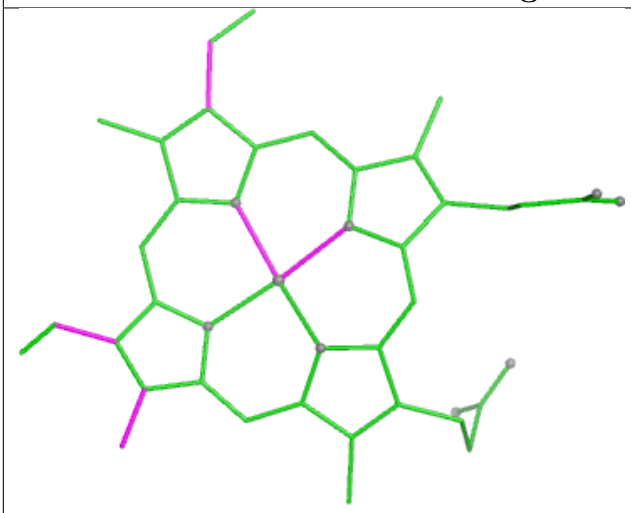
Rings

Ligand MD1 T 5801	
 Bond lengths	 Bond angles
 Torsions	 Rings

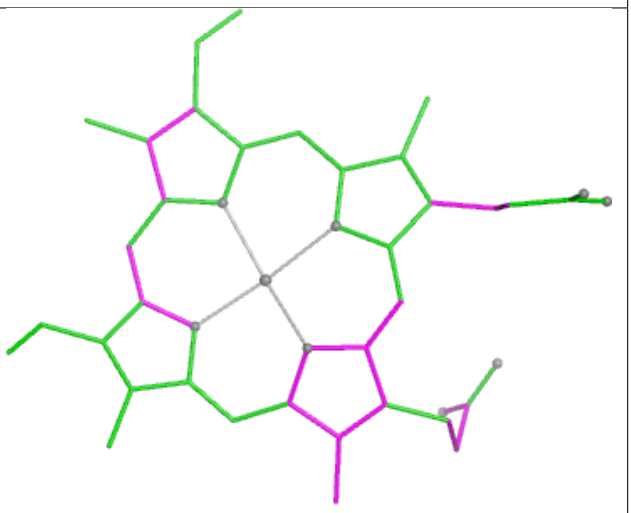
Ligand F3S J 504



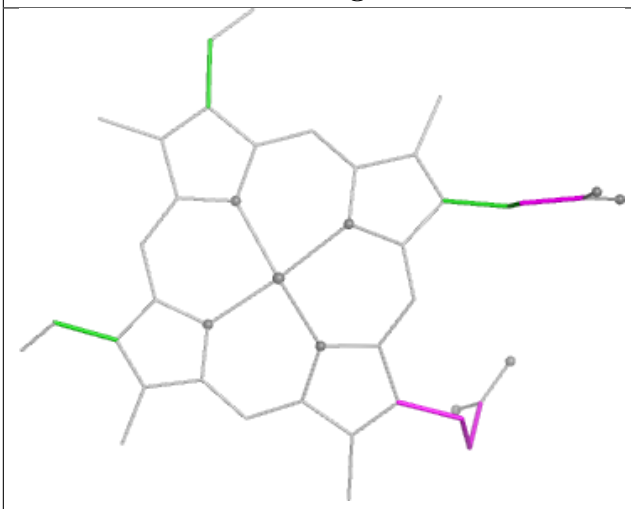
Ligand HEM F 401



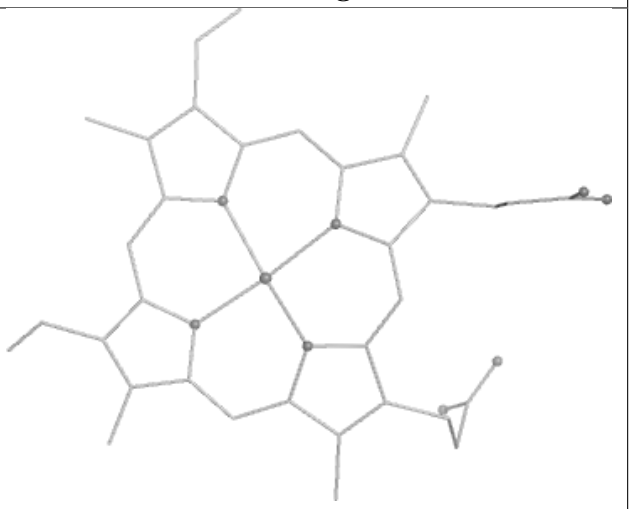
Bond lengths



Bond angles

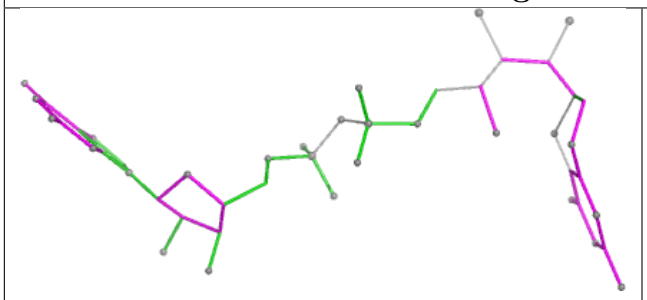


Torsions

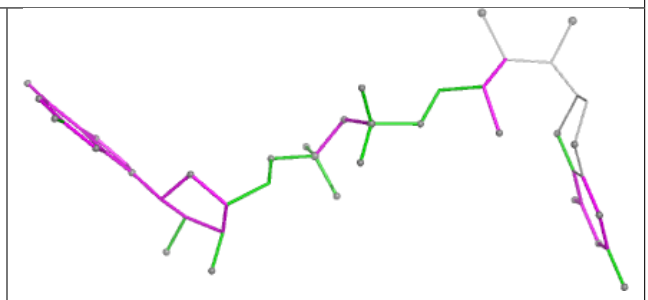


Rings

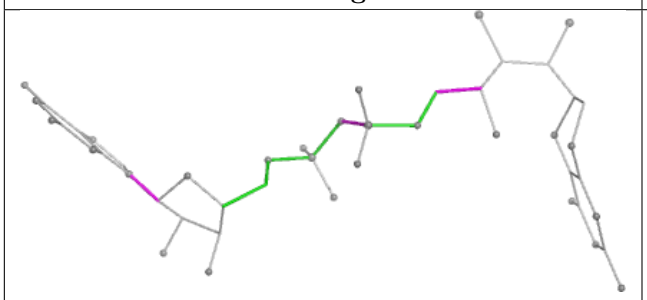
Ligand MD1 H 5802



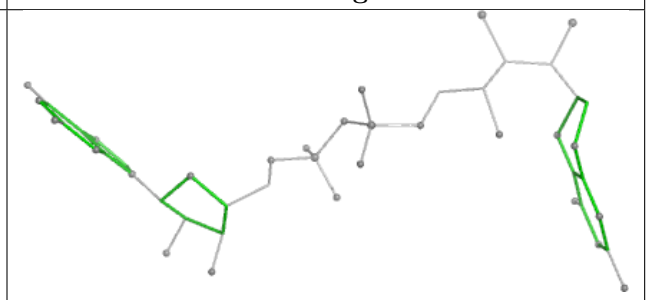
Bond lengths



Bond angles

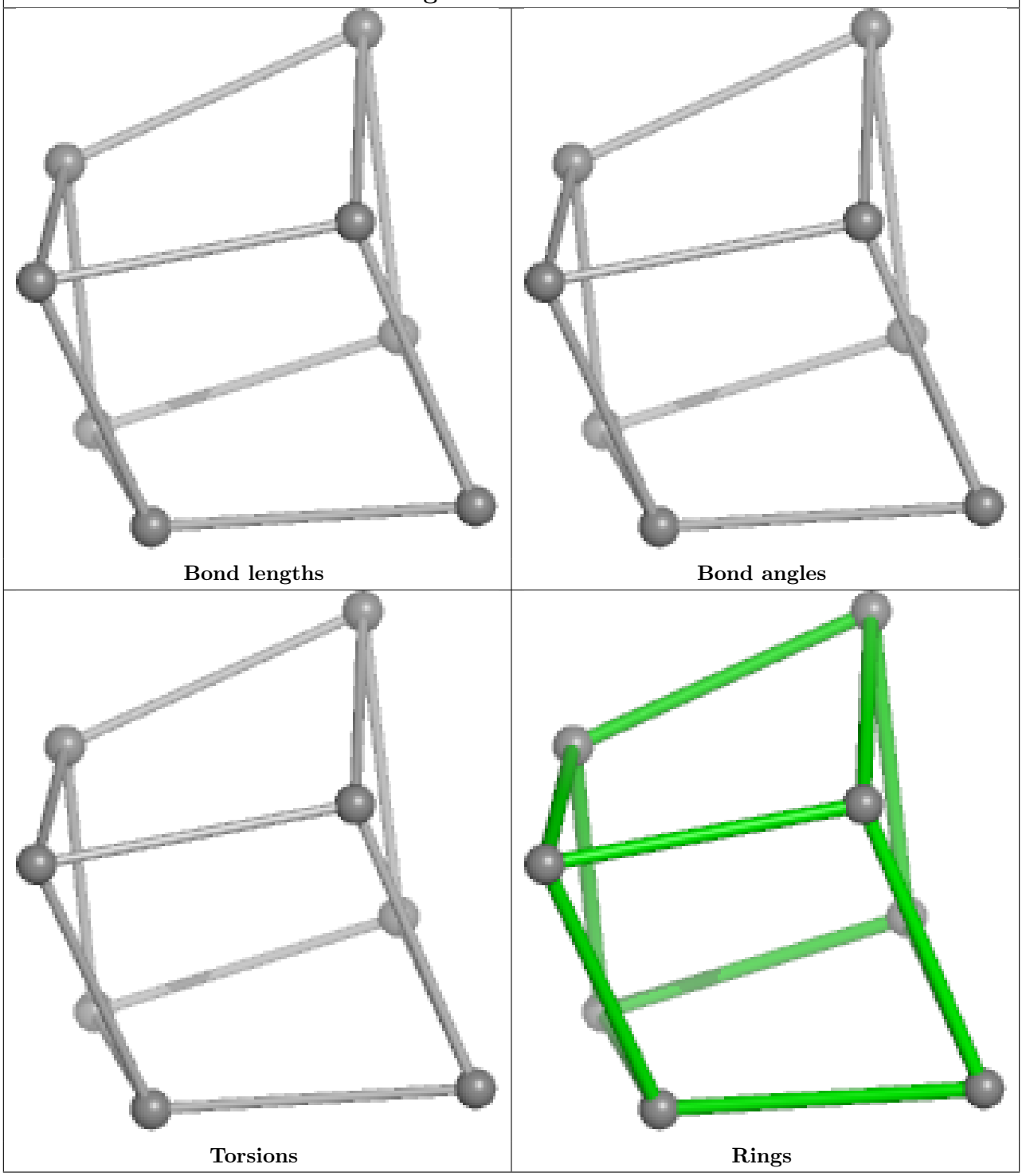


Torsions

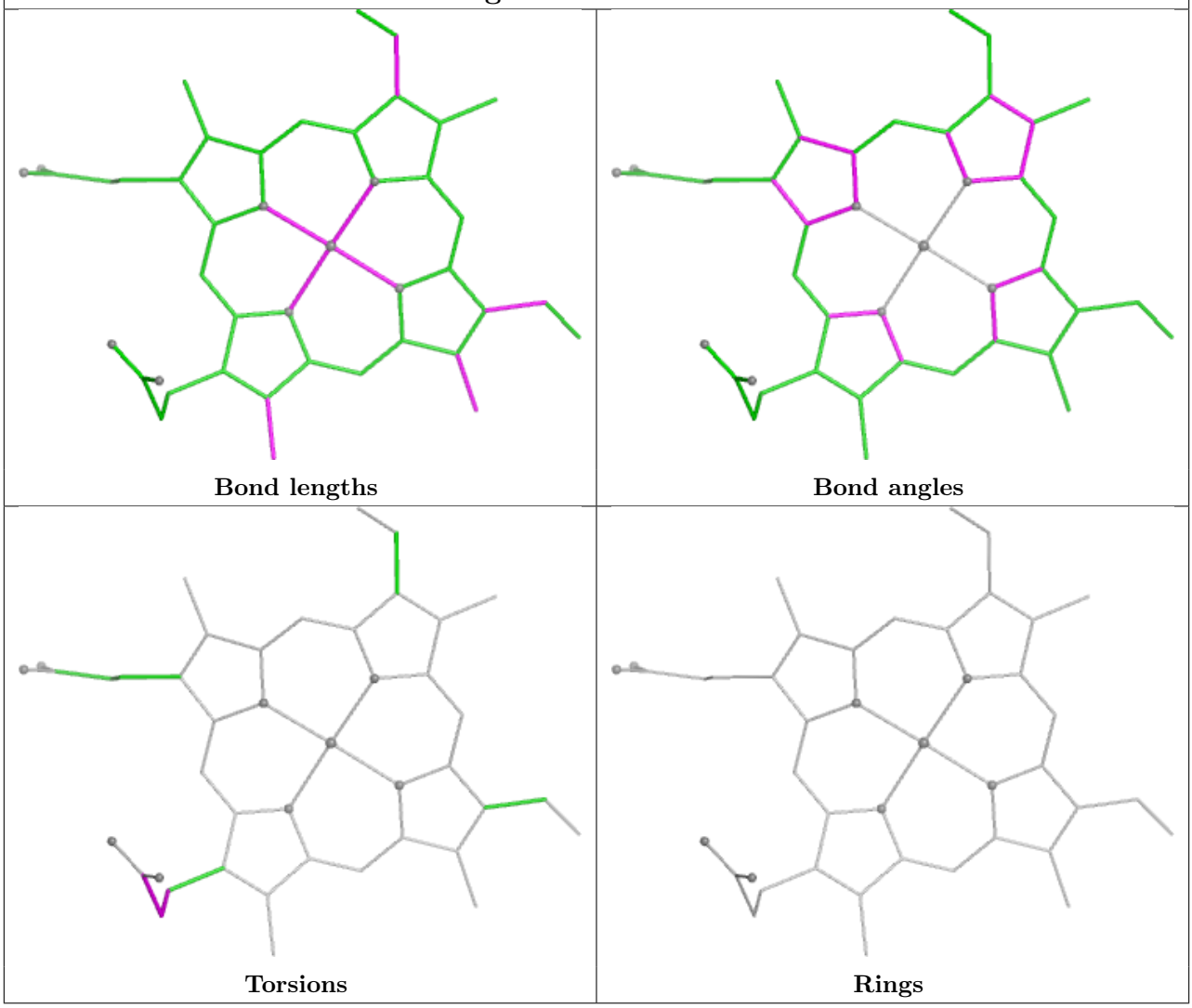


Rings

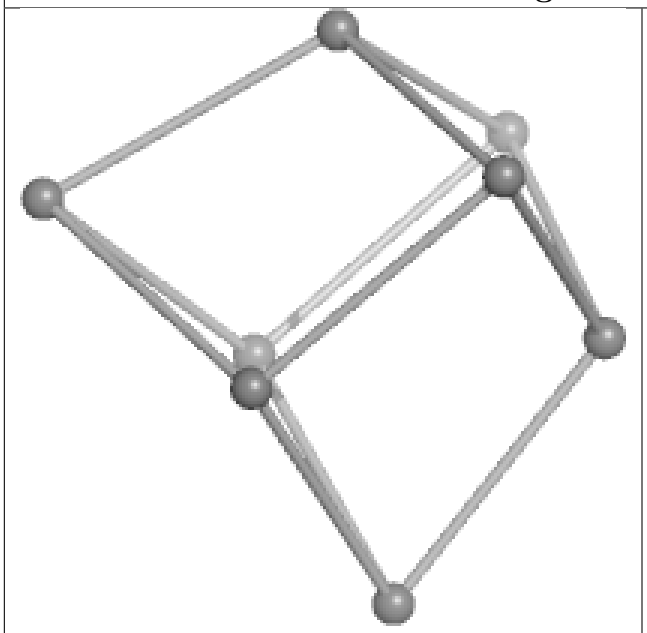
Ligand SF4 A 503



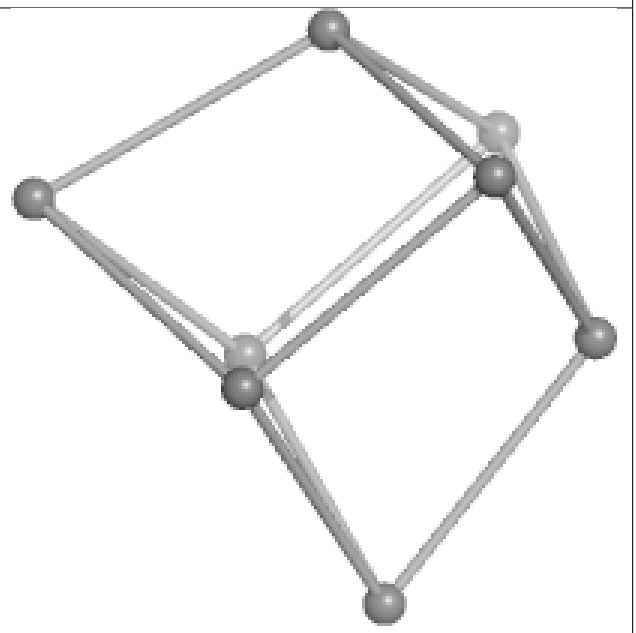
Ligand HEM L 401



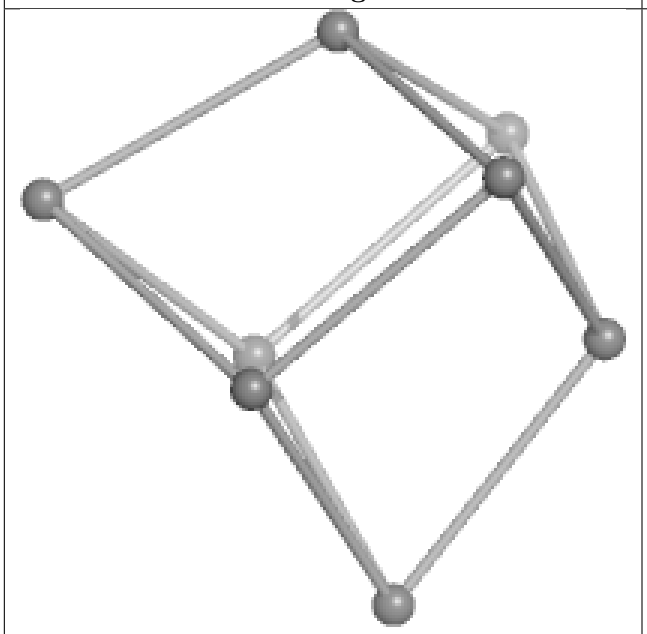
Ligand SF4 S 501



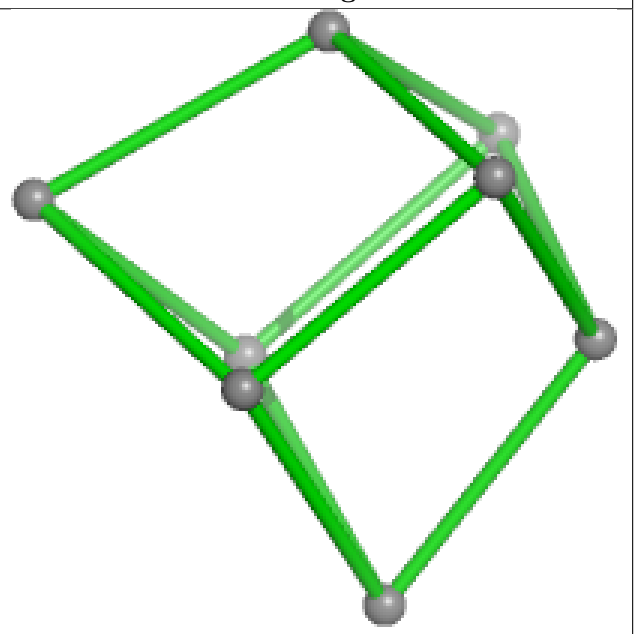
Bond lengths



Bond angles

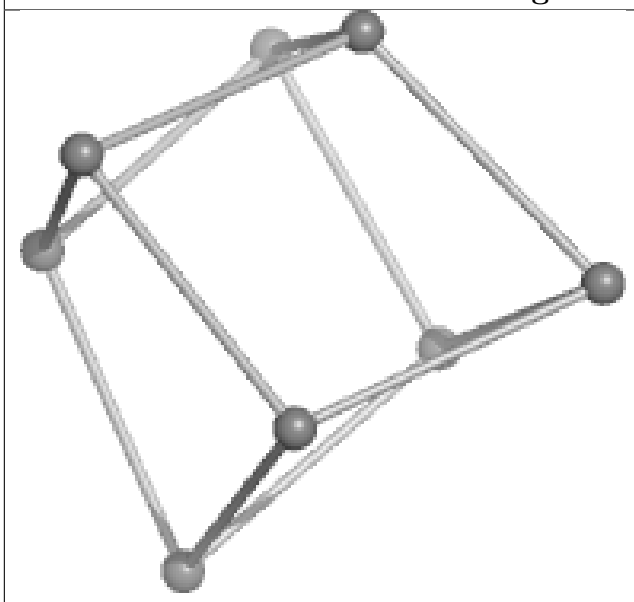


Torsions

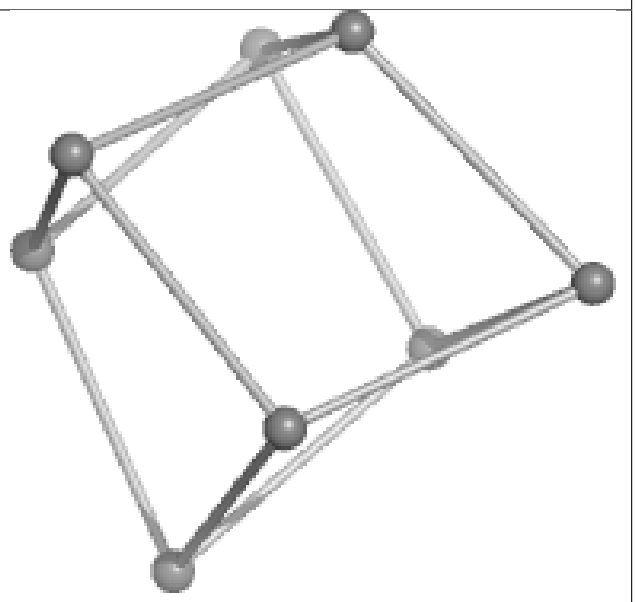


Rings

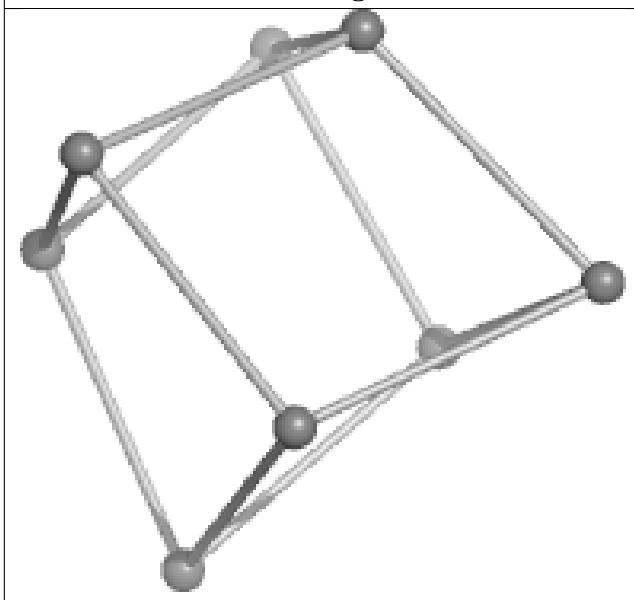
Ligand SF4 A 502



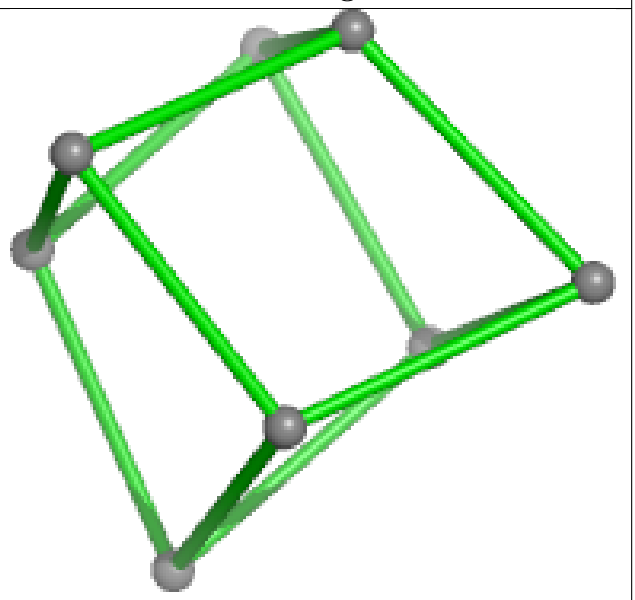
Bond lengths



Bond angles

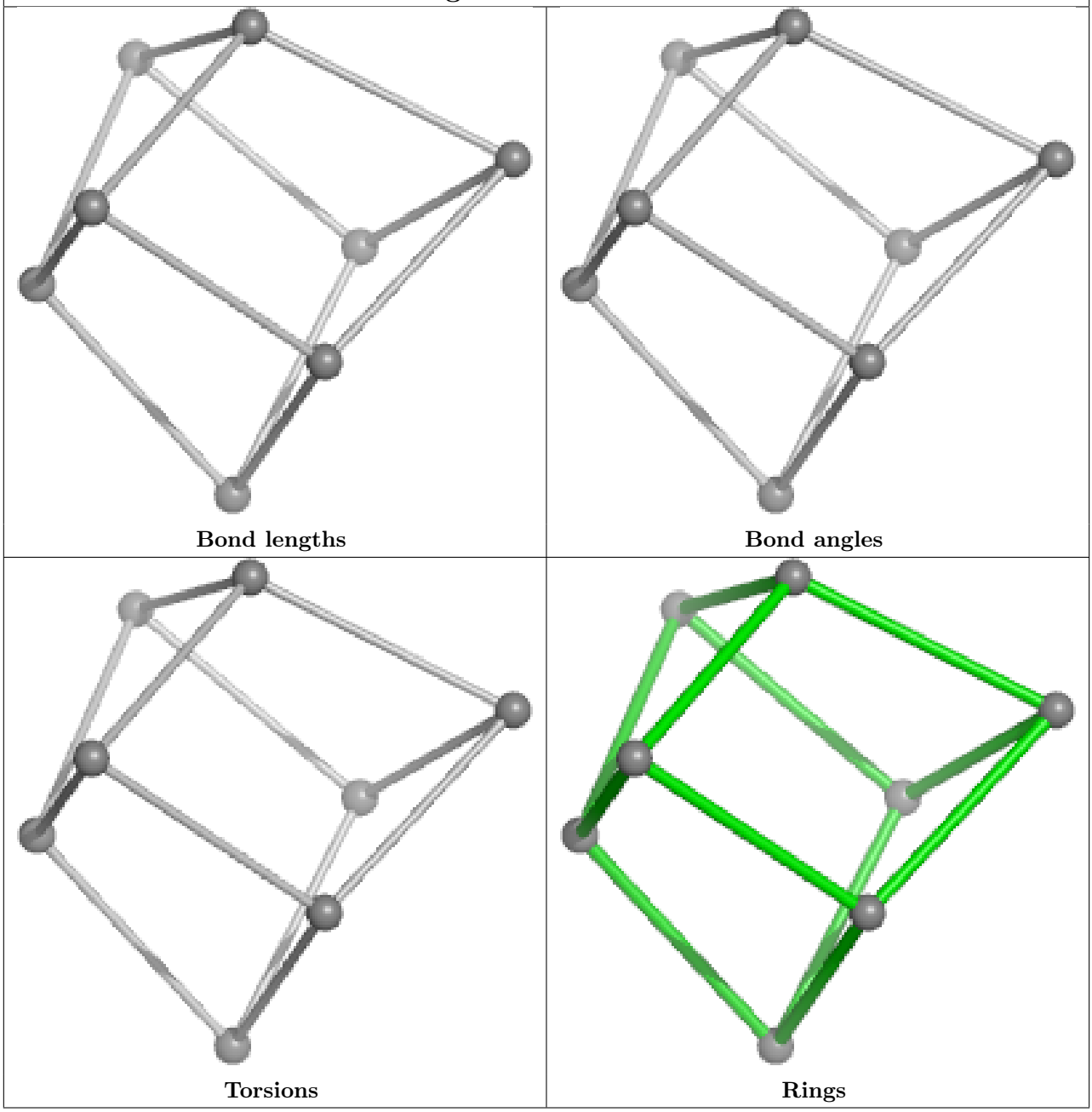


Torsions

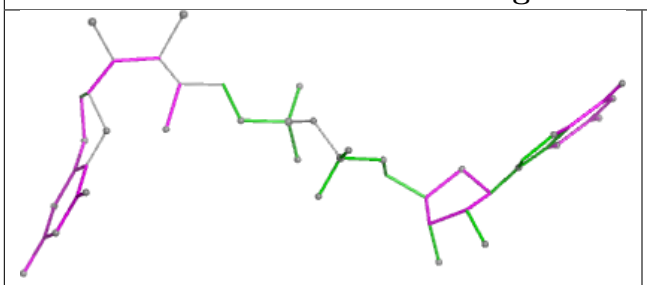


Rings

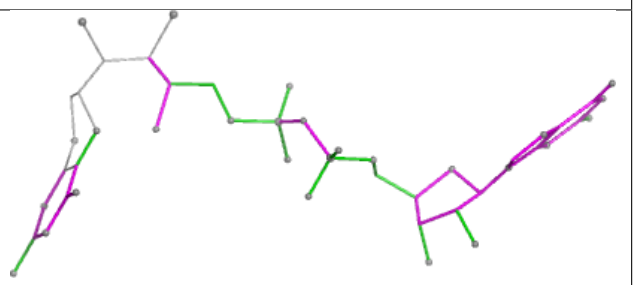
Ligand SF4 T 5804



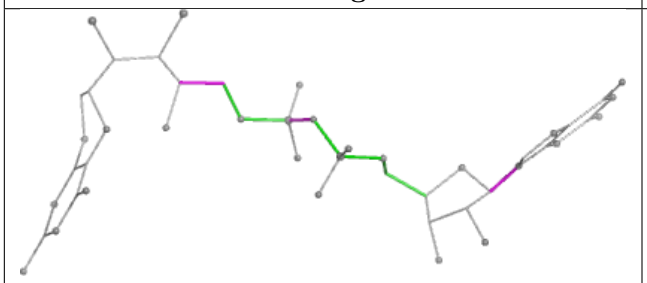
Ligand MD1 N 5802



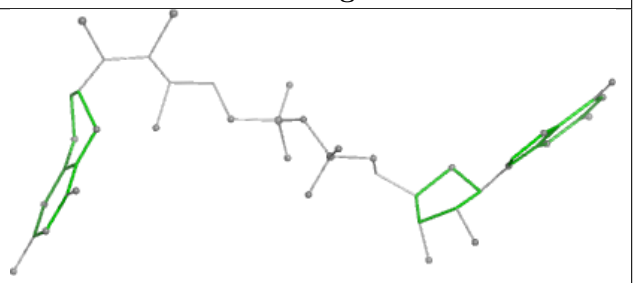
Bond lengths



Bond angles

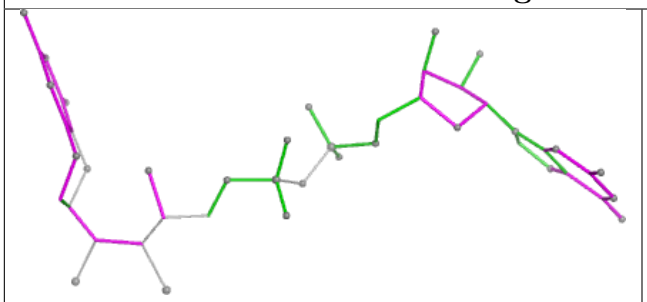


Torsions

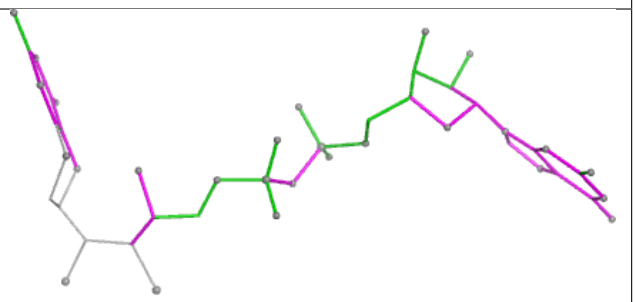


Rings

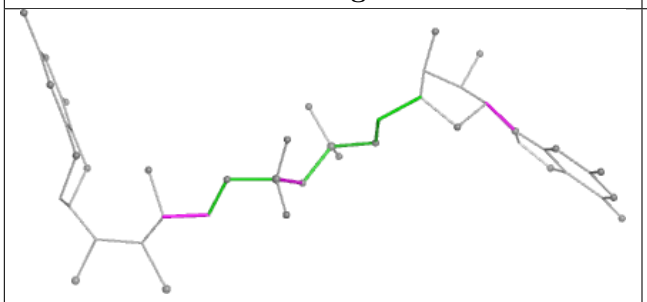
Ligand MD1 B 5802



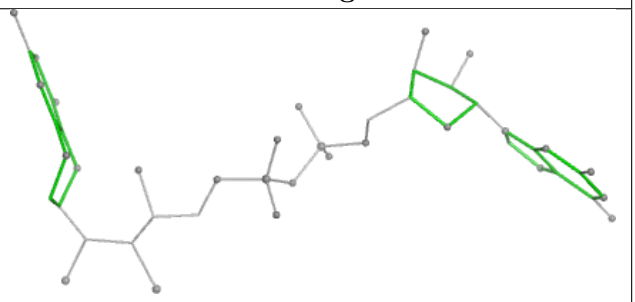
Bond lengths



Bond angles

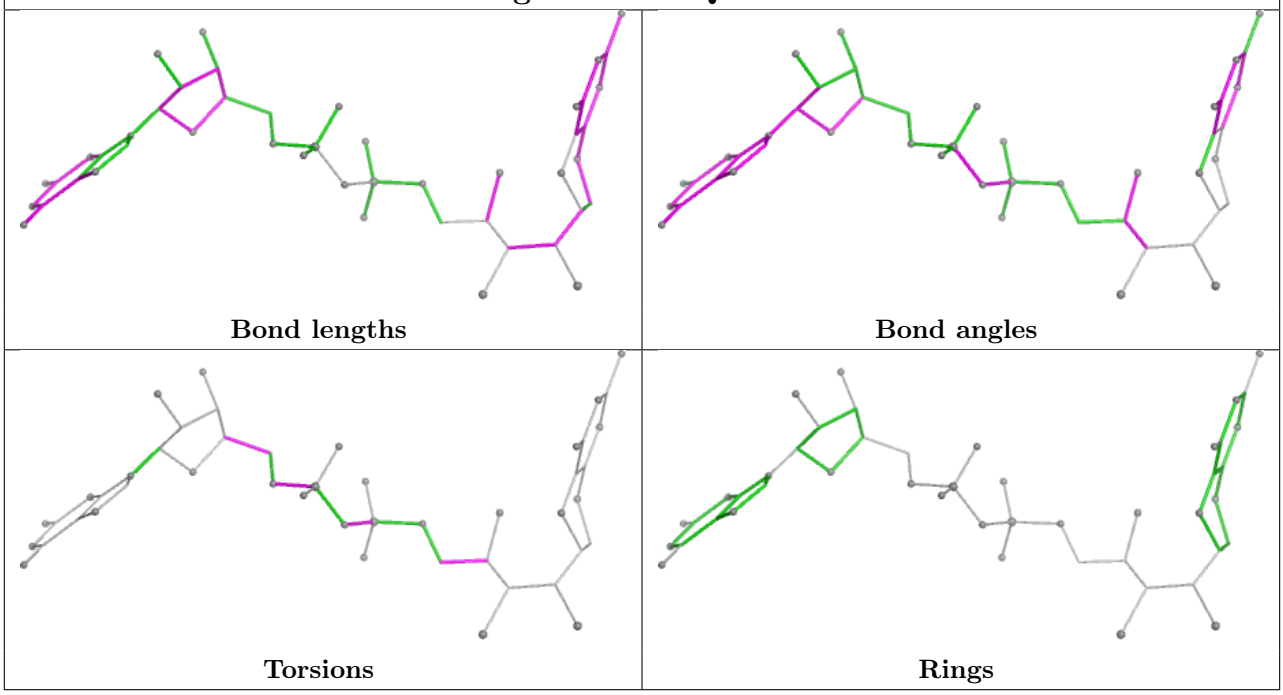


Torsions

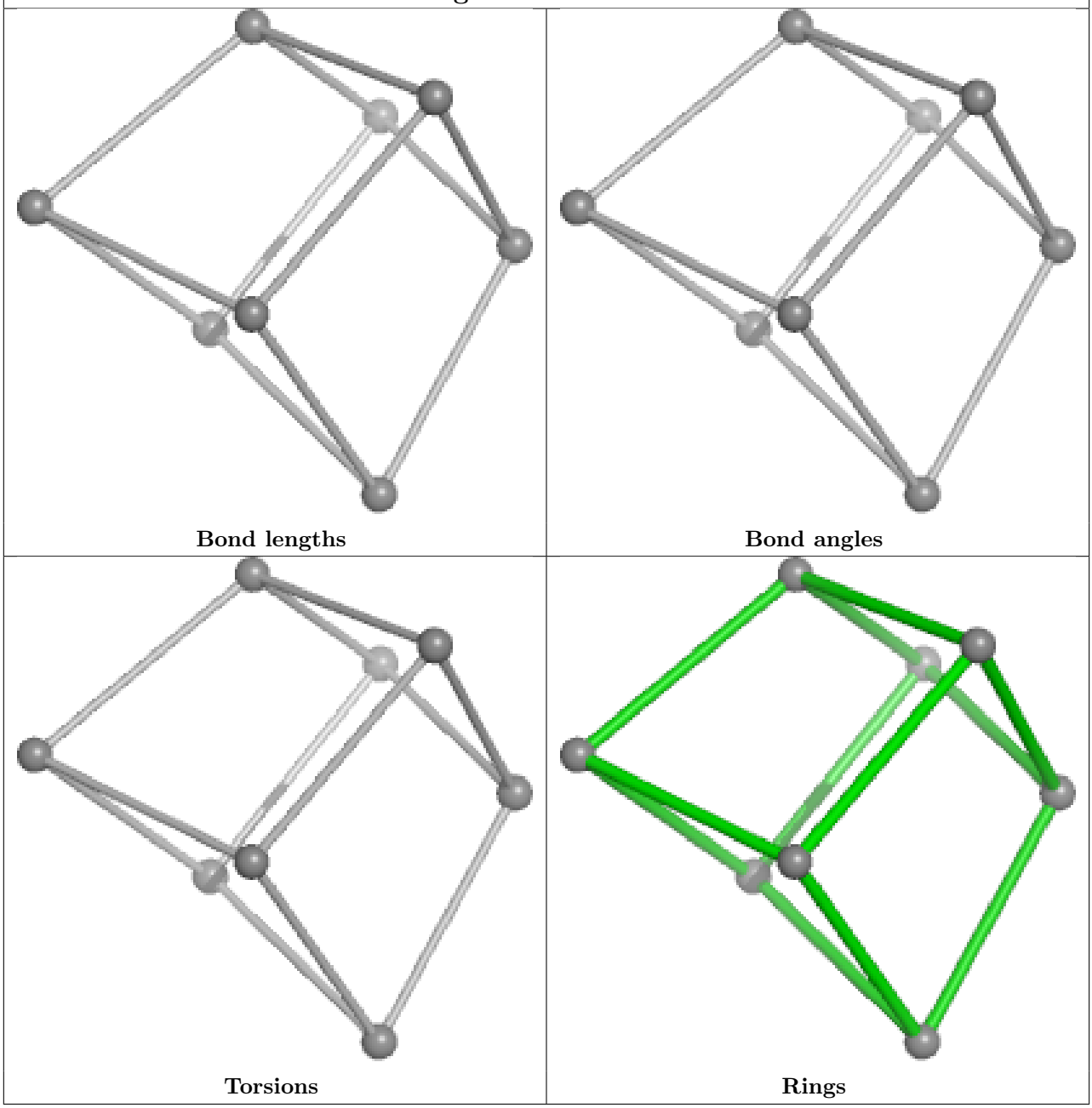


Rings

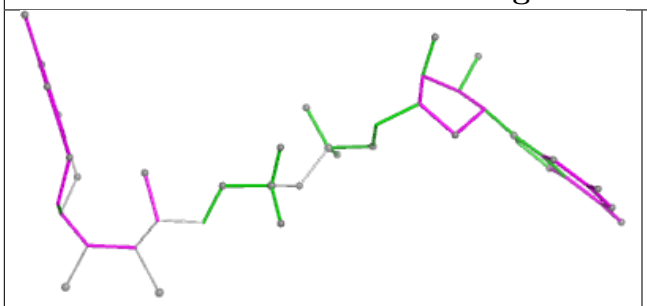
Ligand MD1 Q 5802



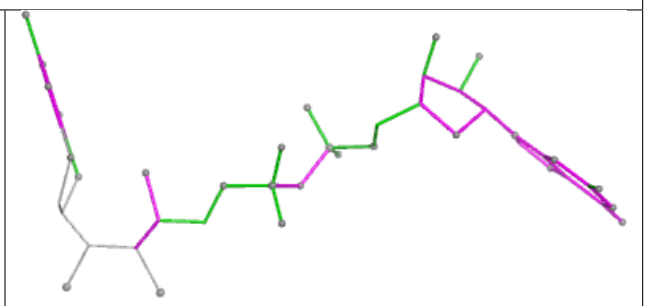
Ligand SF4 P 503



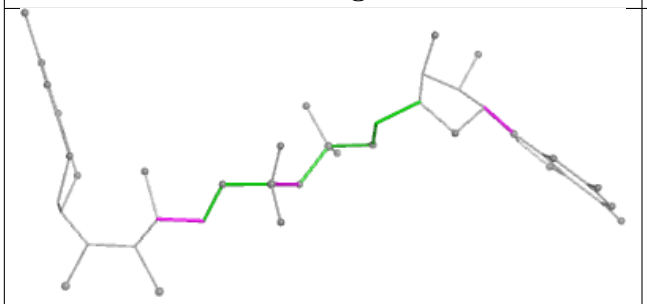
Ligand MD1 K 5802



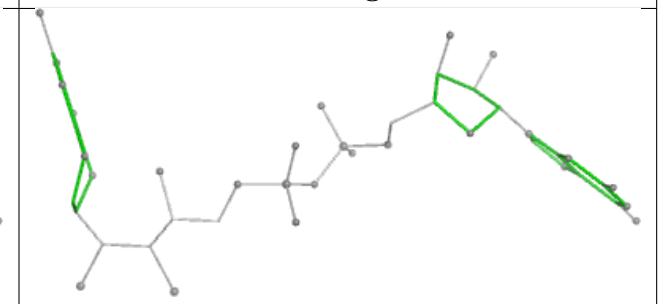
Bond lengths



Bond angles

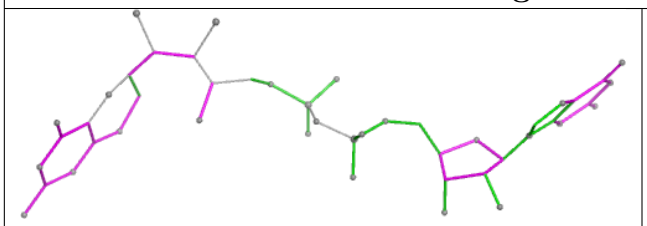


Torsions

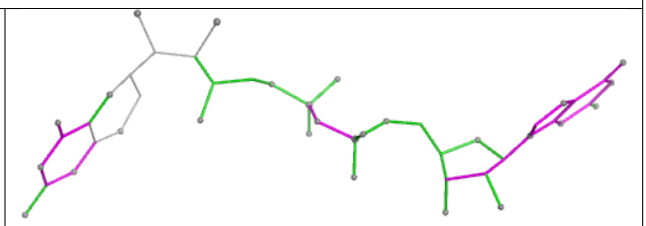


Rings

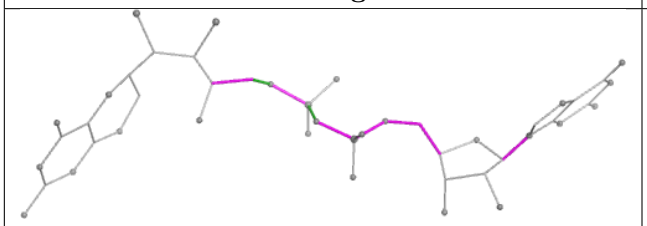
Ligand MD1 H 5801



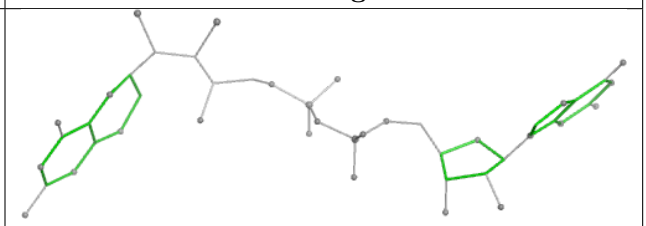
Bond lengths



Bond angles

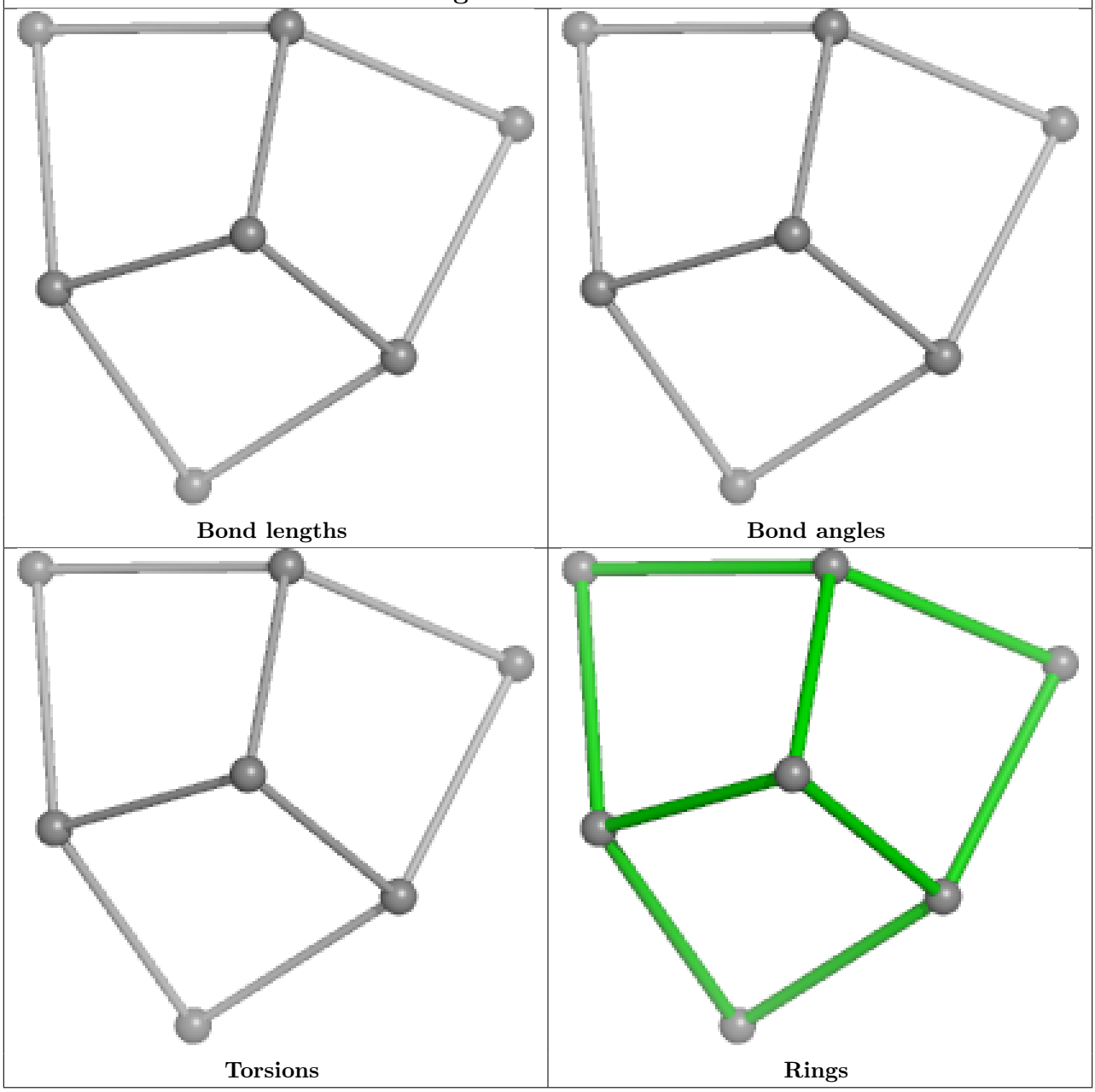


Torsions

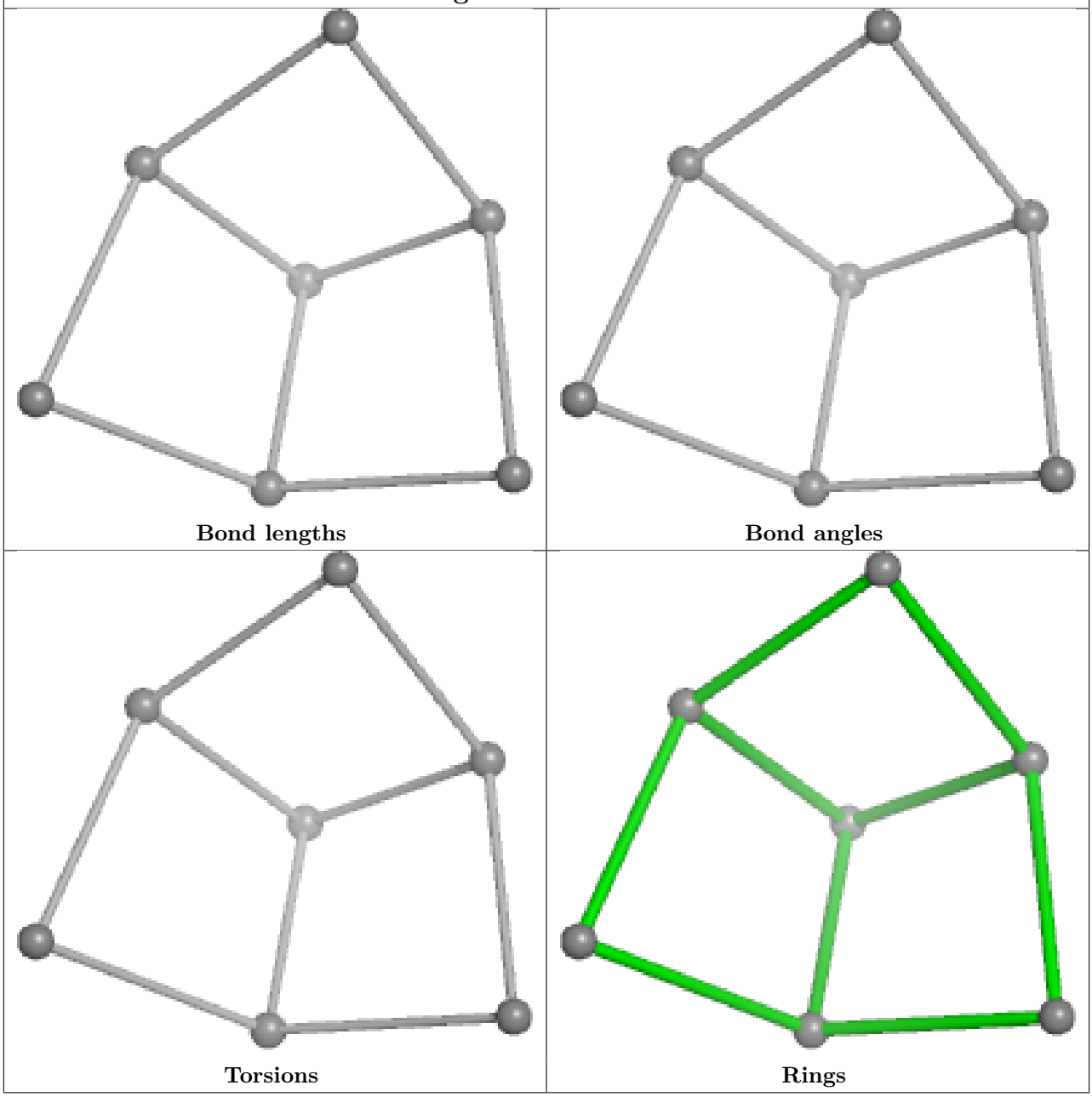


Rings

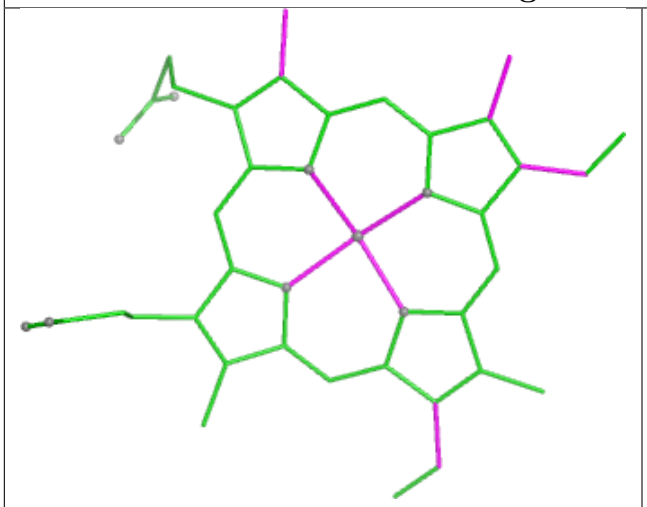
Ligand F3S G 504



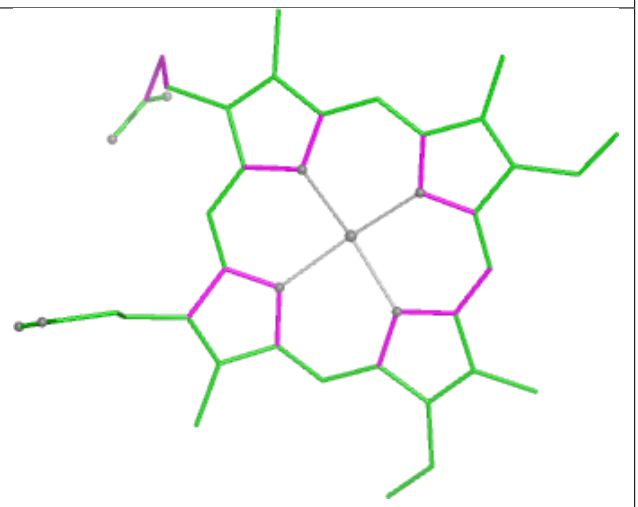
Ligand F3S P 504



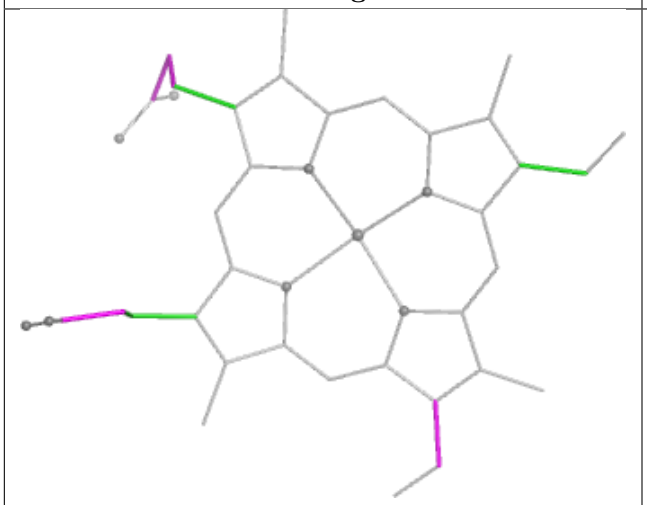
Ligand HEM R 401



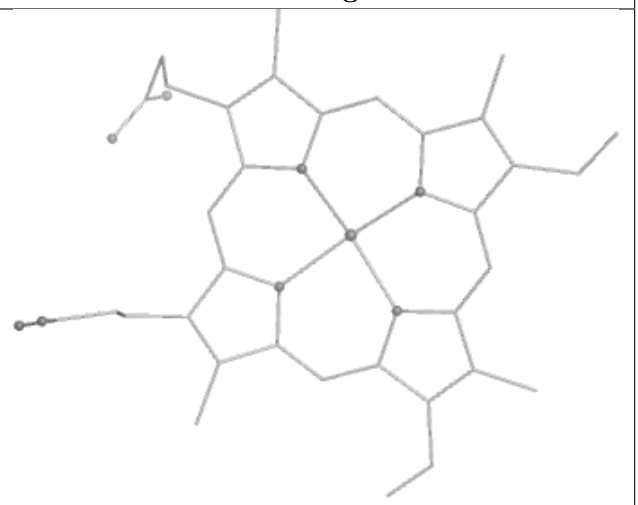
Bond lengths



Bond angles

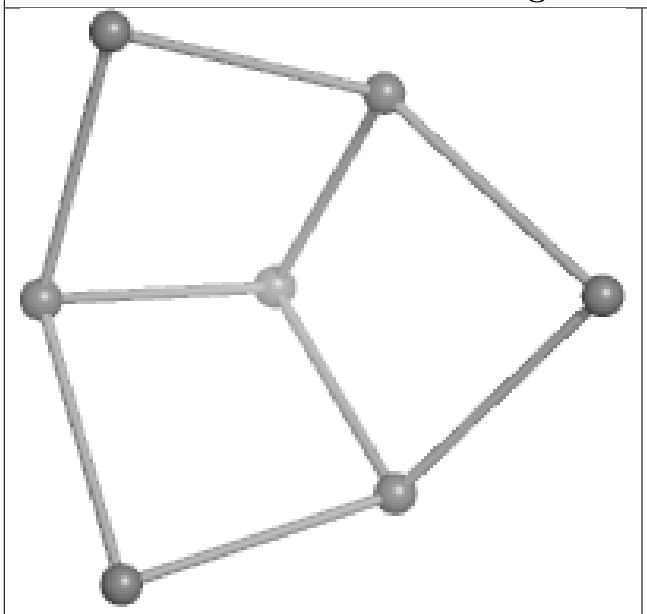


Torsions

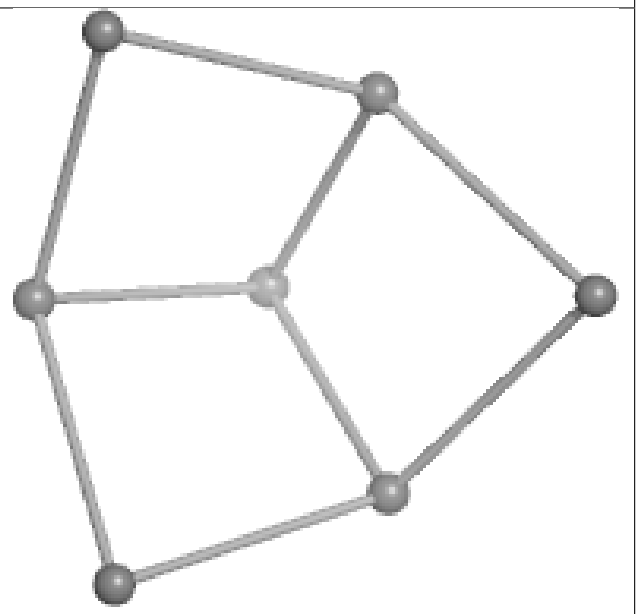


Rings

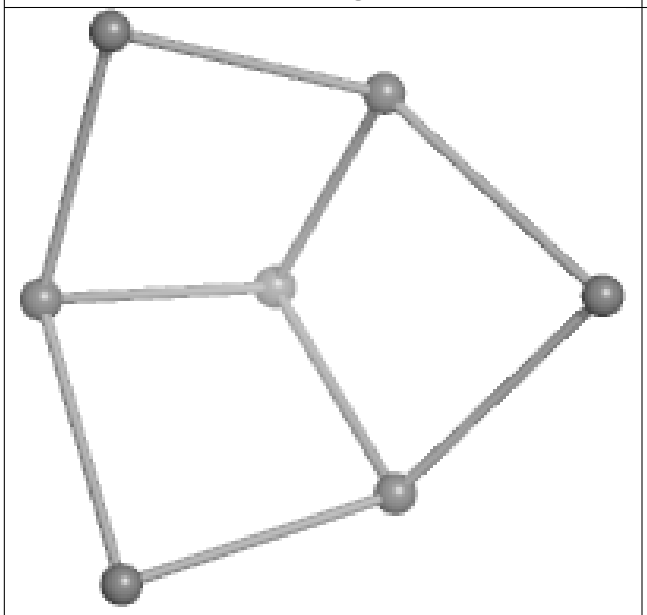
Ligand F3S M 504



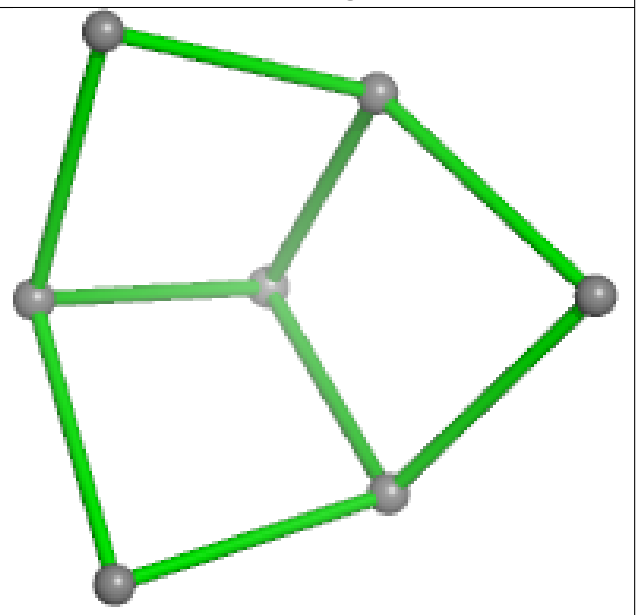
Bond lengths



Bond angles

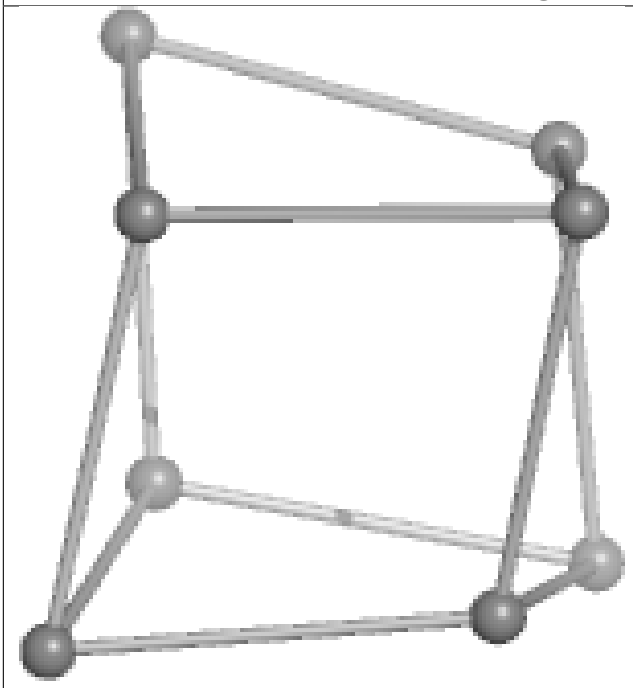


Torsions

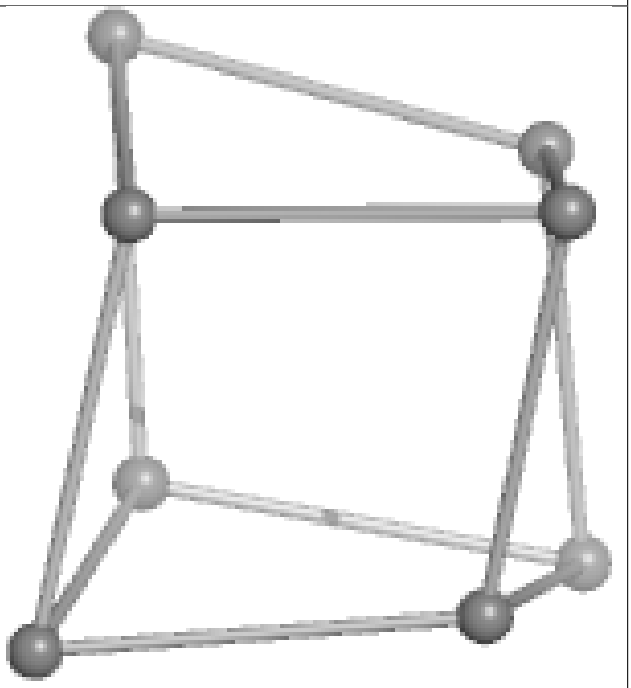


Rings

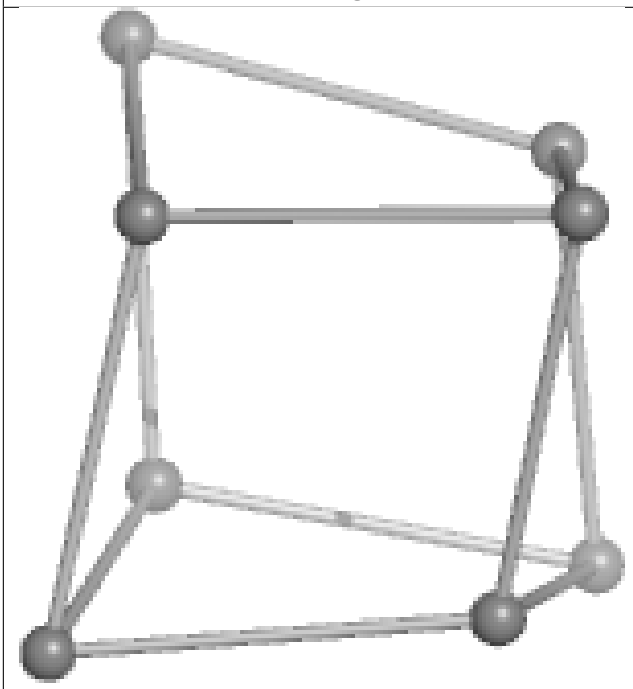
Ligand SF4 J 501



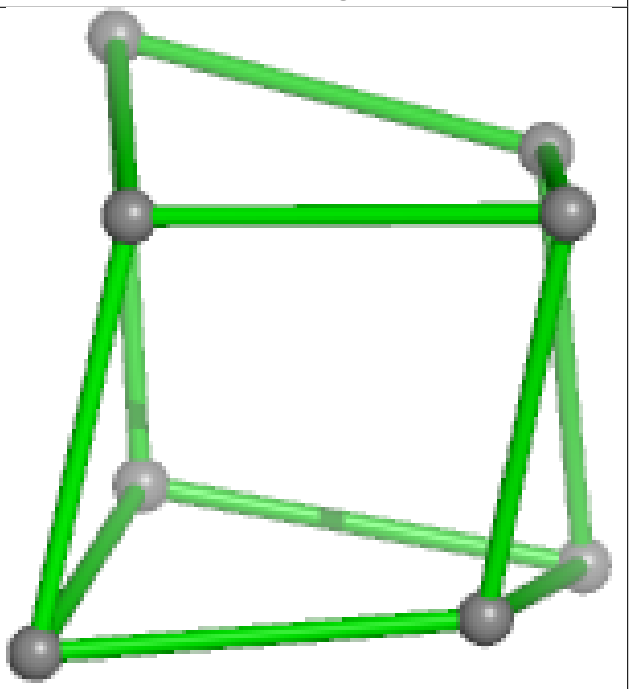
Bond lengths



Bond angles

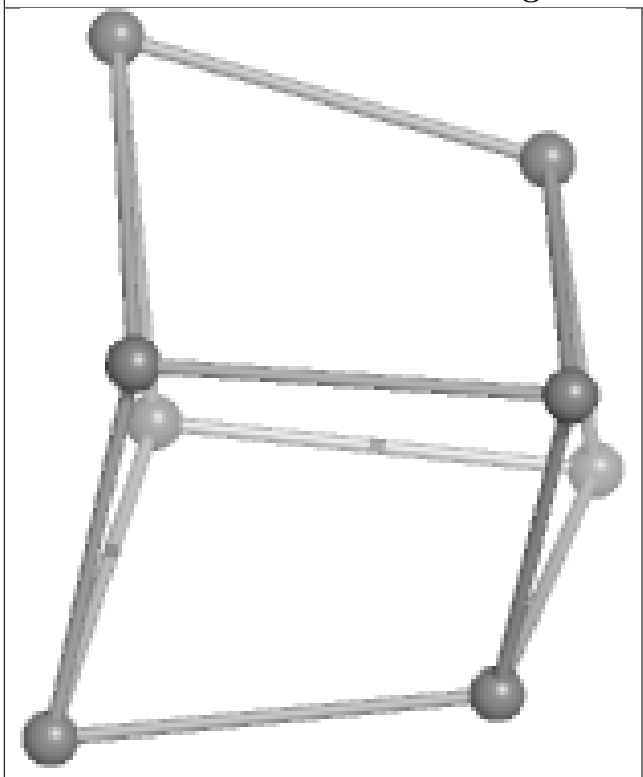


Torsions

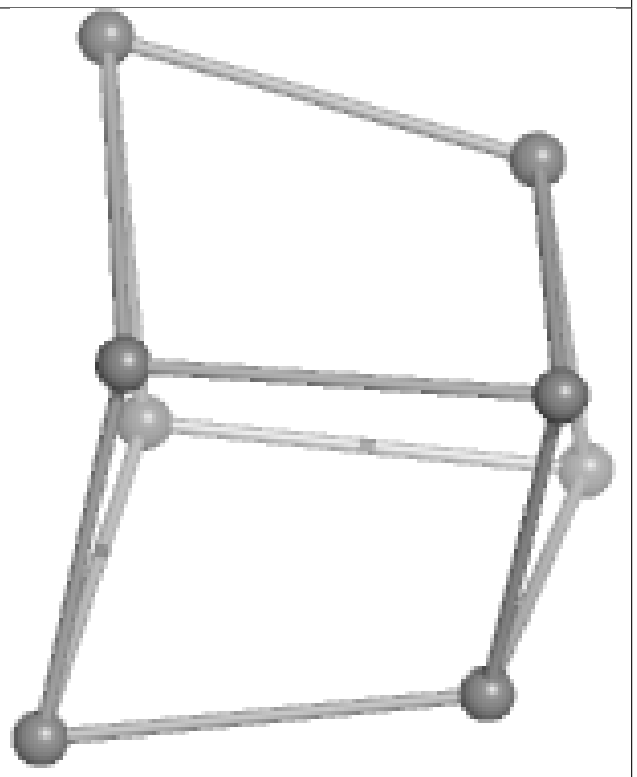


Rings

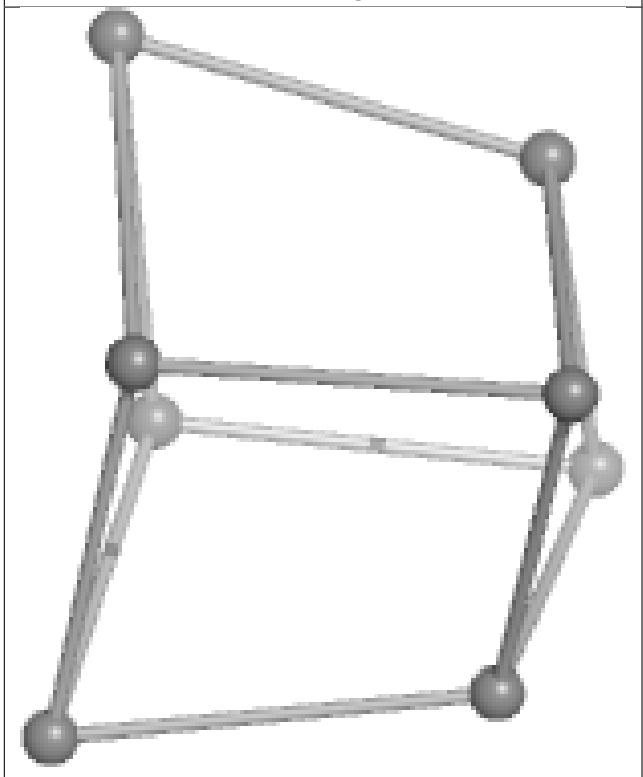
Ligand SF4 H 5804



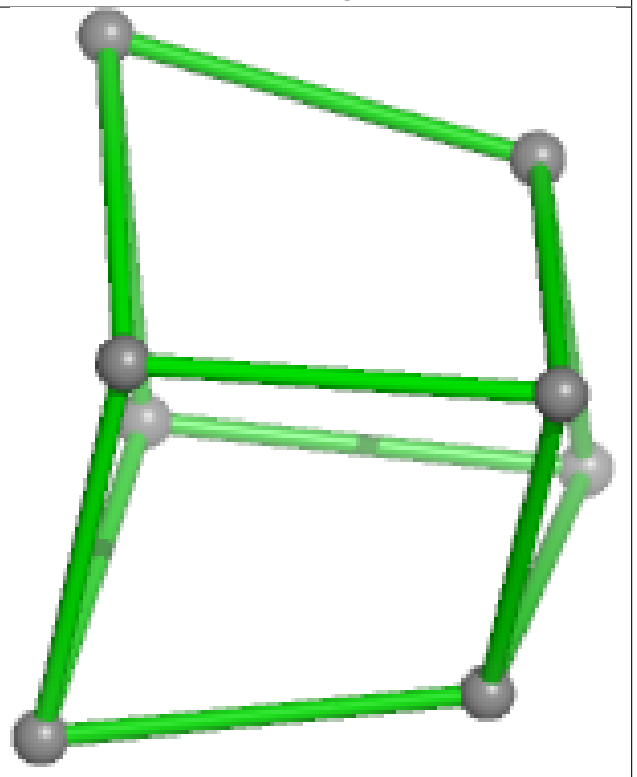
Bond lengths



Bond angles

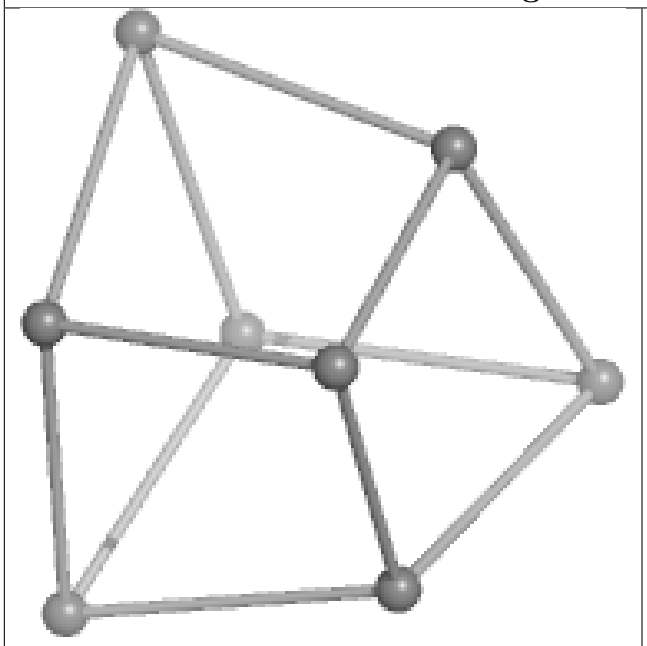


Torsions

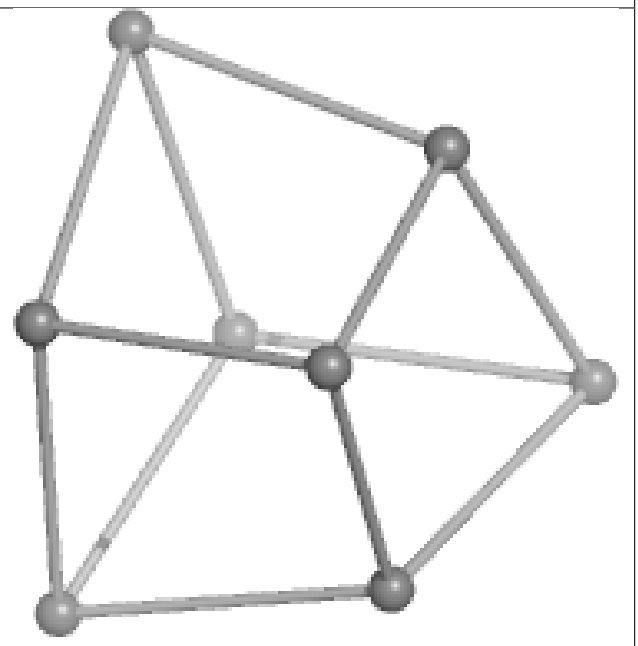


Rings

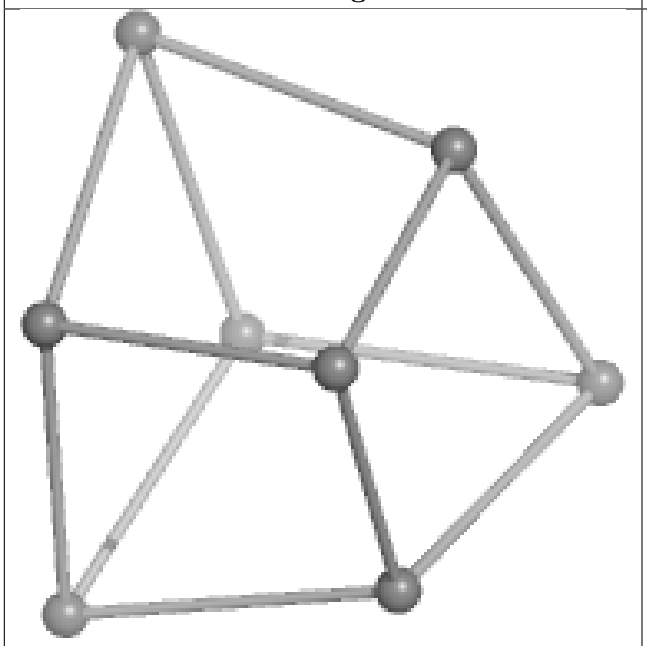
Ligand SF4 N 5804



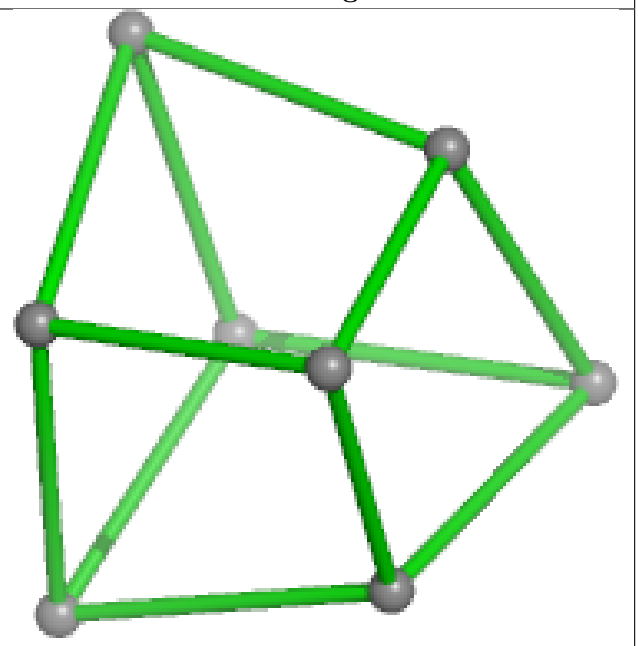
Bond lengths



Bond angles

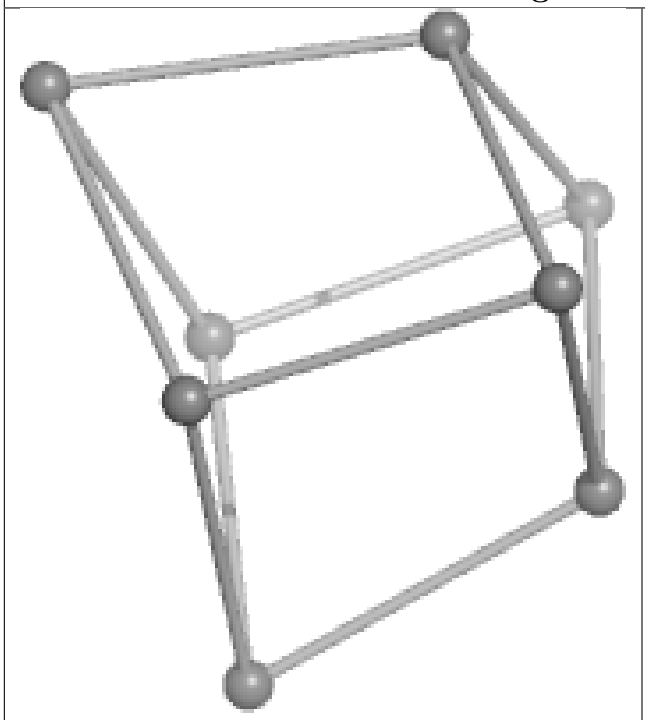


Torsions

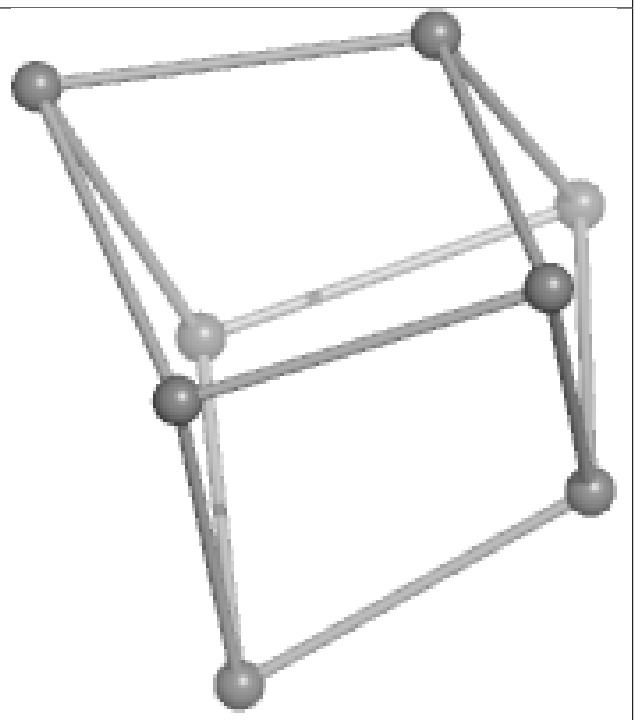


Rings

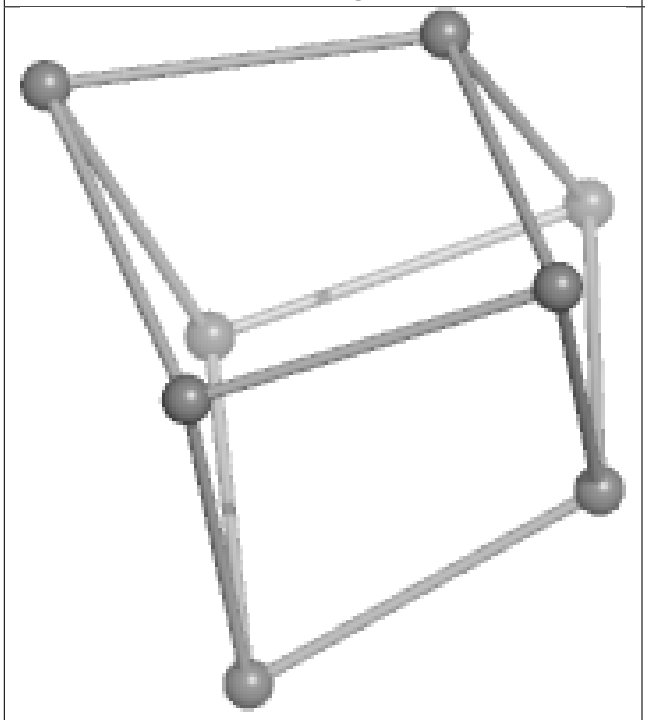
Ligand SF4 V 502



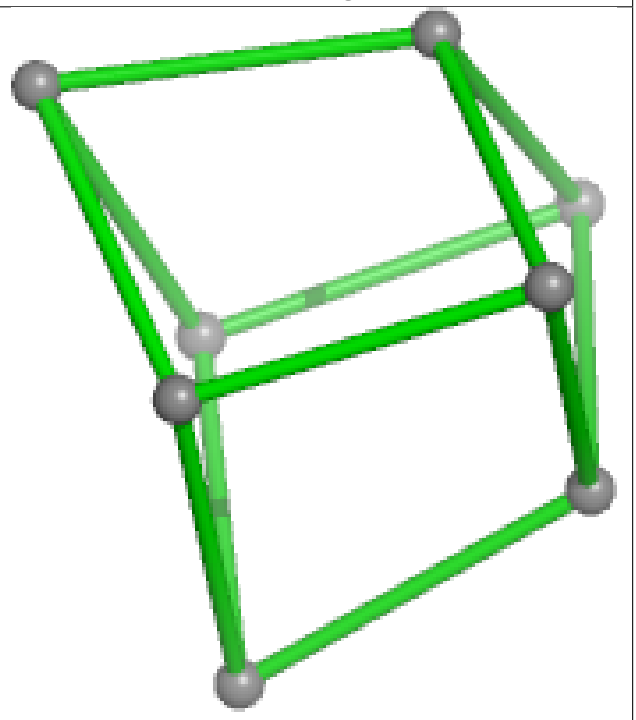
Bond lengths



Bond angles

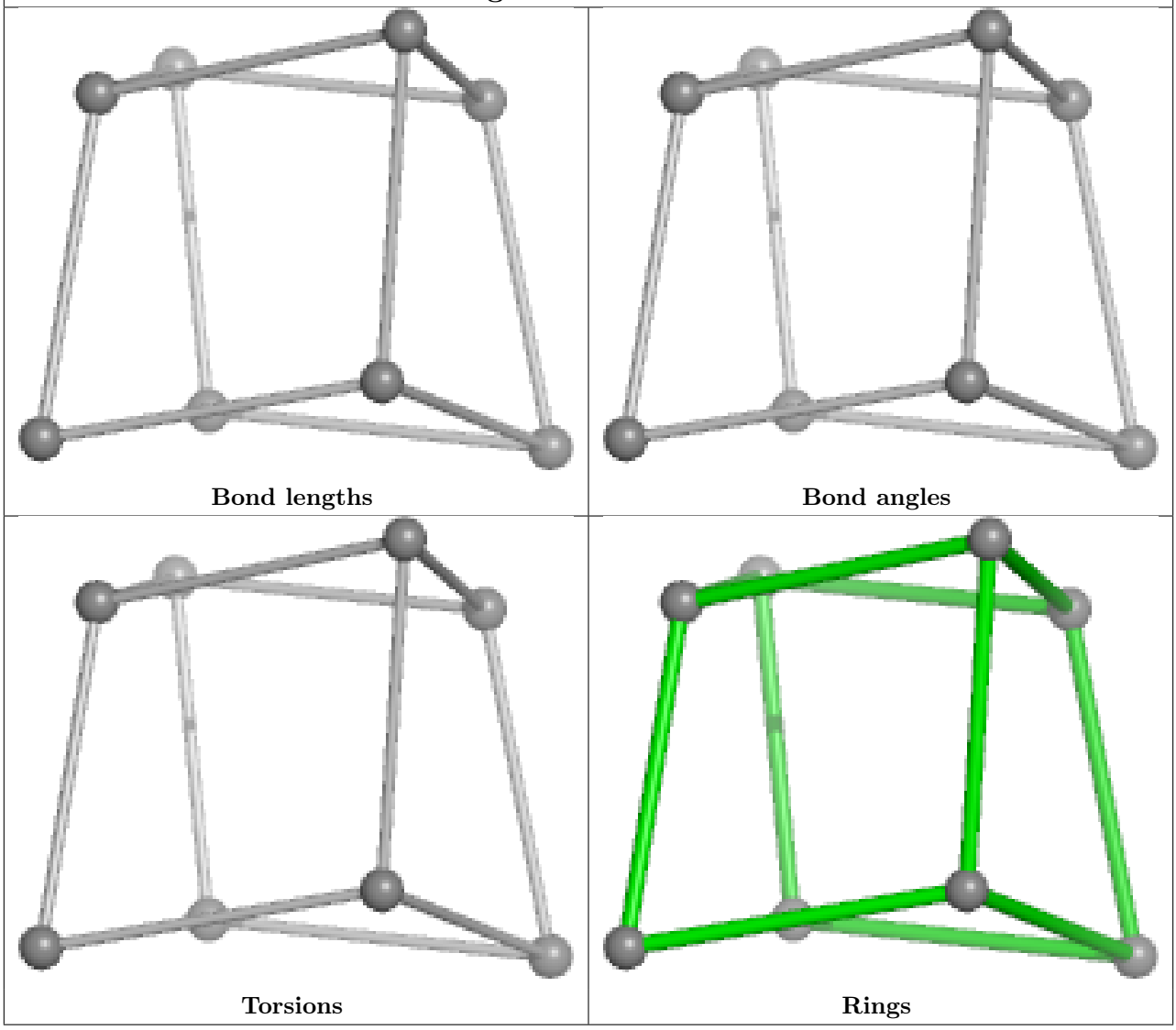


Torsions

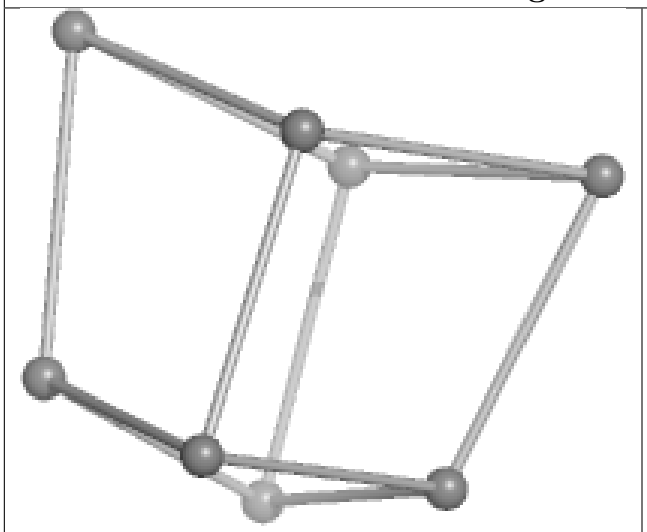


Rings

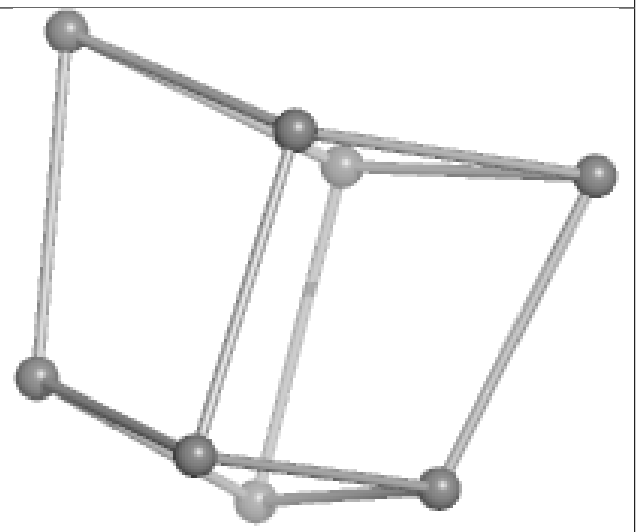
Ligand SF4 D 502



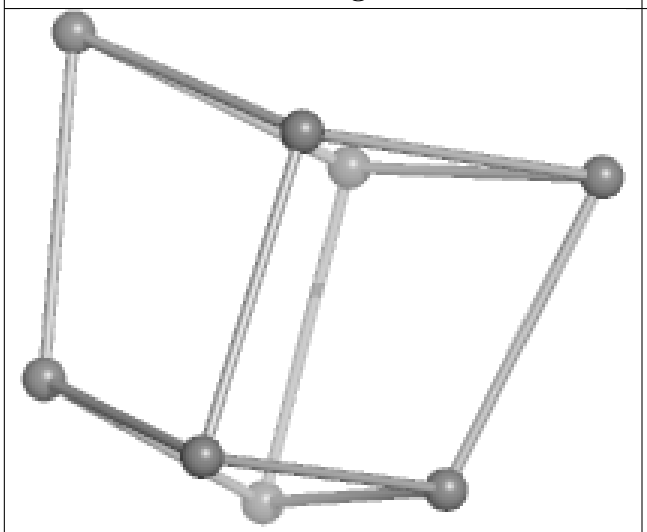
Ligand SF4 M 503



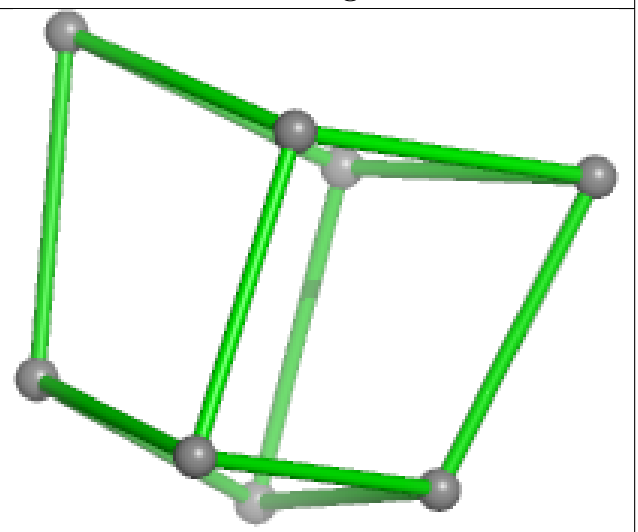
Bond lengths



Bond angles

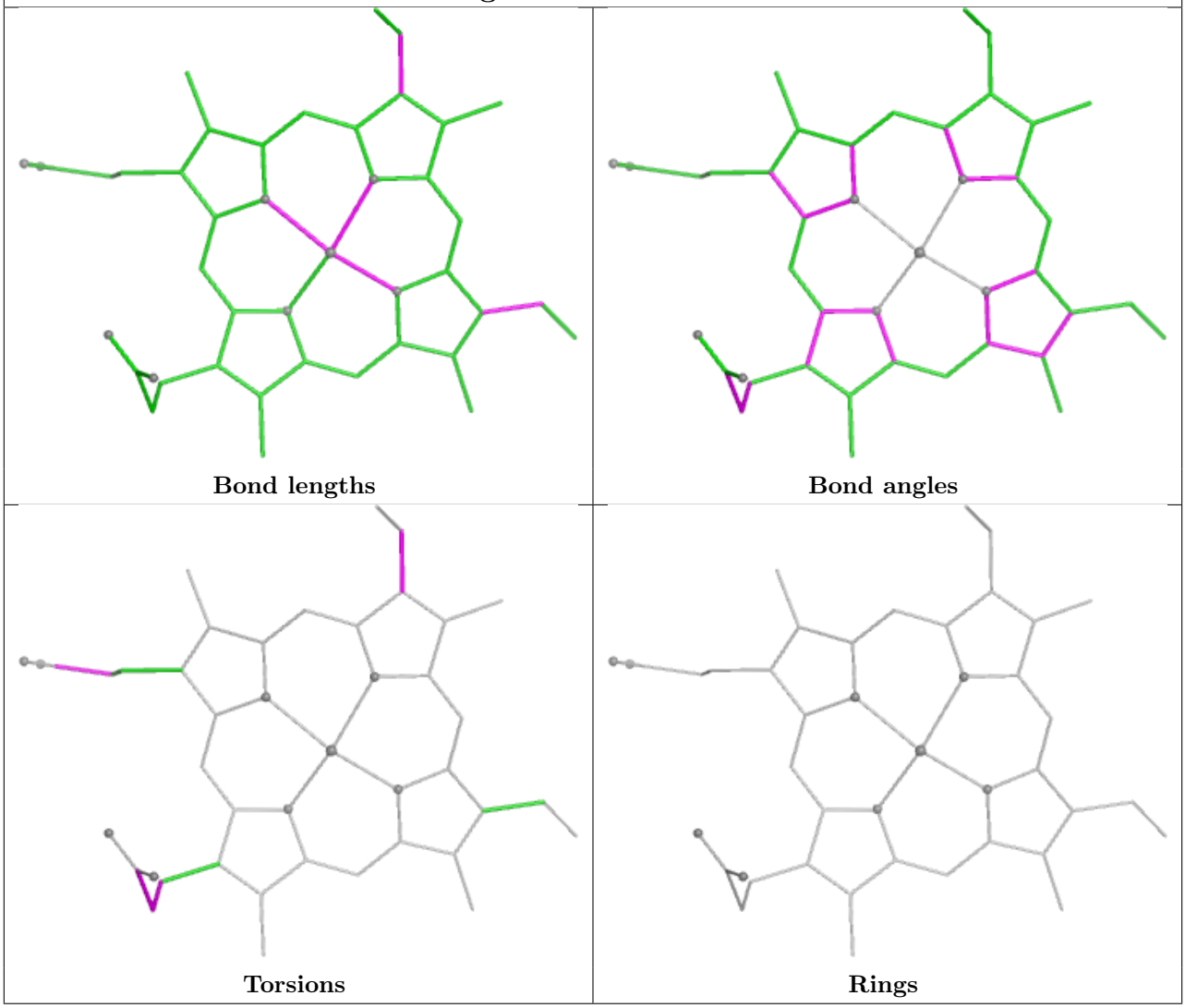


Torsions

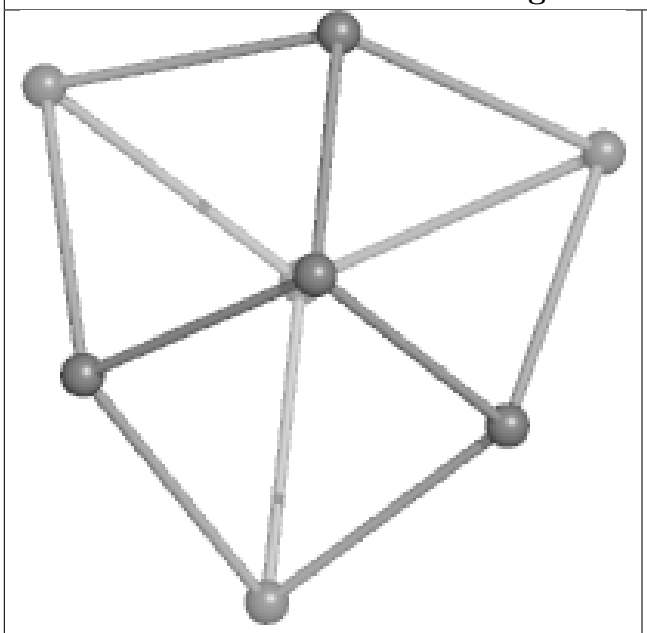


Rings

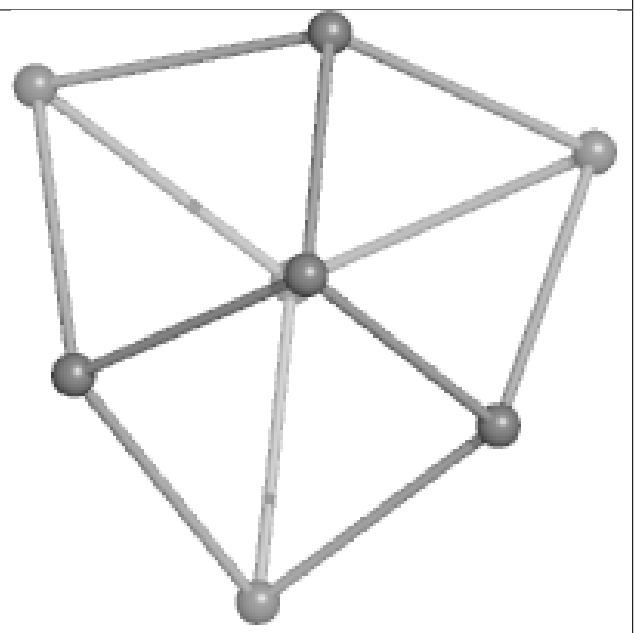
Ligand HEM C 401



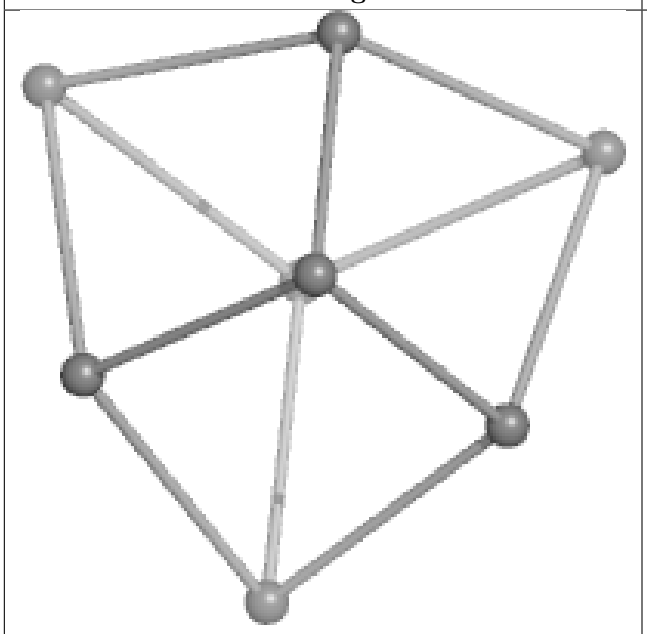
Ligand SF4 M 501



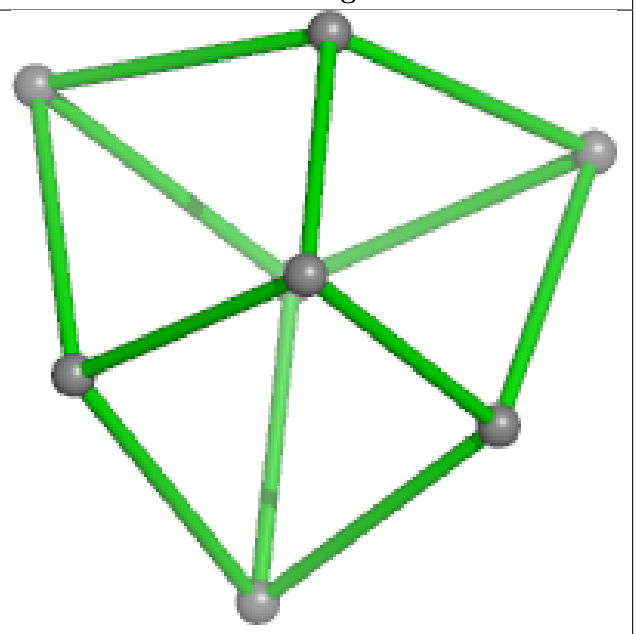
Bond lengths



Bond angles

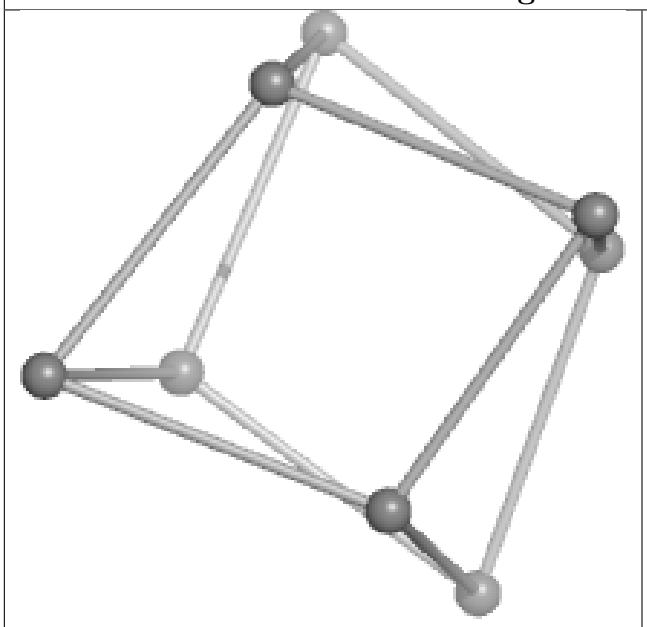


Torsions

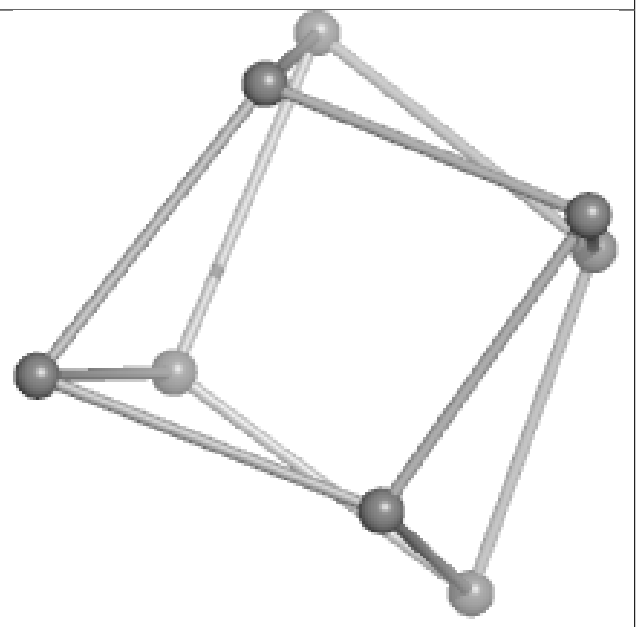


Rings

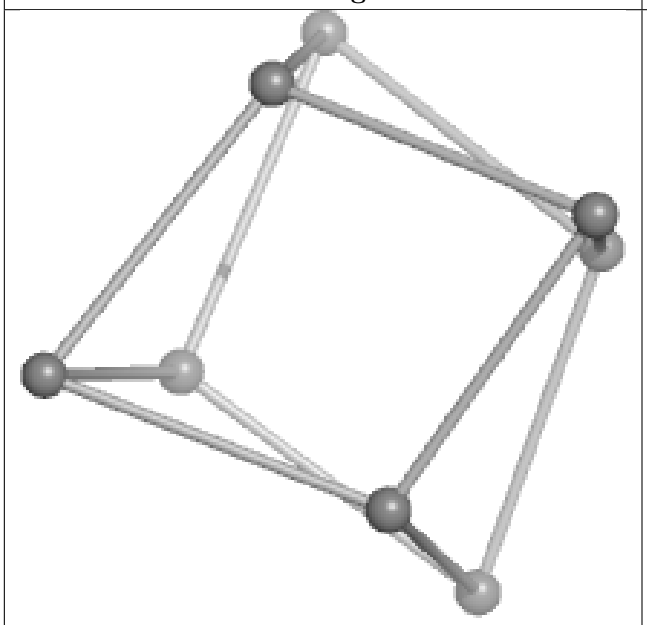
Ligand SF4 W 5804



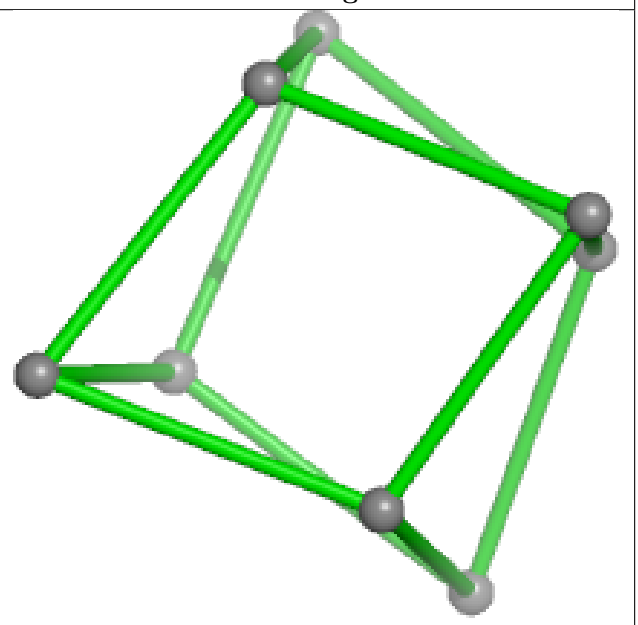
Bond lengths



Bond angles

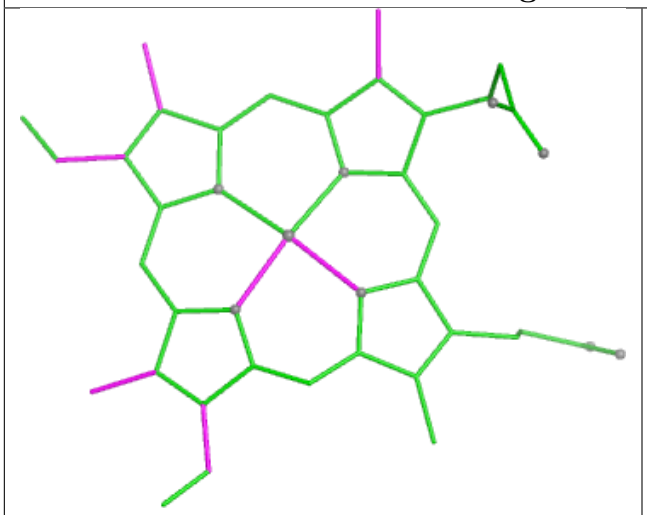


Torsions

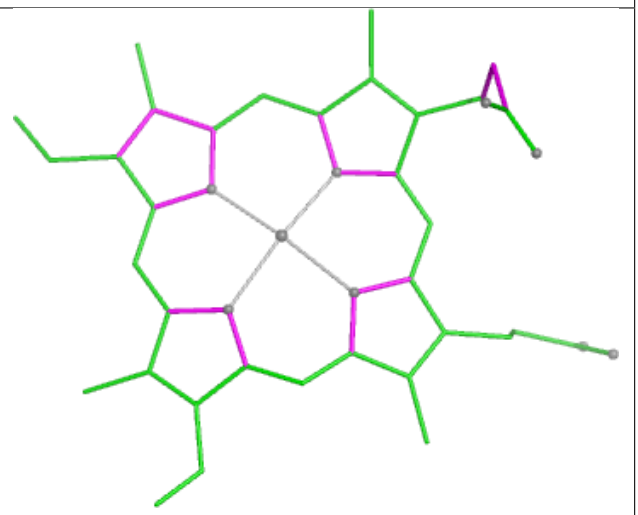


Rings

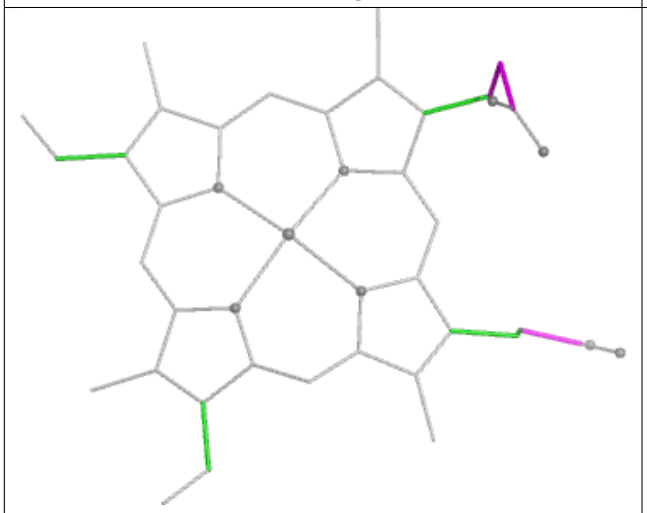
Ligand HEM O 401



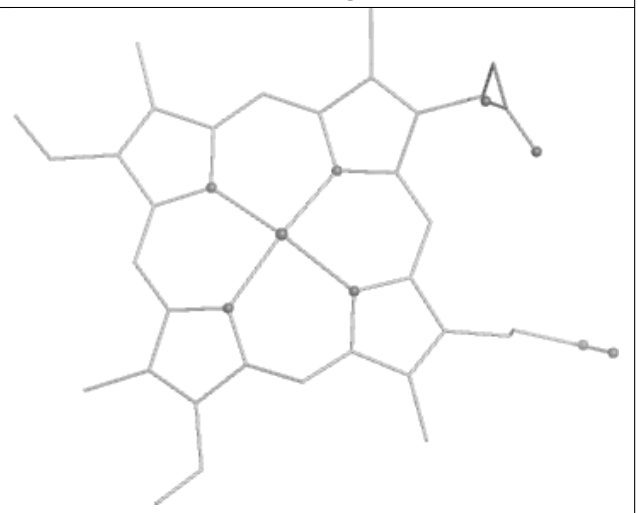
Bond lengths



Bond angles

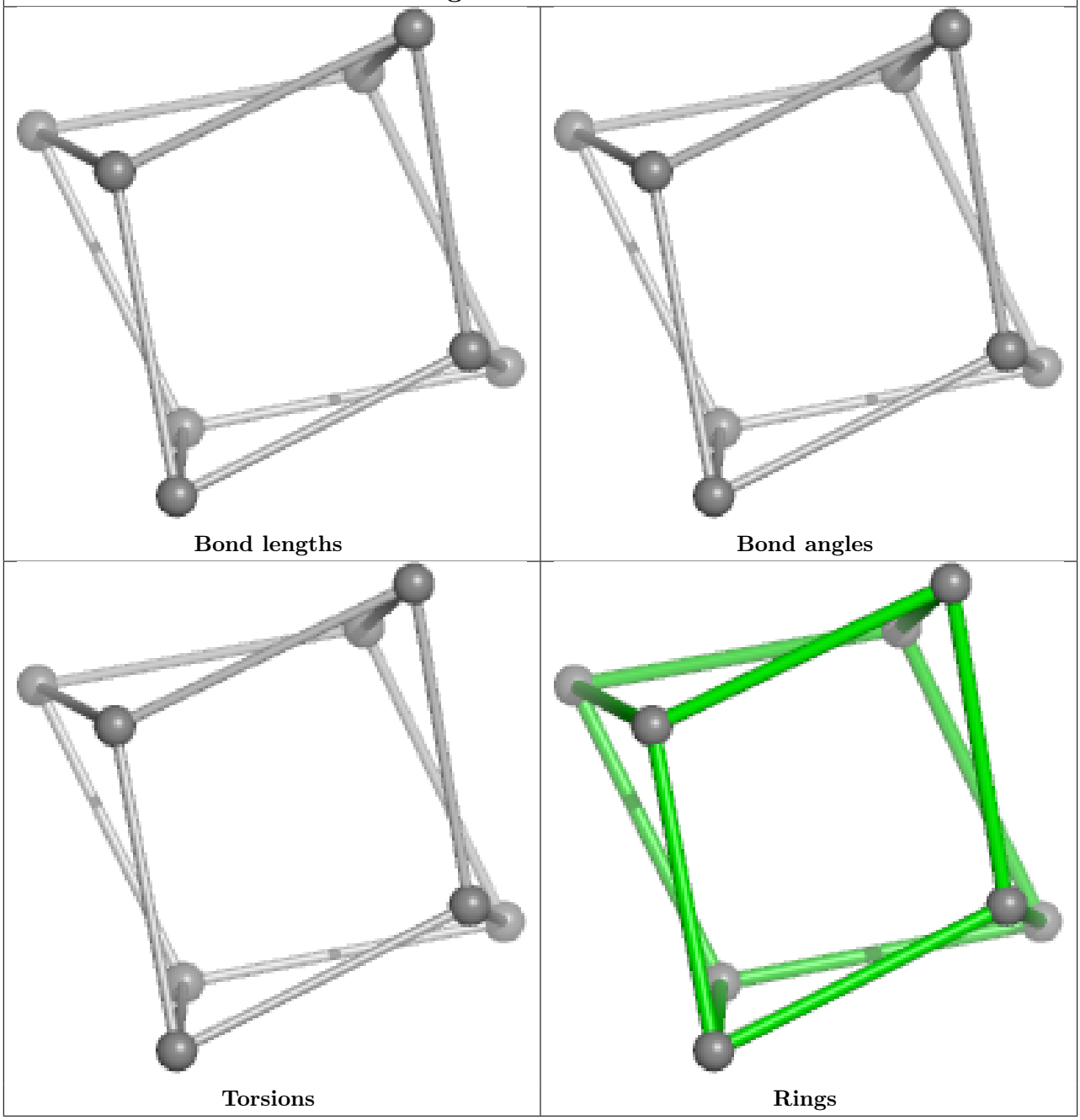


Torsions



Rings

Ligand SF4 G 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	663:VAL	C	664:TYR	N	1.68

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	409/410 (99%)	0.17	1 (0%) 91 85	22, 37, 53, 68	2 (0%)
1	D	408/410 (99%)	2.34	239 (58%) 0 0	66, 97, 117, 133	0
1	G	409/410 (99%)	0.13	6 (1%) 72 53	21, 32, 45, 93	0
1	J	409/410 (99%)	-0.14	1 (0%) 91 85	18, 25, 37, 58	0
1	M	409/410 (99%)	0.53	7 (1%) 69 50	27, 48, 65, 79	0
1	P	409/410 (99%)	0.65	18 (4%) 39 24	26, 46, 64, 77	3 (0%)
1	S	409/410 (99%)	0.22	0 100 100	21, 33, 47, 61	1 (0%)
1	V	409/410 (99%)	1.35	87 (21%) 2 2	43, 61, 79, 86	1 (0%)
2	B	1120/1148 (97%)	0.52	29 (2%) 57 38	19, 41, 62, 92	2 (0%)
2	E	1111/1148 (96%)	3.26	902 (81%) 0 0	61, 117, 155, 175	1 (0%)
2	H	1118/1148 (97%)	0.15	13 (1%) 76 59	16, 29, 45, 85	3 (0%)
2	K	1119/1148 (97%)	0.15	8 (0%) 84 70	17, 32, 47, 76	2 (0%)
2	N	1117/1148 (97%)	0.19	6 (0%) 87 75	18, 33, 54, 85	4 (0%)
2	Q	1116/1148 (97%)	0.65	41 (3%) 45 28	21, 47, 70, 92	6 (0%)
2	T	1119/1148 (97%)	0.32	12 (1%) 78 61	21, 37, 57, 88	2 (0%)
2	W	1118/1148 (97%)	0.83	59 (5%) 32 19	29, 49, 66, 95	5 (0%)
3	C	292/322 (90%)	0.17	7 (2%) 59 40	18, 31, 49, 72	1 (0%)
3	F	292/322 (90%)	1.40	54 (18%) 3 2	57, 83, 104, 121	0
3	I	292/322 (90%)	0.88	25 (8%) 16 10	25, 50, 69, 83	0
3	L	292/322 (90%)	0.20	3 (1%) 79 63	19, 31, 47, 70	1 (0%)
3	O	291/322 (90%)	1.21	54 (18%) 3 2	35, 69, 89, 102	0
3	R	291/322 (90%)	0.19	2 (0%) 84 70	23, 34, 51, 72	1 (0%)
3	U	292/322 (90%)	0.18	5 (1%) 69 50	23, 34, 51, 70	1 (0%)
3	X	292/322 (90%)	1.23	42 (14%) 6 4	30, 62, 76, 81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	14543/15040 (96%)	0.72	1621 (11%)	10	7	16, 41, 109, 175	36 (0%)

The worst 5 of 1621 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	710	ASN	9.7
2	E	112	PRO	8.8
2	E	713	SER	8.8
2	E	91	GLN	8.6
2	E	283	SER	8.5

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
6	MD1	E	5801	47/47	0.60	0.19	75,111,136,150	0
6	MD1	E	5802	47/47	0.70	0.17	80,117,133,137	0
8	HEM	F	401	43/43	0.81	0.18	77,97,112,116	0
4	SF4	D	503	8/8	0.83	0.11	107,133,158,166	0
9	CA	F	403	1/1	0.83	0.11	104,104,104,104	0
4	SF4	D	501	8/8	0.85	0.18	91,115,146,160	0
5	F3S	V	504	7/7	0.87	0.14	65,87,97,112	0
8	HEM	X	401	43/43	0.88	0.17	59,75,81,89	0
4	SF4	E	5804	8/8	0.88	0.12	119,125,139,167	0
5	F3S	D	504	7/7	0.89	0.10	99,113,128,134	0
9	CA	F	402	1/1	0.90	0.11	76,76,76,76	0
8	HEM	O	401	43/43	0.90	0.15	57,69,75,84	0
6	MD1	Q	5802	47/47	0.91	0.13	30,43,56,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SF4	D	502	8/8	0.91	0.09	112,118,142,149	0
9	CA	U	403	1/1	0.91	0.07	29,29,29,29	0
8	HEM	I	401	43/43	0.92	0.12	38,55,65,66	0
6	MD1	W	5802	47/47	0.92	0.12	28,47,62,72	0
6	MD1	Q	5801	47/47	0.92	0.11	21,34,44,54	0
4	SF4	V	501	8/8	0.93	0.10	43,63,75,78	0
6	MD1	W	5801	47/47	0.93	0.12	31,46,57,69	0
6	MD1	N	5802	47/47	0.94	0.11	26,34,44,46	0
6	MD1	B	5801	47/47	0.94	0.12	24,34,40,41	0
9	CA	L	403	1/1	0.94	0.08	29,29,29,29	0
6	MD1	B	5802	47/47	0.94	0.11	28,42,50,56	0
9	CA	X	403	1/1	0.94	0.07	71,71,71,71	0
4	SF4	W	5804	8/8	0.95	0.10	40,57,63,72	0
6	MD1	H	5801	47/47	0.95	0.09	16,24,36,38	0
6	MD1	H	5802	47/47	0.95	0.10	15,30,36,47	0
9	CA	C	403	1/1	0.95	0.06	35,35,35,35	0
6	MD1	T	5802	47/47	0.95	0.10	22,31,41,45	0
6	MD1	K	5801	47/47	0.95	0.09	20,25,33,37	0
9	CA	I	403	1/1	0.95	0.07	69,69,69,69	0
6	MD1	K	5802	47/47	0.95	0.10	15,29,38,45	0
8	HEM	C	401	43/43	0.95	0.12	19,27,32,49	0
6	MD1	N	5801	47/47	0.95	0.10	21,28,34,48	0
8	HEM	L	401	43/43	0.96	0.10	17,24,30,33	0
4	SF4	K	5804	8/8	0.96	0.09	18,32,40,42	0
8	HEM	R	401	43/43	0.96	0.10	23,33,40,46	0
8	HEM	U	401	43/43	0.96	0.10	23,30,34,43	0
6	MD1	T	5801	47/47	0.96	0.09	23,29,35,38	0
5	F3S	M	504	7/7	0.96	0.08	46,67,69,70	0
4	SF4	N	5804	8/8	0.96	0.10	40,42,48,51	0
4	SF4	Q	5804	8/8	0.96	0.09	26,43,57,67	0
7	MO	E	5803	1/1	0.96	0.06	139,139,139,139	0
9	CA	L	402	1/1	0.96	0.05	27,27,27,27	0
4	SF4	B	5804	8/8	0.96	0.10	22,38,47,49	0
9	CA	O	402	1/1	0.96	0.05	61,61,61,61	0
9	CA	O	403	1/1	0.96	0.06	73,73,73,73	0
4	SF4	V	502	8/8	0.96	0.08	62,72,89,95	0
9	CA	X	402	1/1	0.96	0.05	56,56,56,56	0
4	SF4	H	5804	8/8	0.96	0.09	15,35,41,43	0
4	SF4	V	503	8/8	0.97	0.09	50,65,72,83	0
9	CA	C	402	1/1	0.97	0.04	33,33,33,33	0
4	SF4	M	502	8/8	0.97	0.07	58,64,82,84	0
5	F3S	A	504	7/7	0.97	0.07	24,32,43,44	0

Continued on next page...

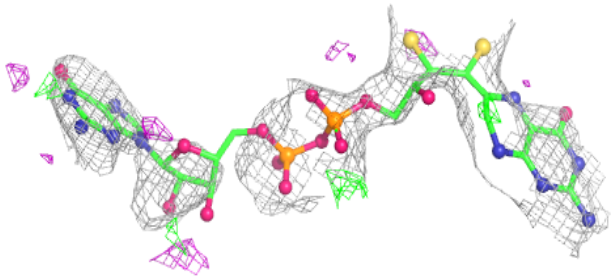
Continued from previous page...

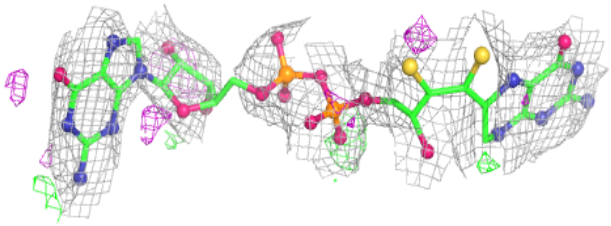
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MO	Q	5803	1/1	0.97	0.04	46,46,46,46	0
7	MO	T	5803	1/1	0.97	0.04	37,37,37,37	0
4	SF4	J	501	8/8	0.97	0.07	16,26,33,33	0
4	SF4	P	503	8/8	0.97	0.07	30,39,51,60	0
4	SF4	J	502	8/8	0.97	0.07	24,36,52,52	0
4	SF4	S	501	8/8	0.97	0.09	21,32,42,43	0
9	CA	R	403	1/1	0.97	0.04	35,35,35,35	0
4	SF4	T	5804	8/8	0.97	0.09	27,42,48,57	0
4	SF4	A	501	8/8	0.97	0.08	26,27,41,46	0
4	SF4	M	501	8/8	0.97	0.08	35,47,52,54	0
5	F3S	G	504	7/7	0.98	0.08	26,42,51,52	0
5	F3S	J	504	7/7	0.98	0.07	14,25,31,32	0
4	SF4	G	501	8/8	0.98	0.08	24,29,42,43	0
9	CA	I	402	1/1	0.98	0.04	46,46,46,46	0
5	F3S	P	504	7/7	0.98	0.07	24,34,45,47	0
5	F3S	S	504	7/7	0.98	0.06	19,29,43,43	0
4	SF4	P	501	8/8	0.98	0.08	30,35,42,42	0
4	SF4	P	502	8/8	0.98	0.08	37,47,60,63	0
4	SF4	G	502	8/8	0.98	0.07	30,38,54,60	0
9	CA	R	402	1/1	0.98	0.03	31,31,31,31	0
4	SF4	G	503	8/8	0.98	0.07	17,27,33,35	0
9	CA	U	402	1/1	0.98	0.06	32,32,32,32	0
4	SF4	M	503	8/8	0.98	0.06	32,44,56,57	0
4	SF4	S	502	8/8	0.98	0.08	29,39,52,53	0
7	MO	B	5803	1/1	0.98	0.04	45,45,45,45	0
4	SF4	A	503	8/8	0.99	0.07	27,34,49,51	0
4	SF4	A	502	8/8	0.99	0.05	27,43,54,56	0
7	MO	H	5803	1/1	0.99	0.04	38,38,38,38	0
7	MO	K	5803	1/1	0.99	0.03	36,36,36,36	0
7	MO	N	5803	1/1	0.99	0.03	30,30,30,30	0
4	SF4	S	503	8/8	0.99	0.05	28,33,41,47	0
4	SF4	J	503	8/8	0.99	0.05	25,29,37,38	0
7	MO	W	5803	1/1	0.99	0.04	61,61,61,61	0

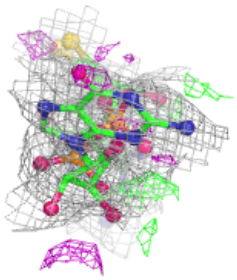
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MD1 E 5801:

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

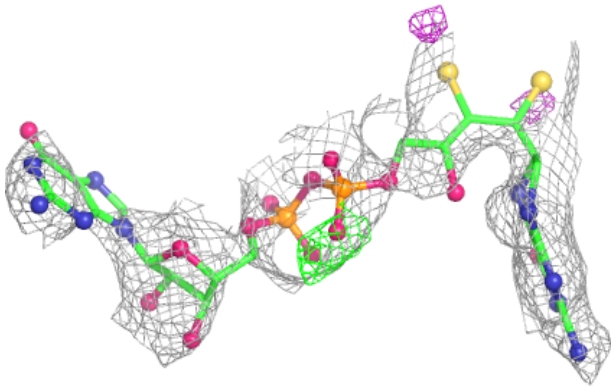


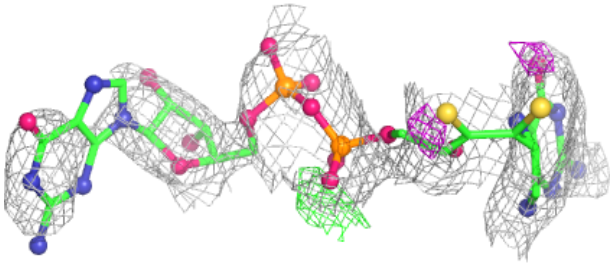


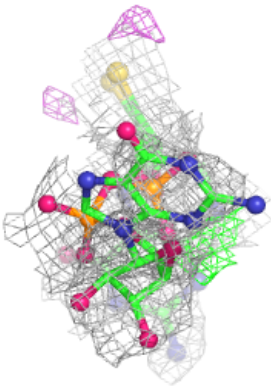


Electron density around MD1 E 5802:

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

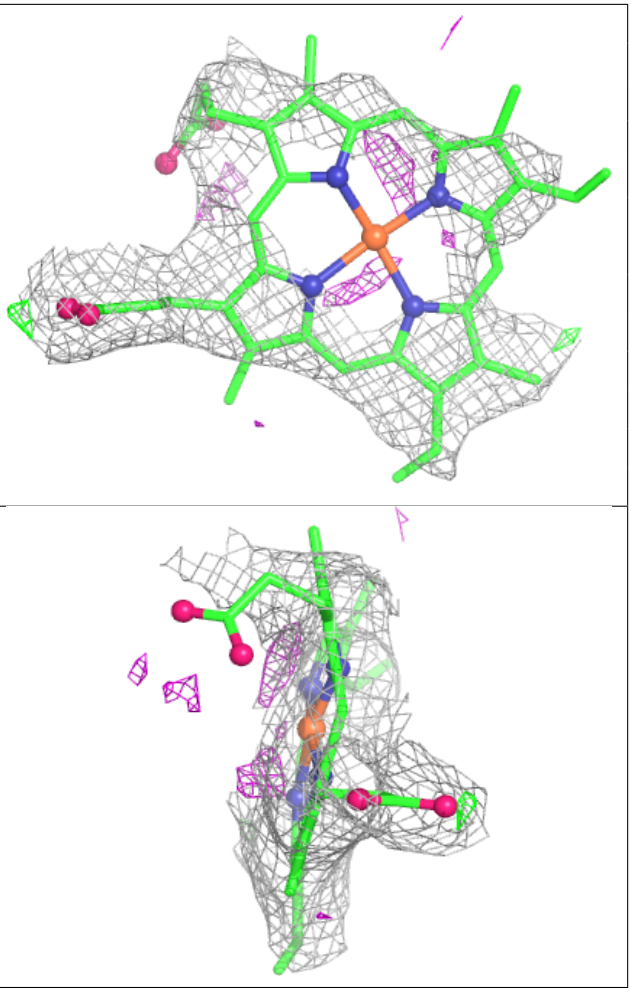






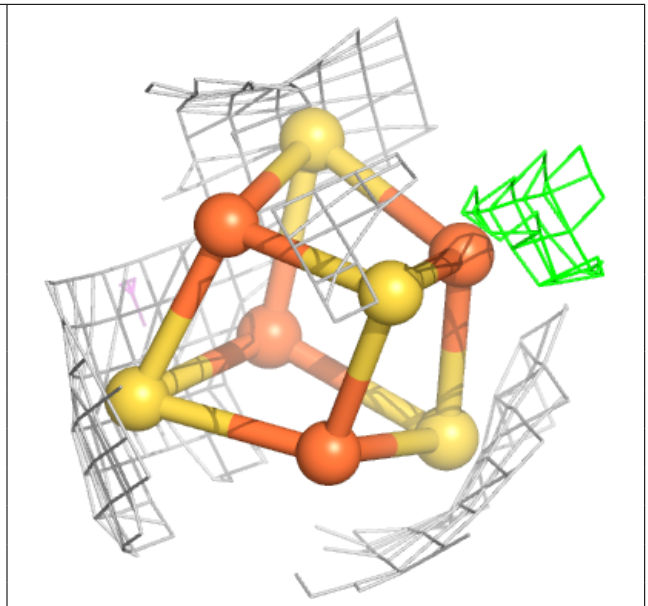
Electron density around HEM F 401:

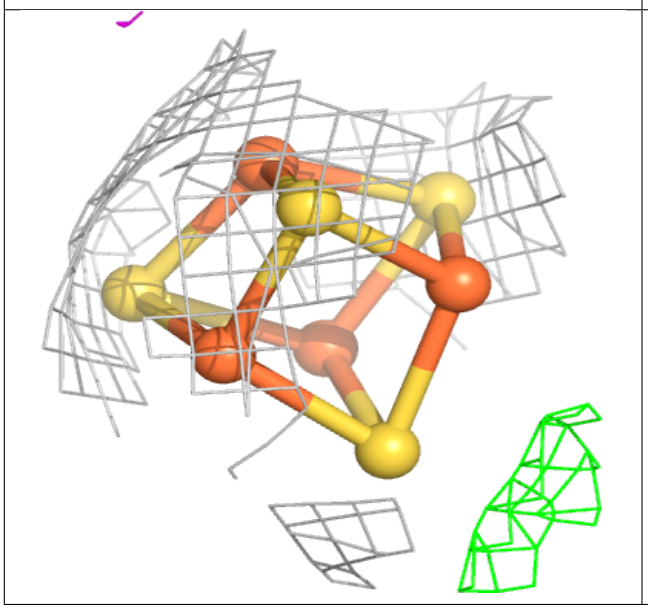
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

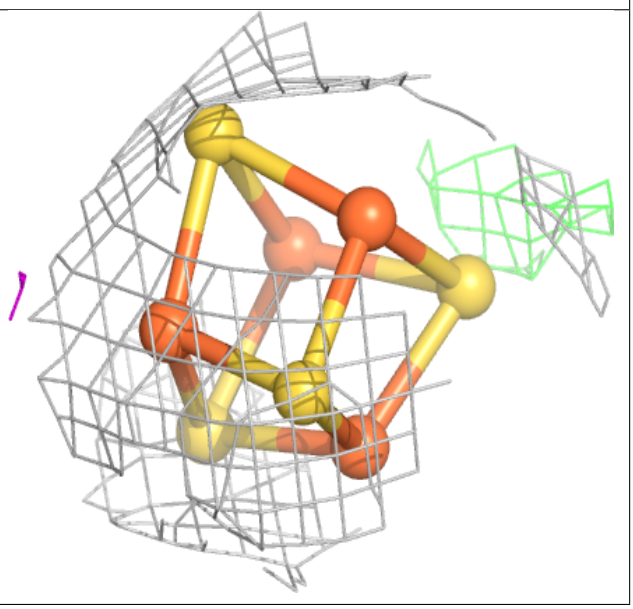


Electron density around SF4 D 503:

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

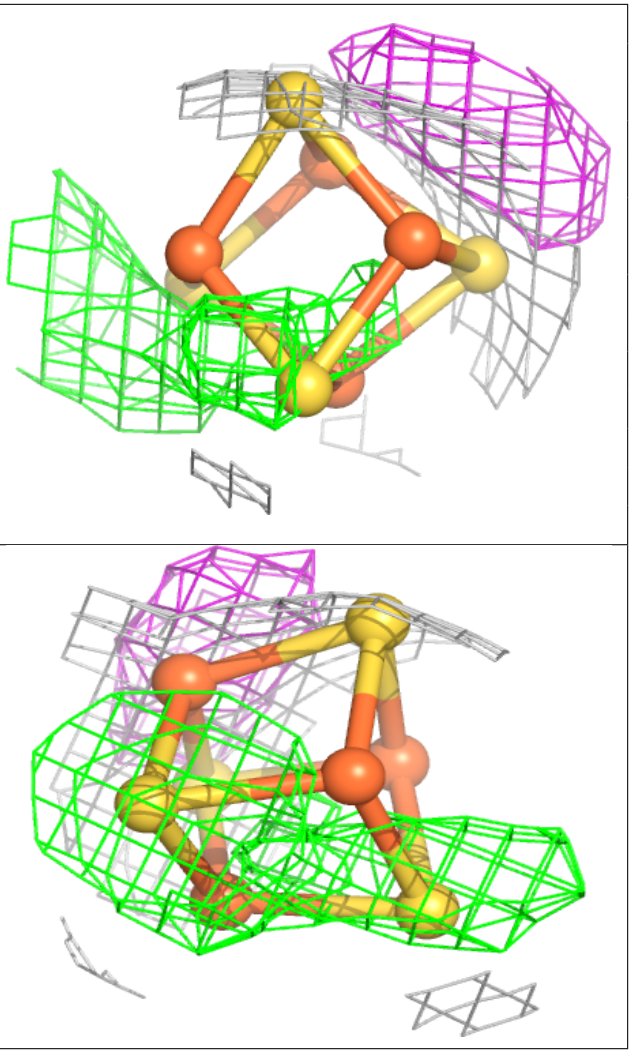






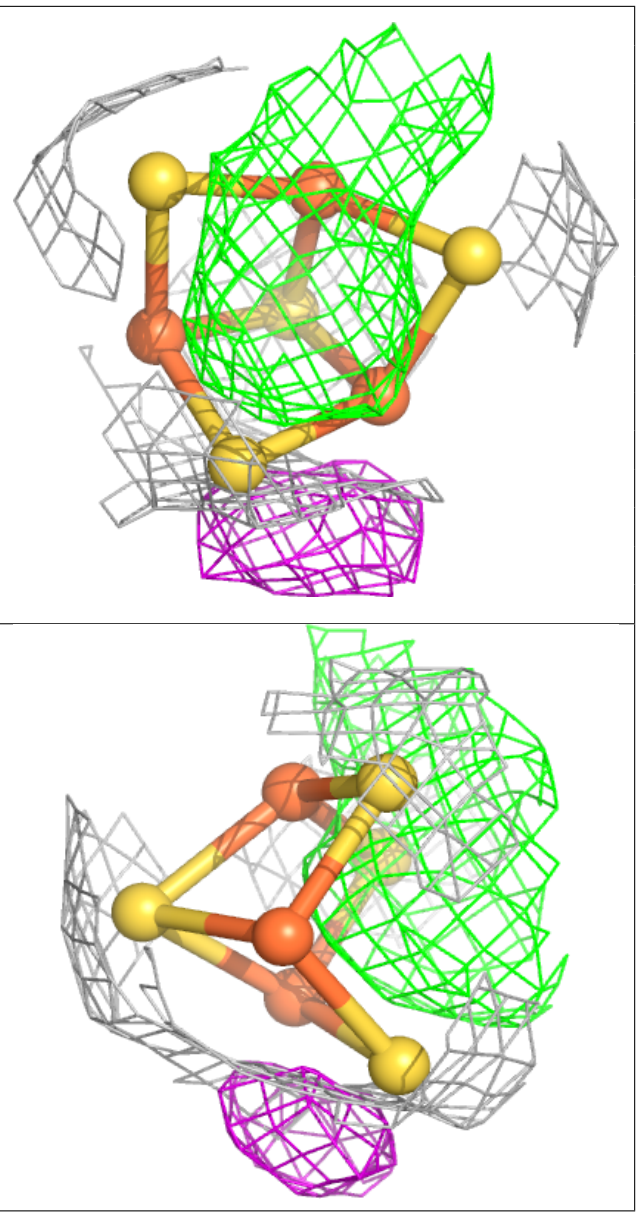
Electron density around SF4 D 501:

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



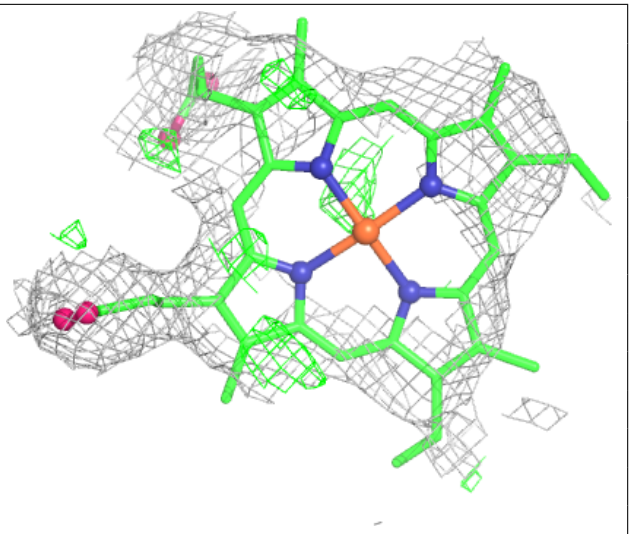
Electron density around F3S V 504:

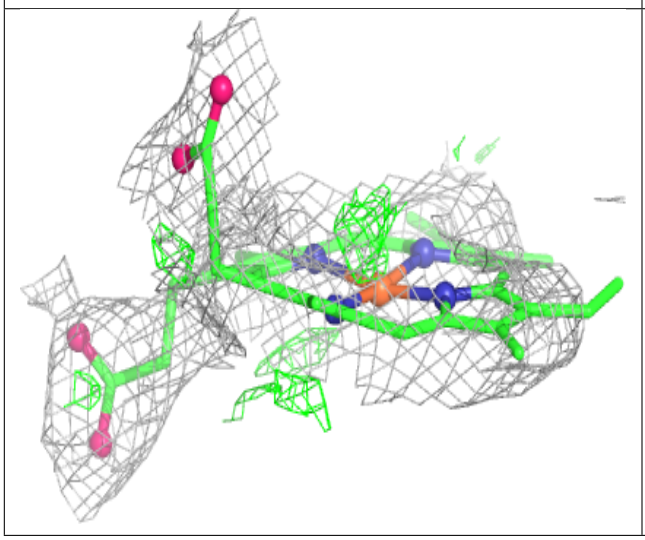
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM X 401:

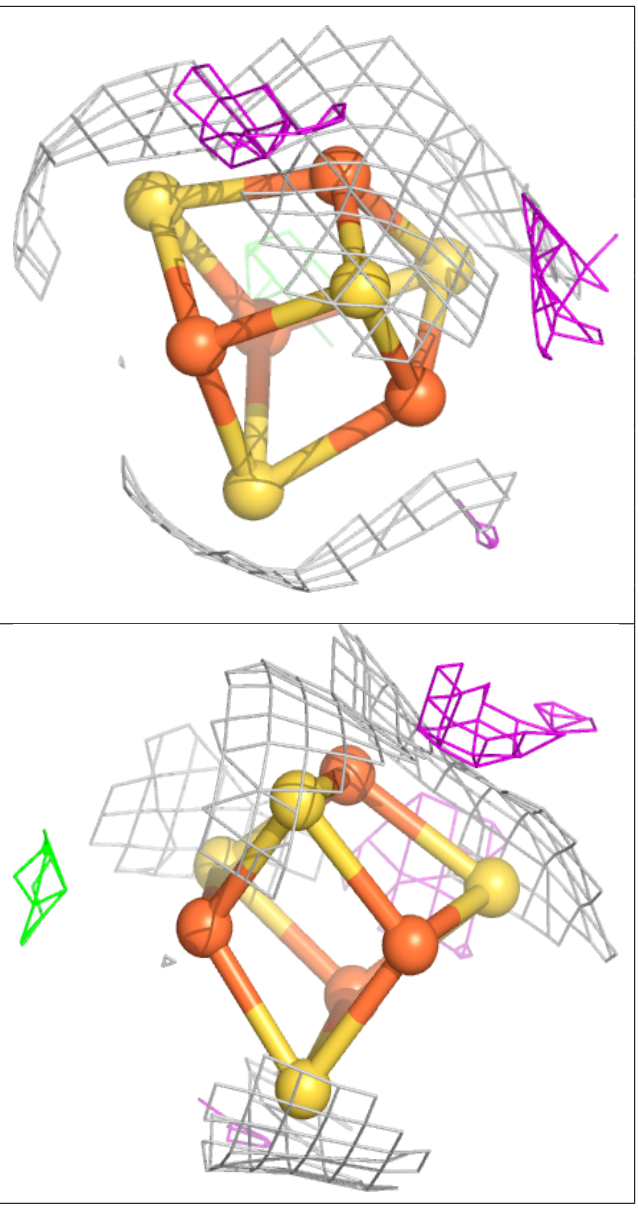
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





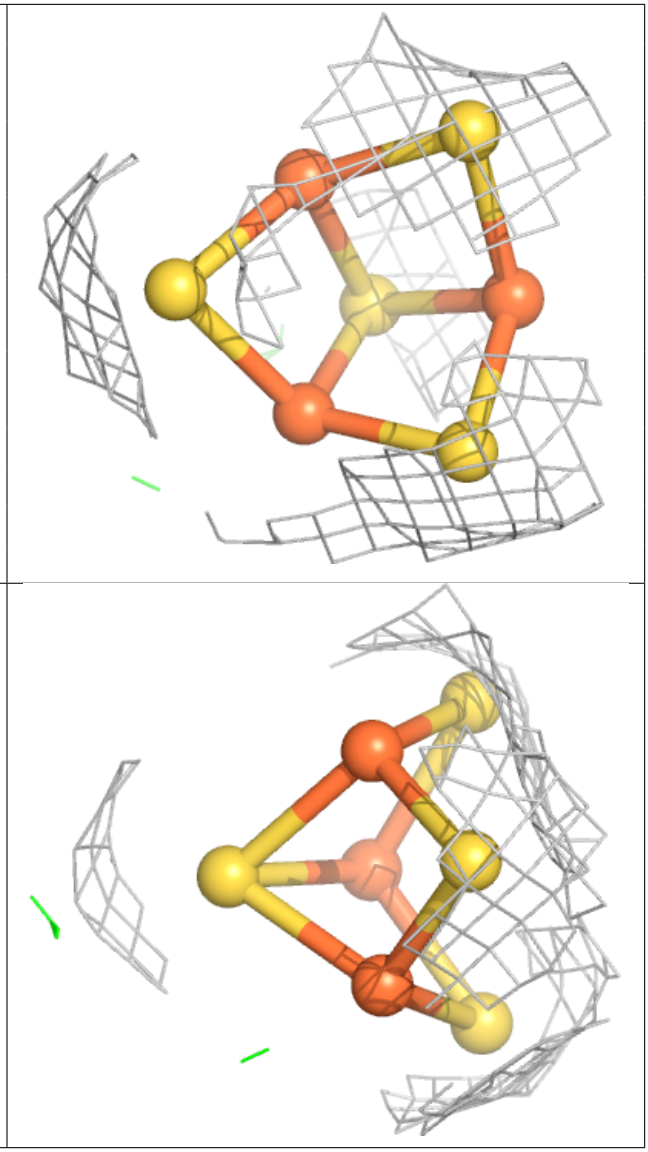
Electron density around SF4 E 5804:

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



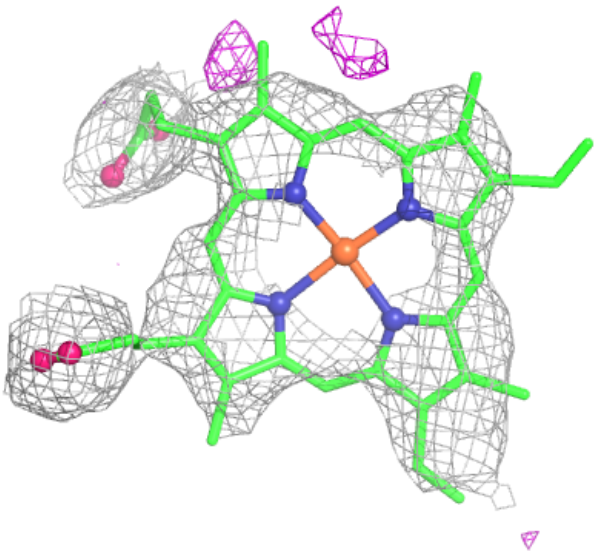
Electron density around F3S D 504:

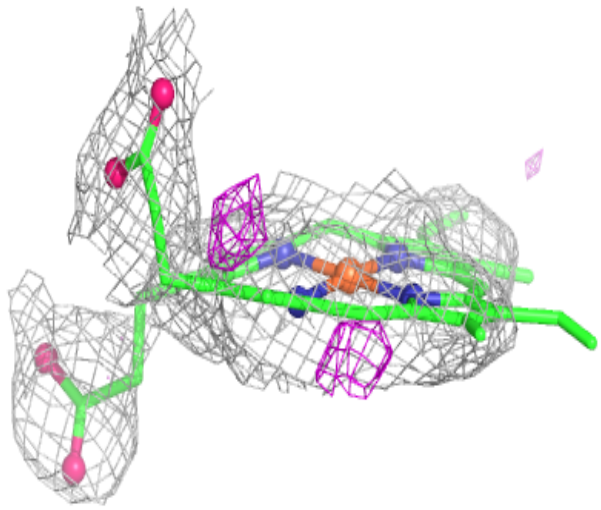
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

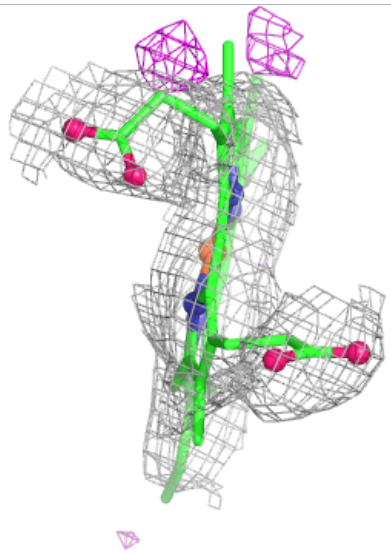


Electron density around HEM O 401:

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

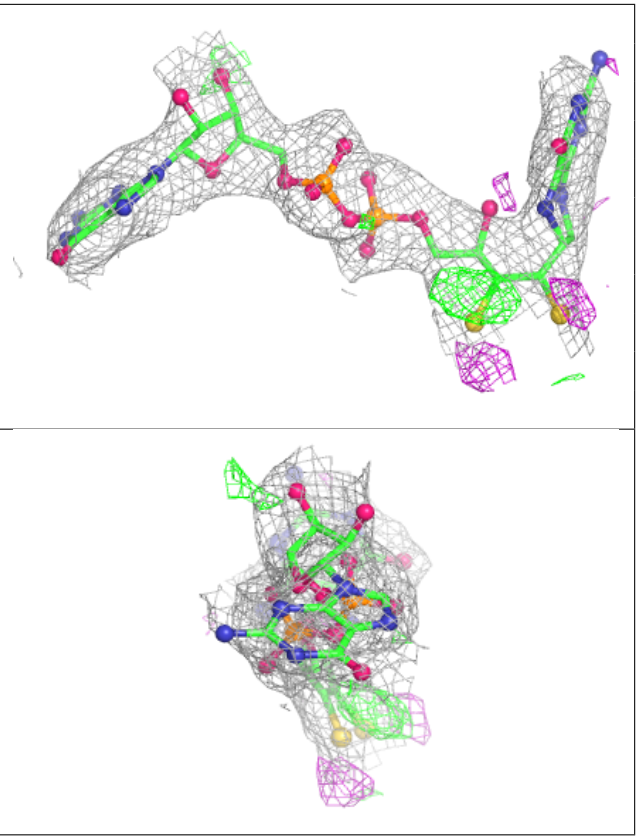






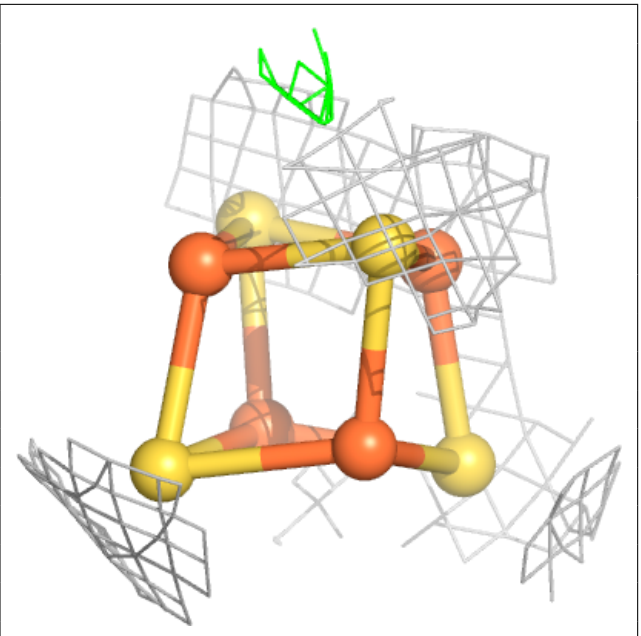
Electron density around MD1 Q 5802:

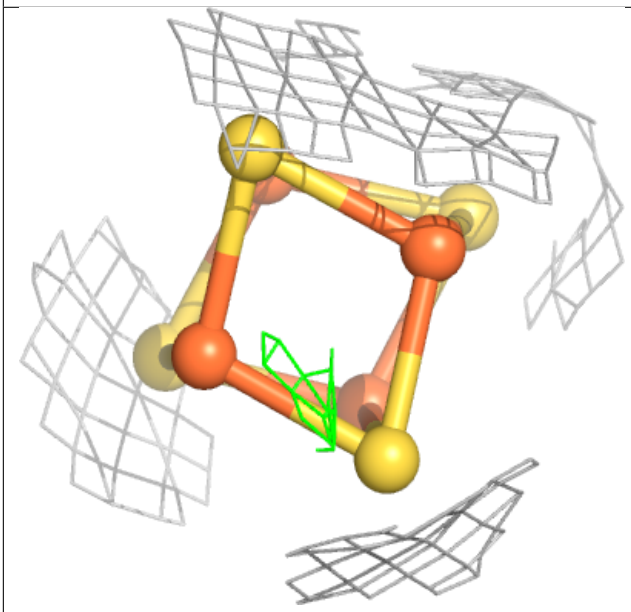
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

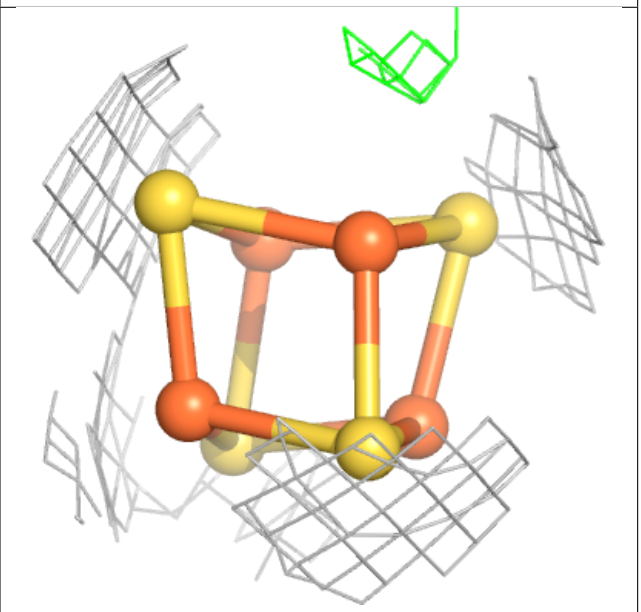


Electron density around SF4 D 502:

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

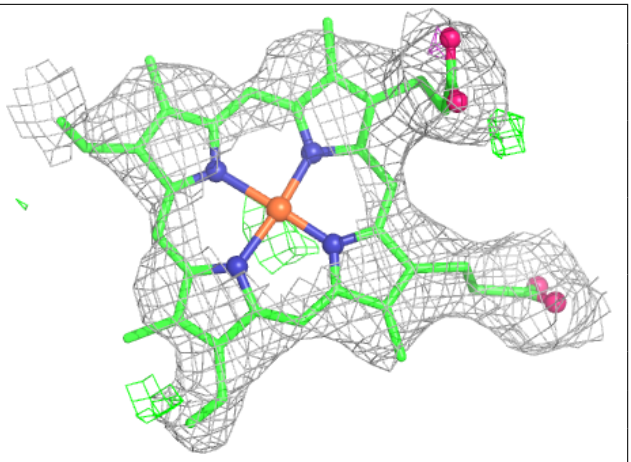


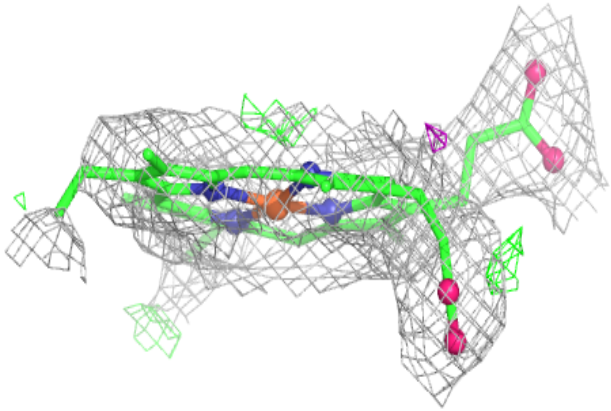


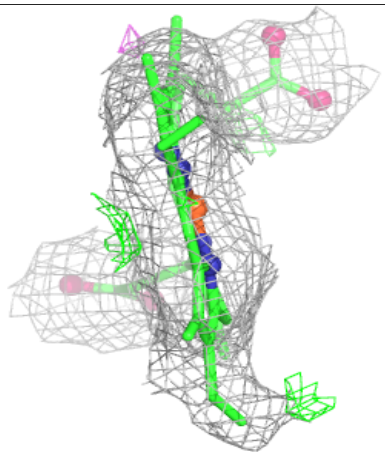


Electron density around HEM I 401:

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

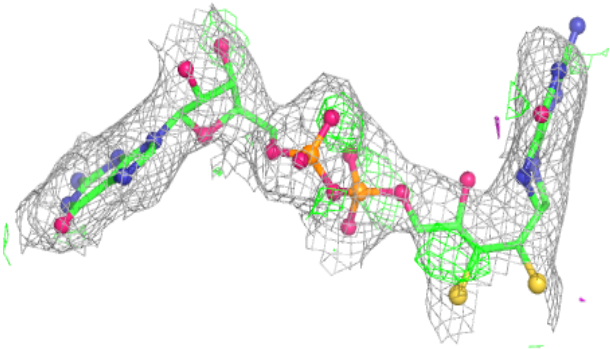


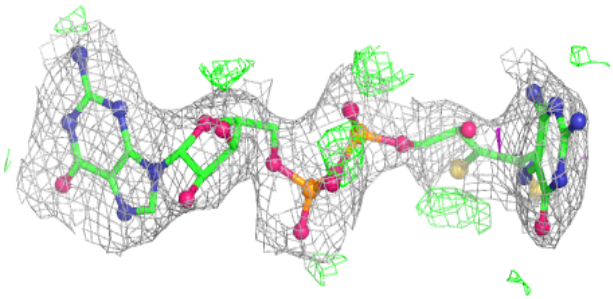


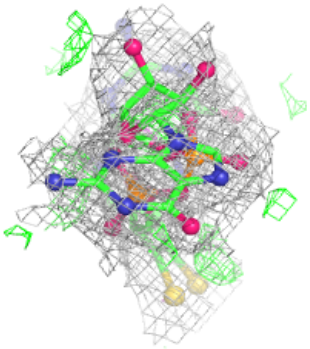


Electron density around MD1 W 5802:

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

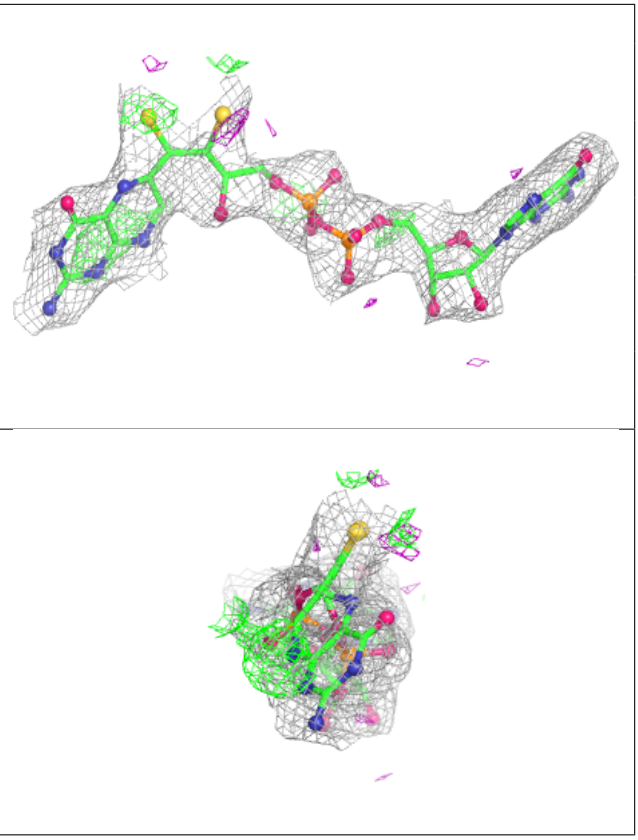






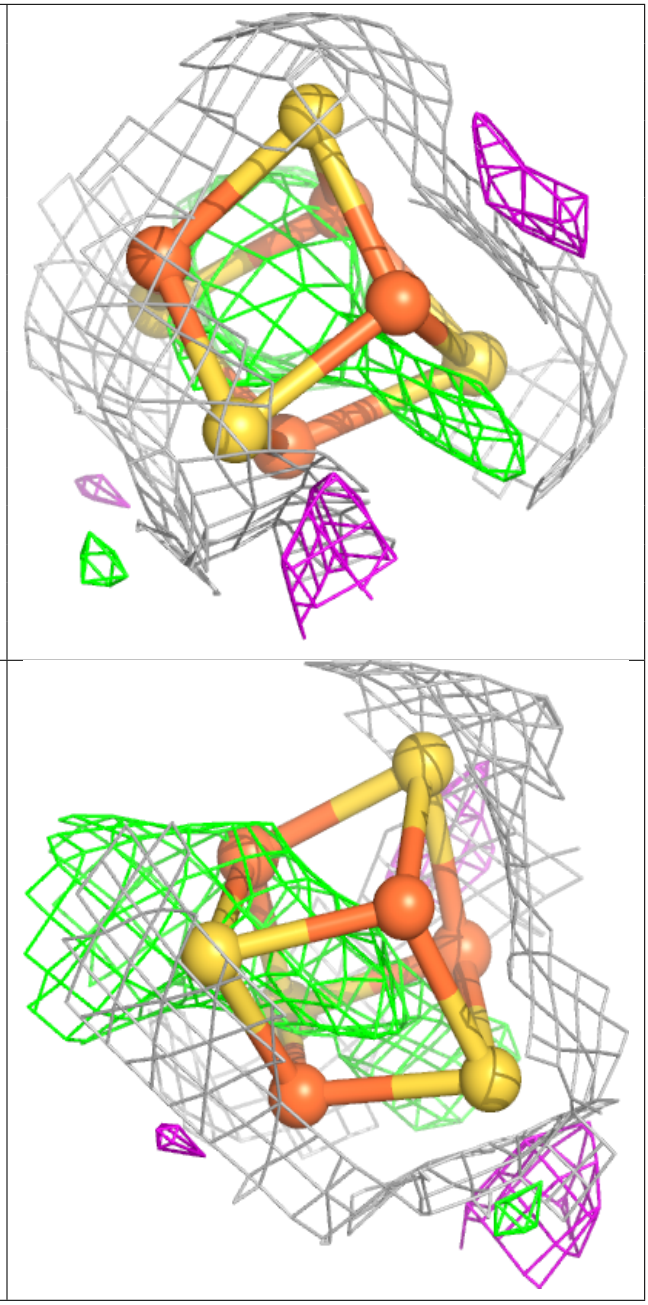
Electron density around MD1 Q 5801:

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



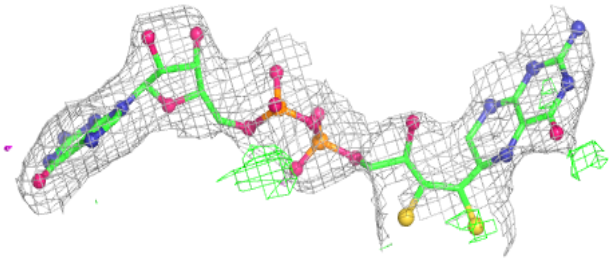
Electron density around SF4 V 501:

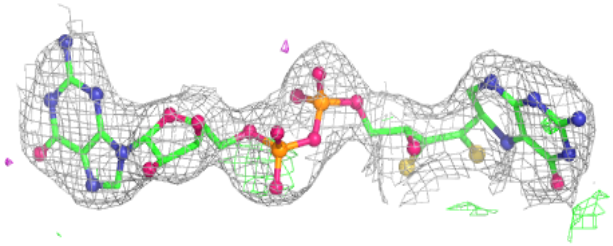
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

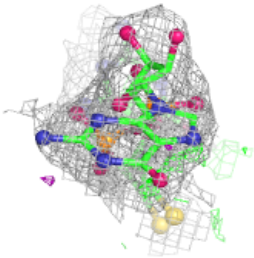


Electron density around MD1 W 5801:

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

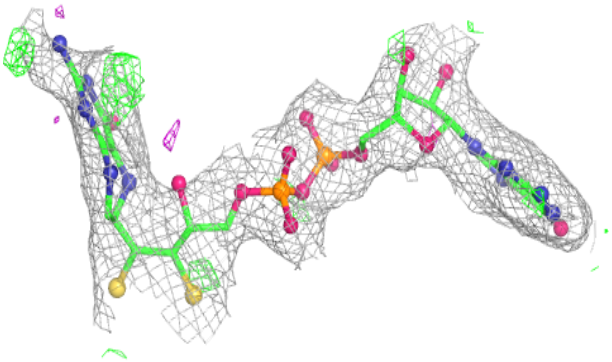


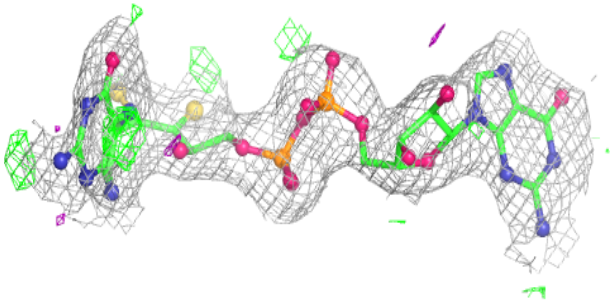


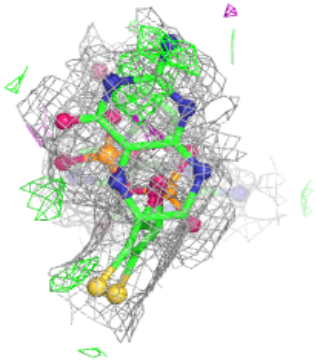


Electron density around MD1 N 5802:

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

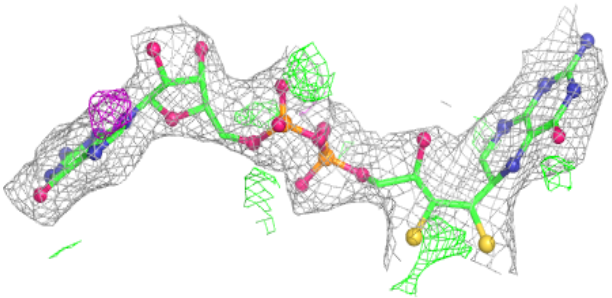


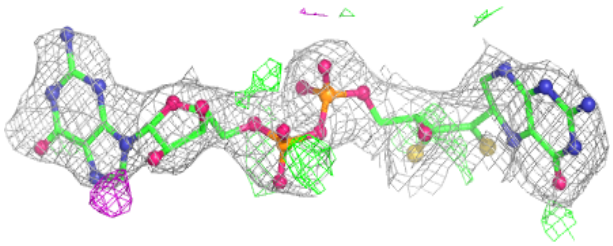


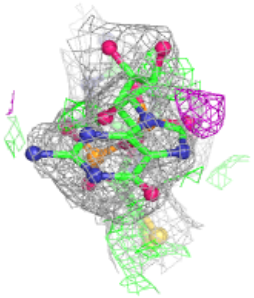


Electron density around MD1 B 5801:

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

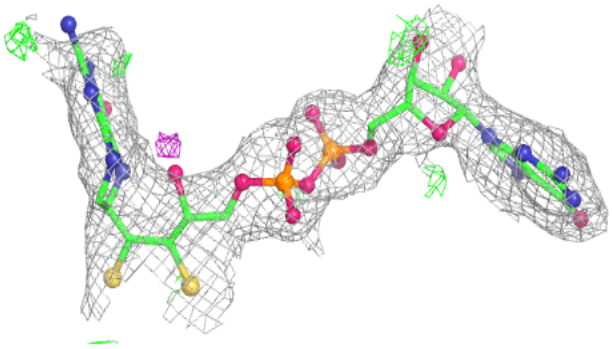


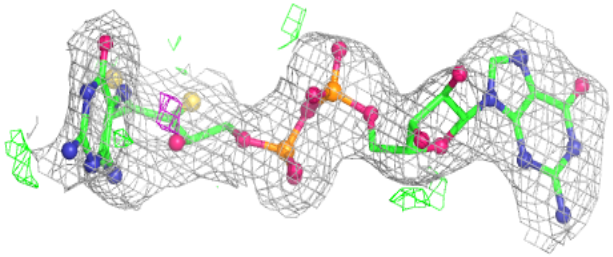


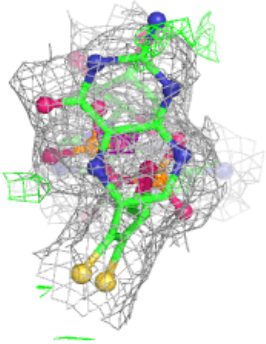


Electron density around MD1 B 5802:

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

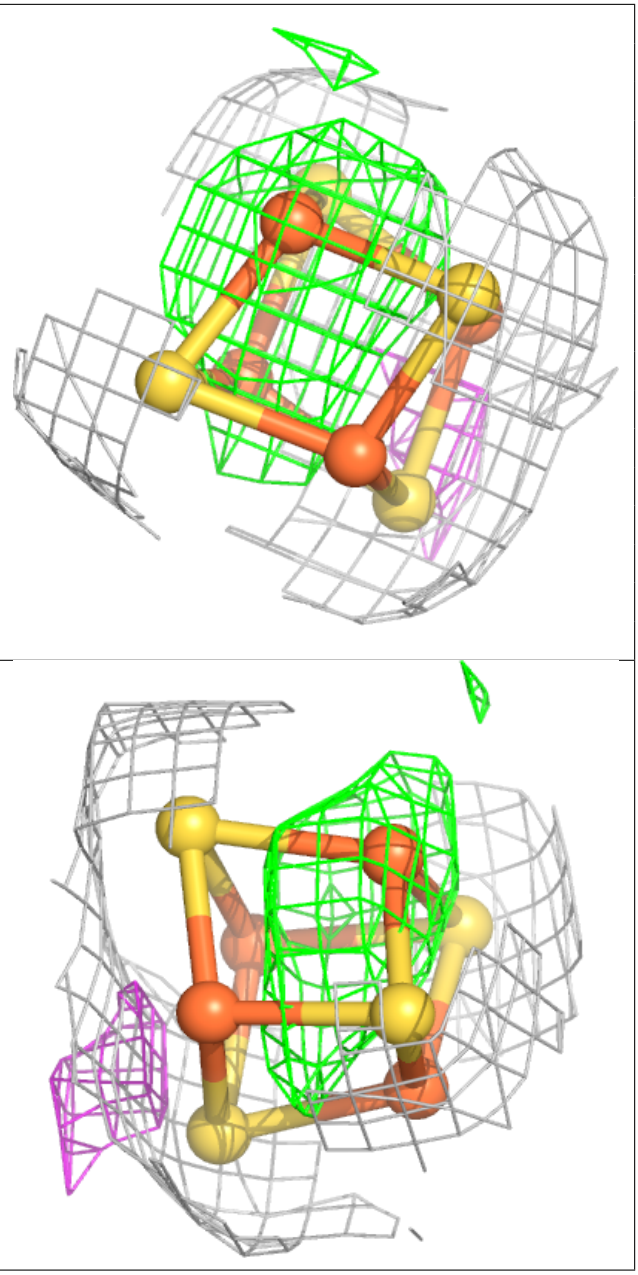






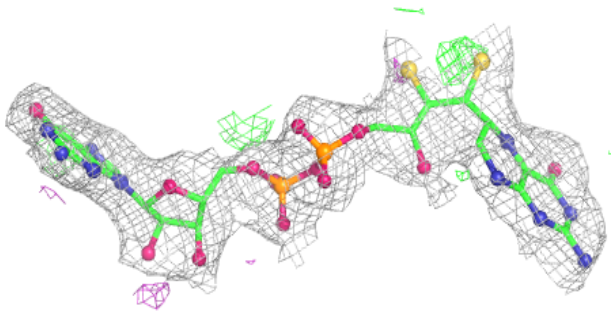
Electron density around SF4 W 5804:

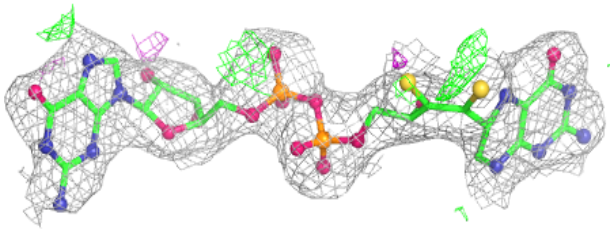
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

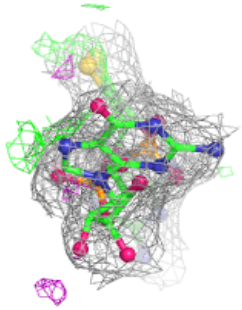


Electron density around MD1 H 5801:

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

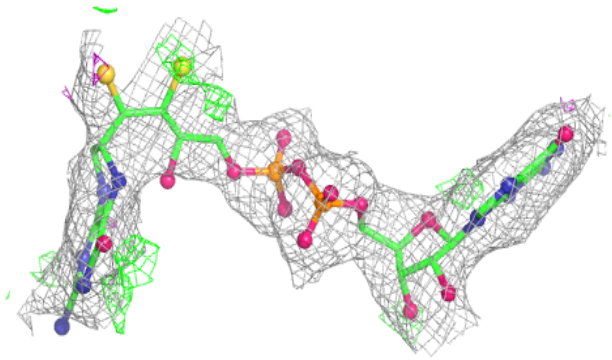


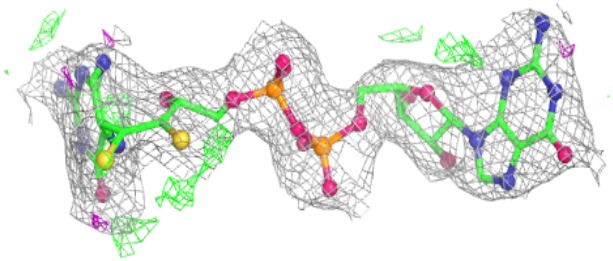


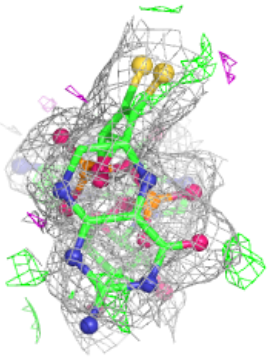


Electron density around MD1 H 5802:

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

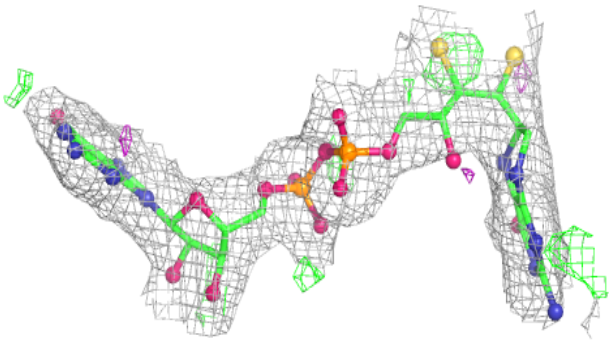


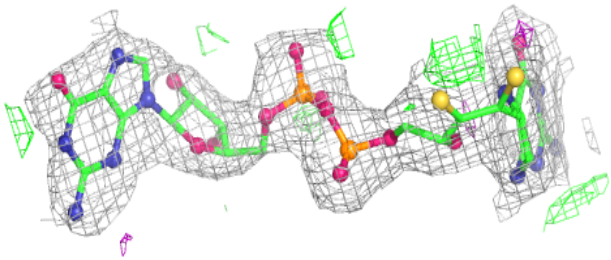


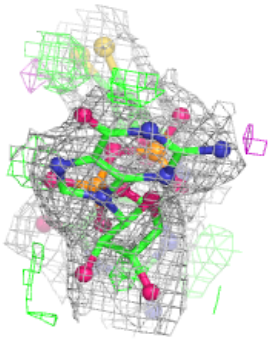


Electron density around MD1 T 5802:

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

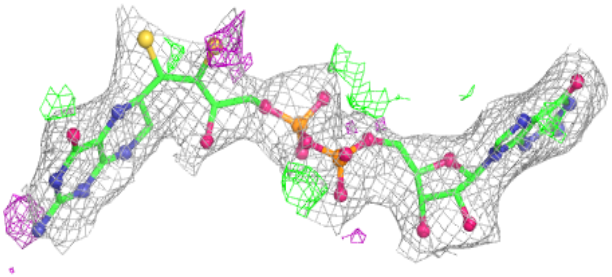


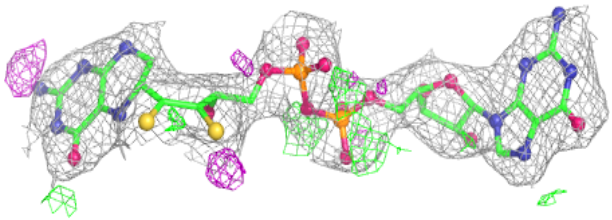


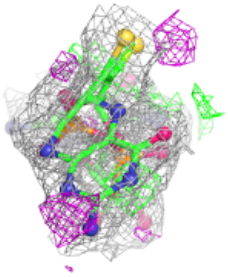


Electron density around MD1 K 5801:

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

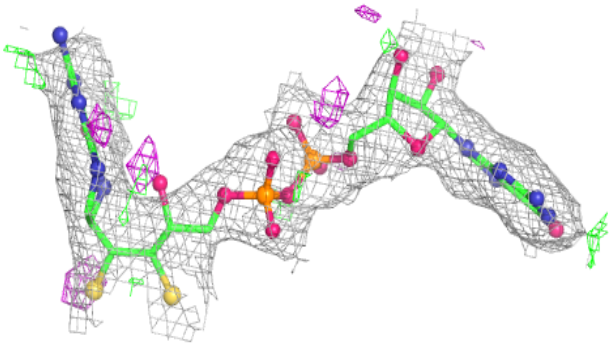


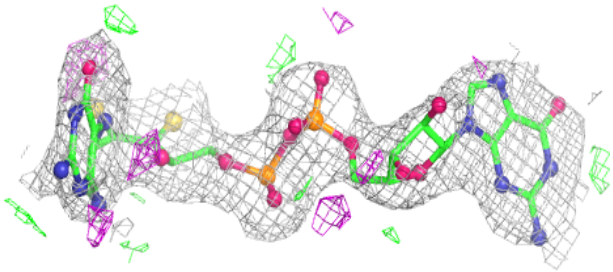


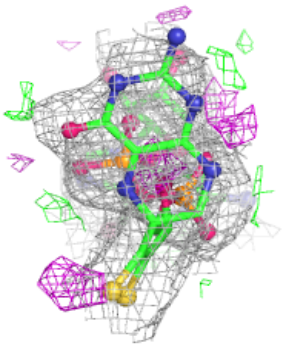


Electron density around MD1 K 5802:

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

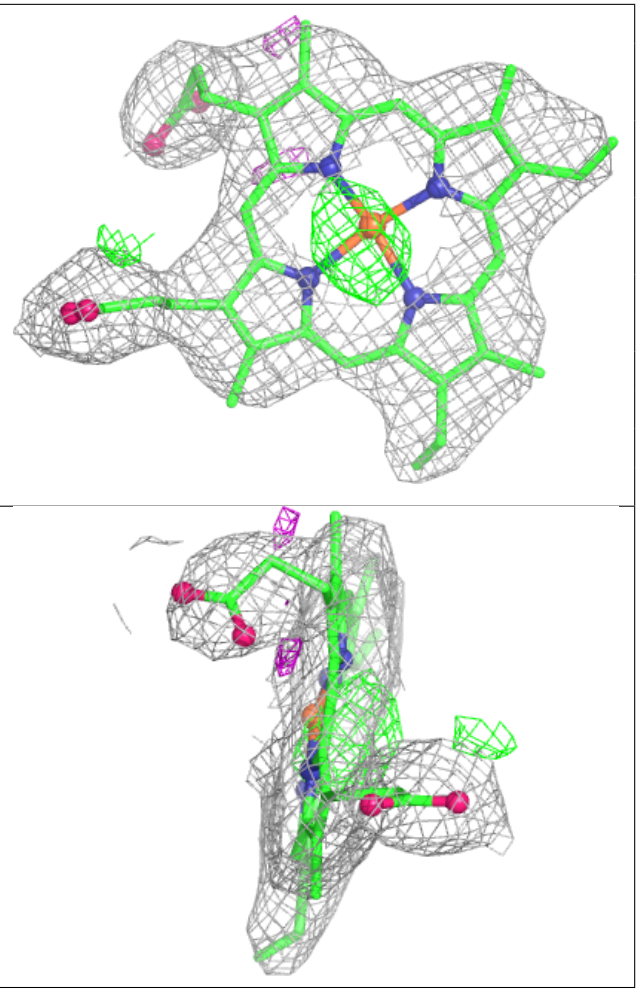






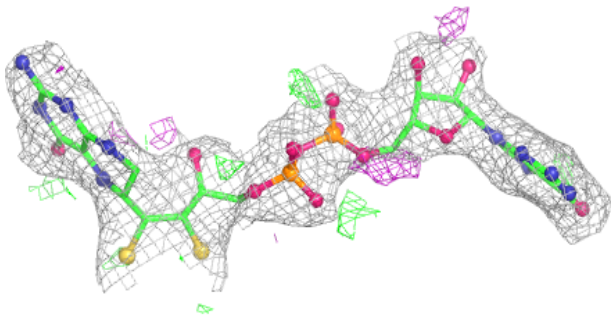
Electron density around HEM C 401:

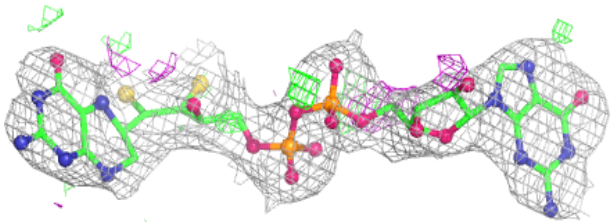
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

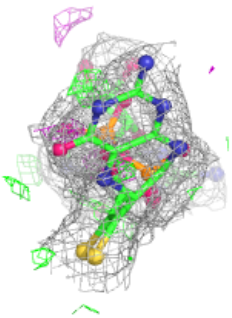


Electron density around MD1 N 5801:

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

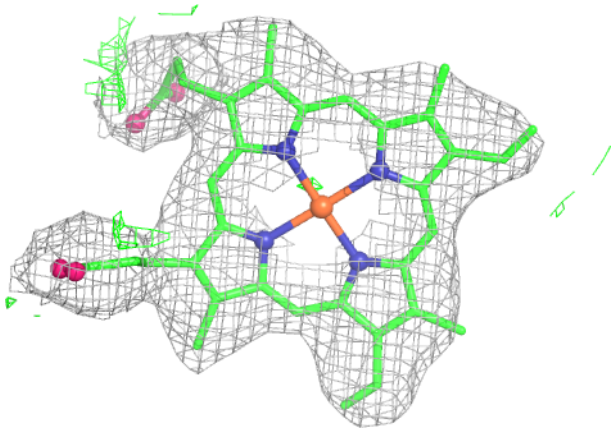


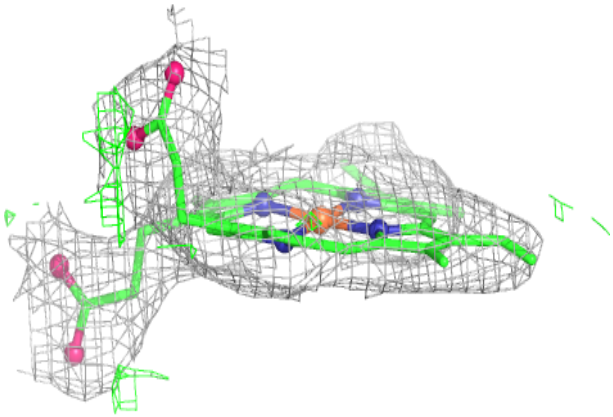


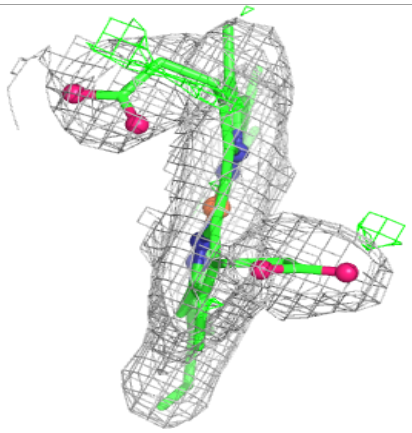


Electron density around HEM L 401:

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

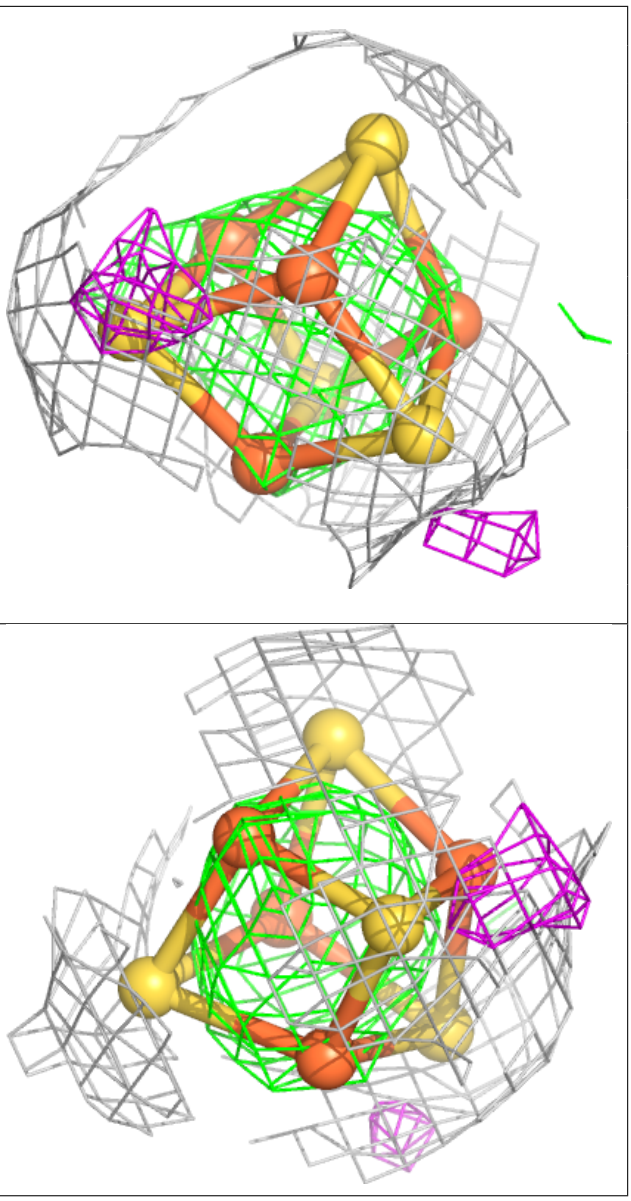






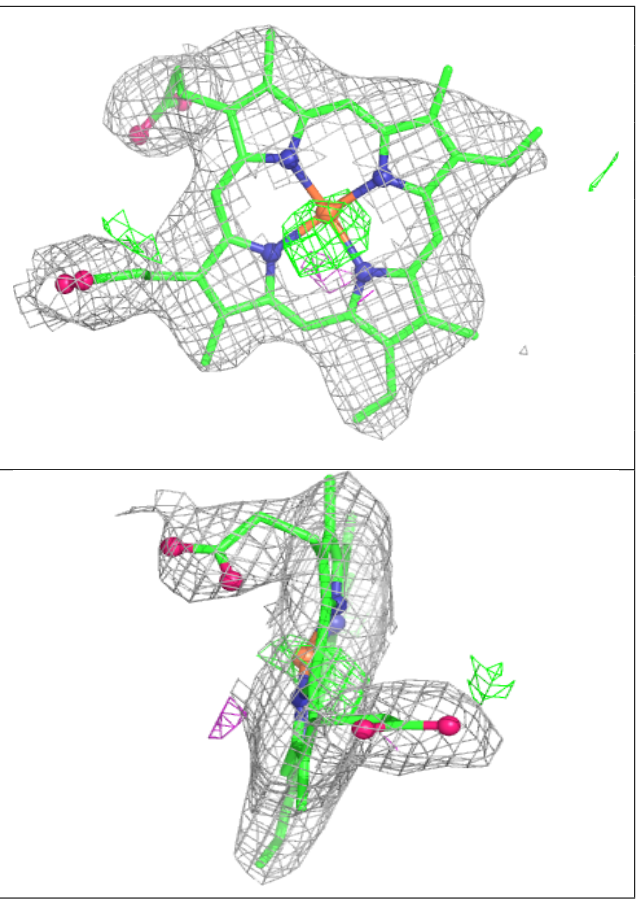
Electron density around SF4 K 5804:

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



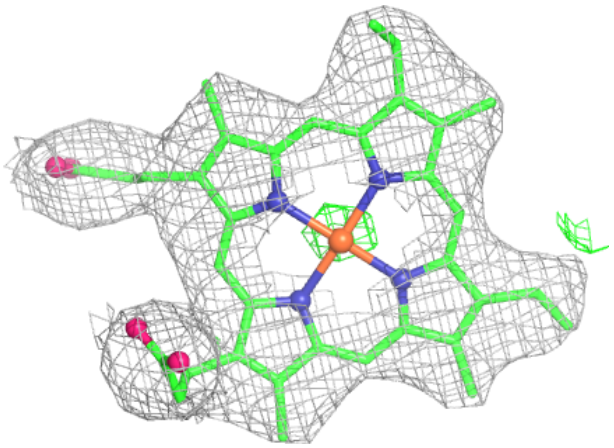
Electron density around HEM R 401:

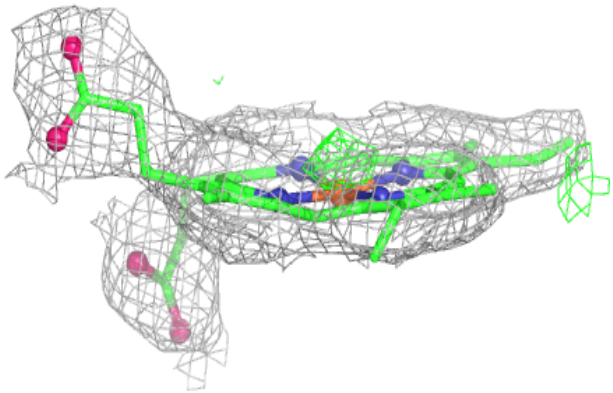
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

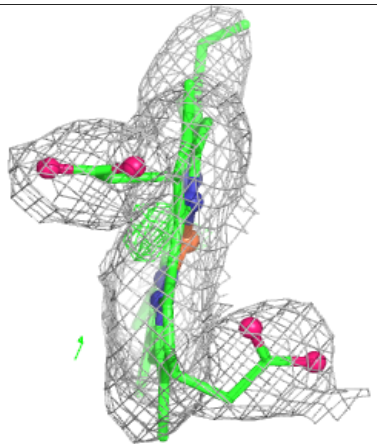


Electron density around HEM U 401:

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

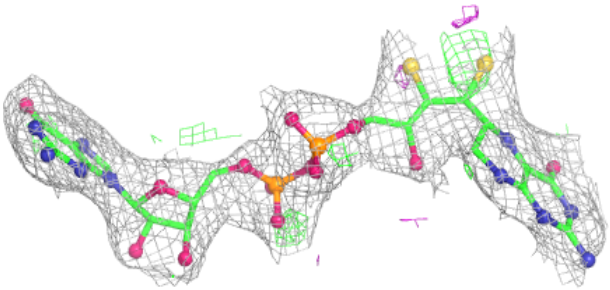


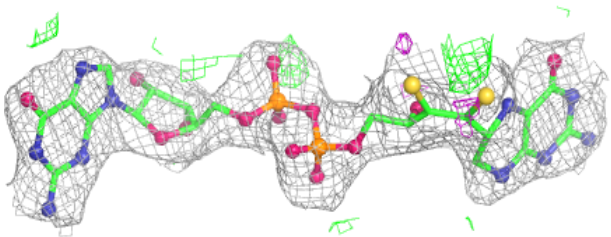


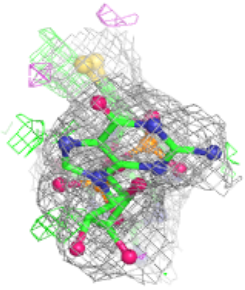


Electron density around MD1 T 5801:

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

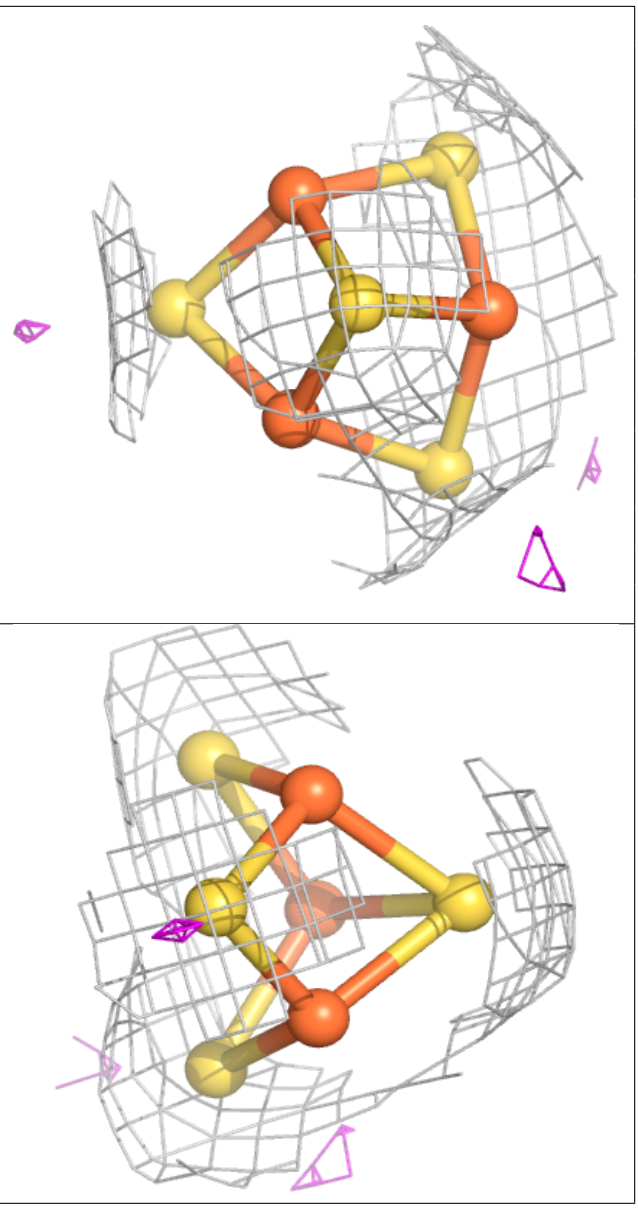






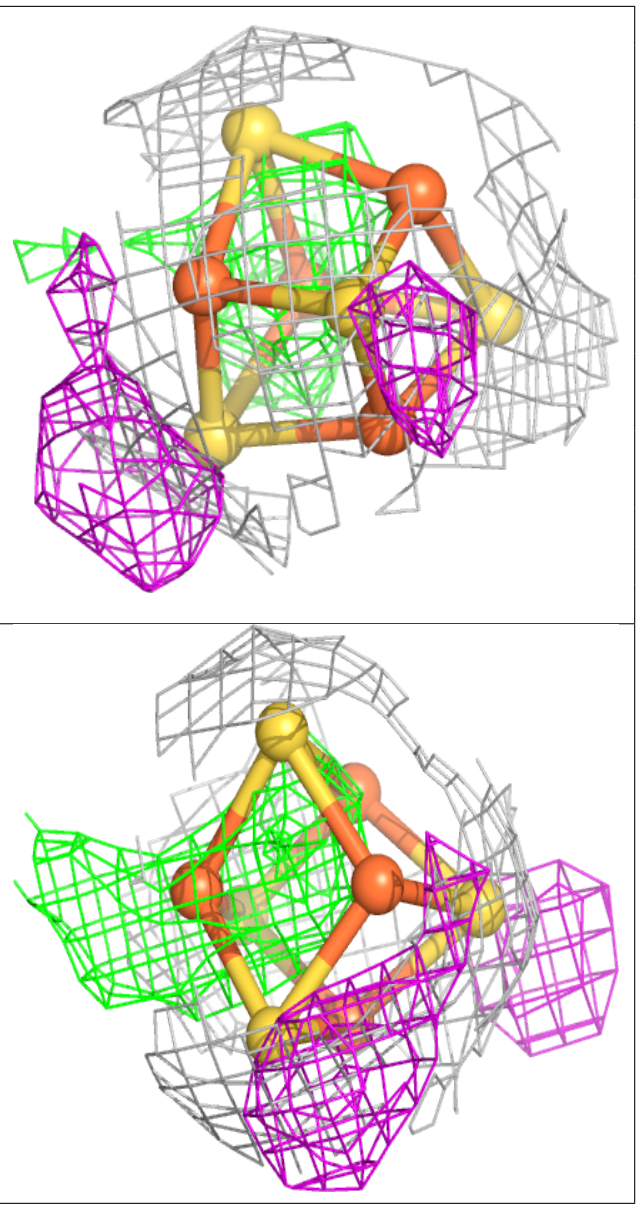
Electron density around F3S M 504:

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



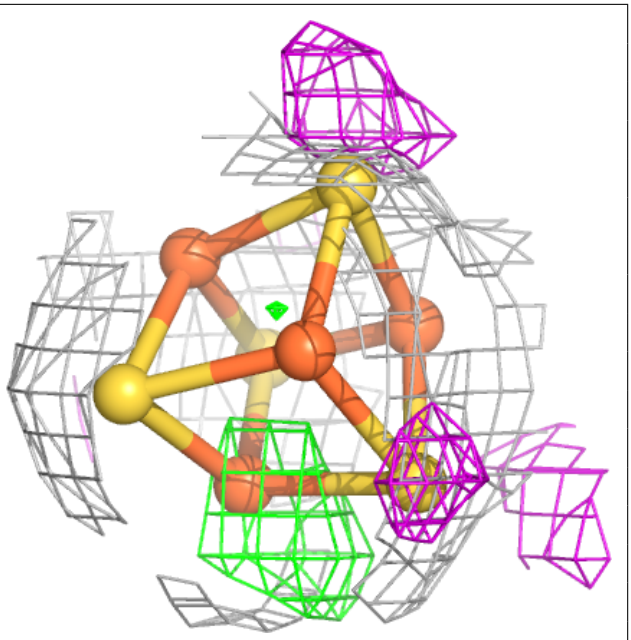
Electron density around SF4 N 5804:

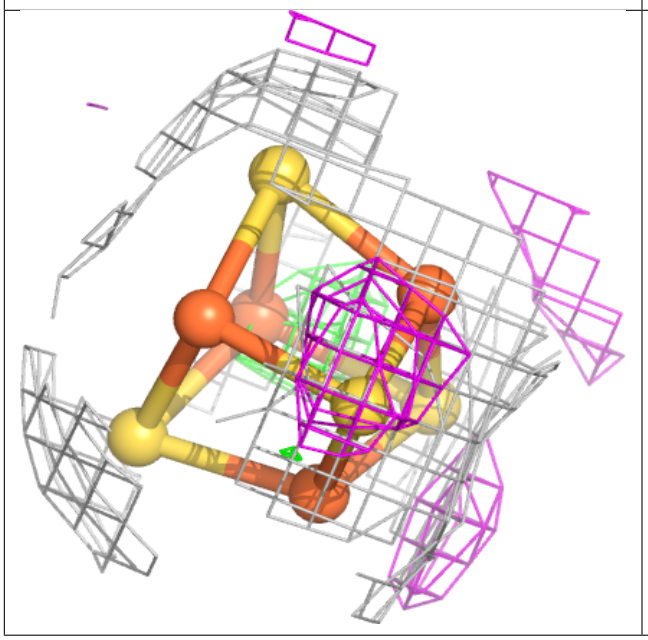
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

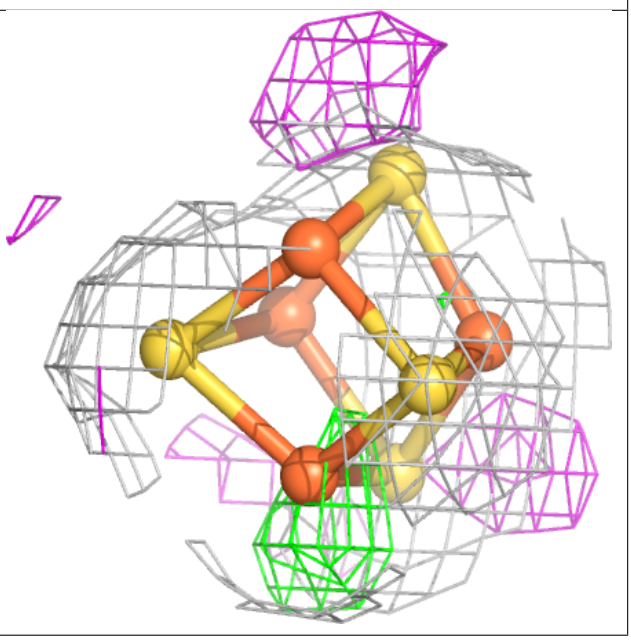


Electron density around SF4 Q 5804:

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

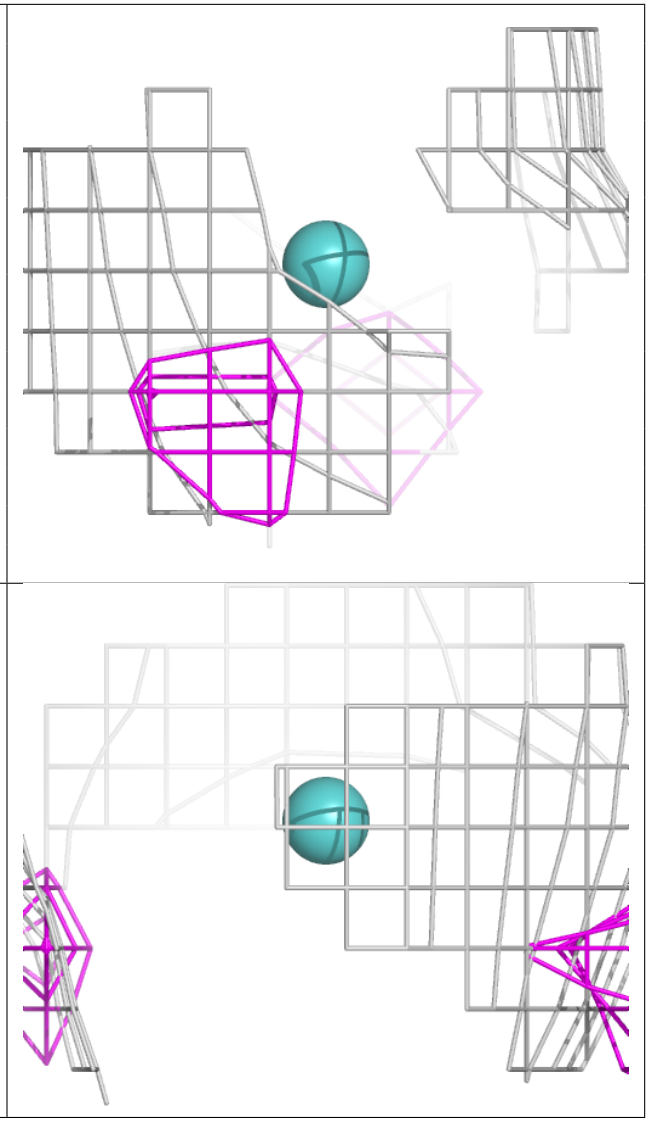






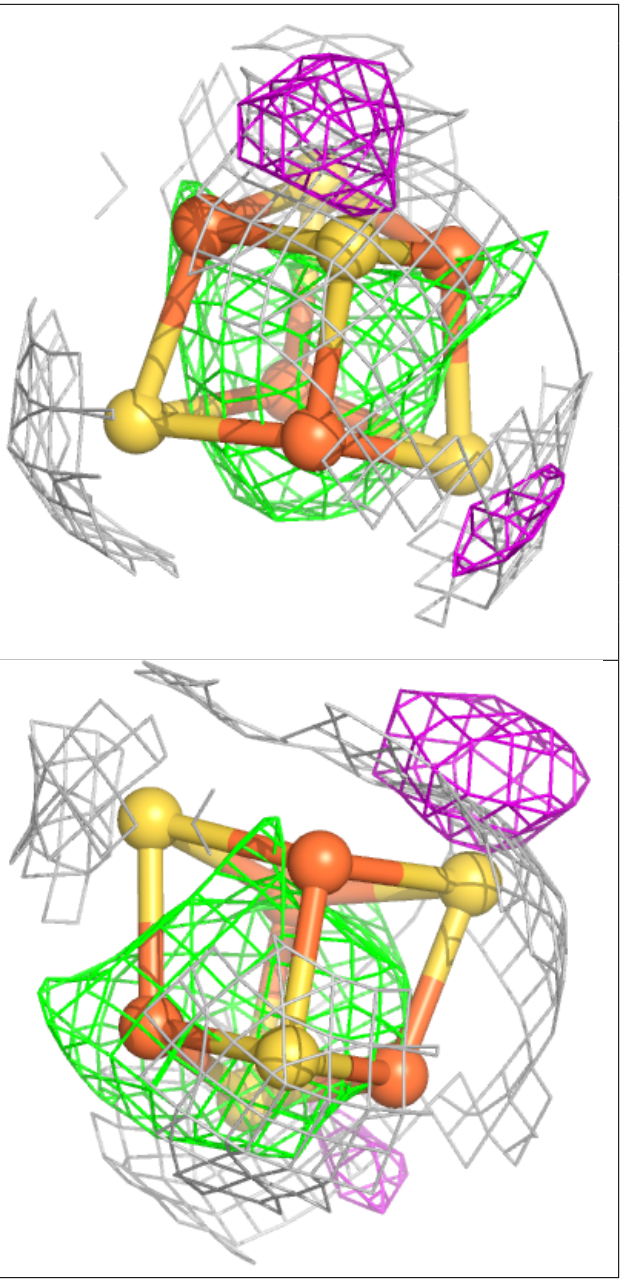
Electron density around MO E 5803:

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



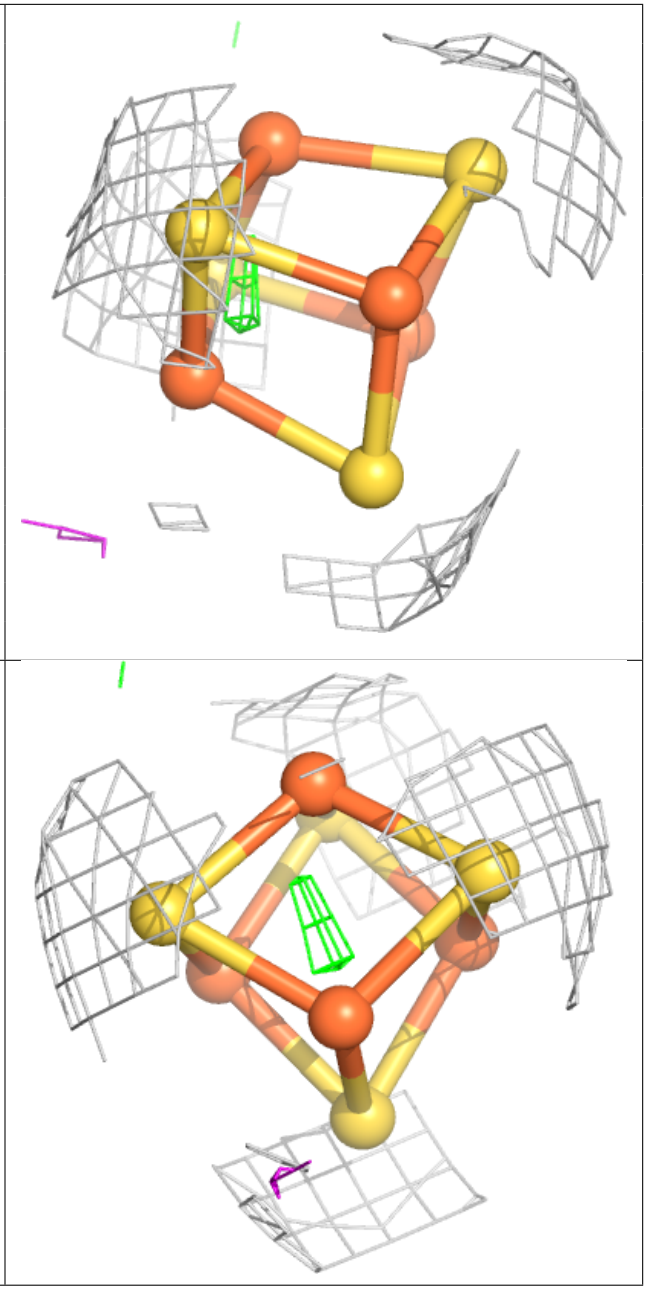
Electron density around SF4 B 5804:

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



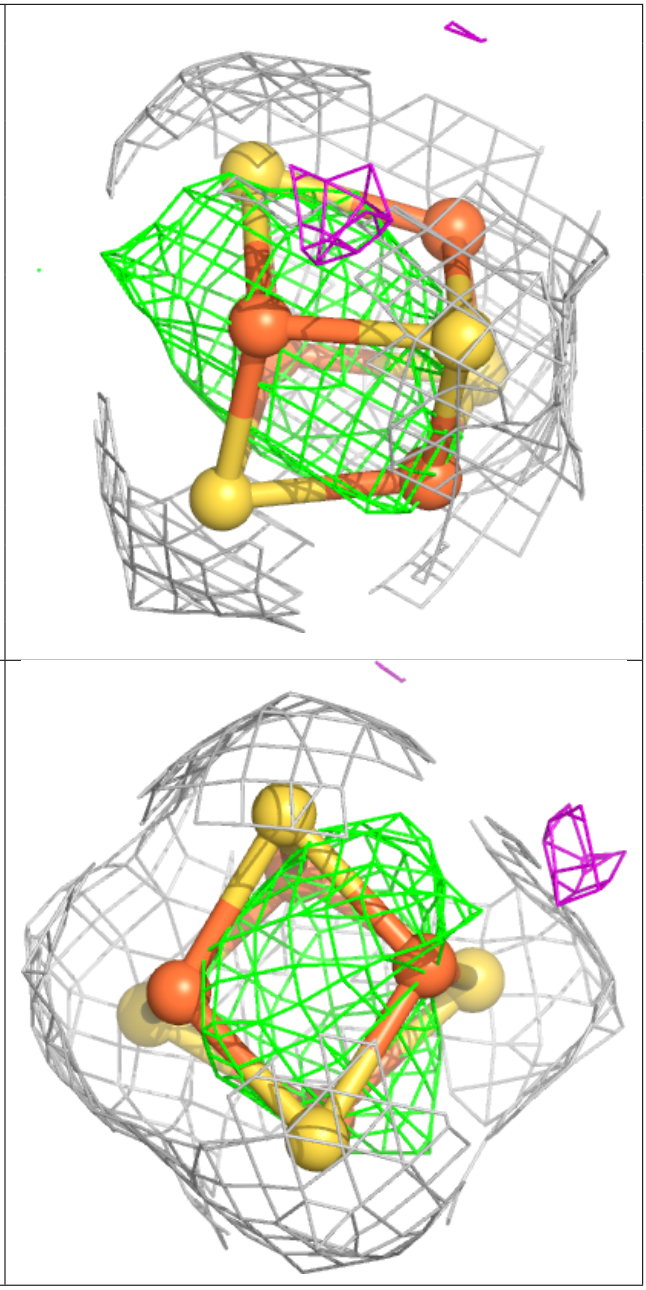
Electron density around SF4 V 502:

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



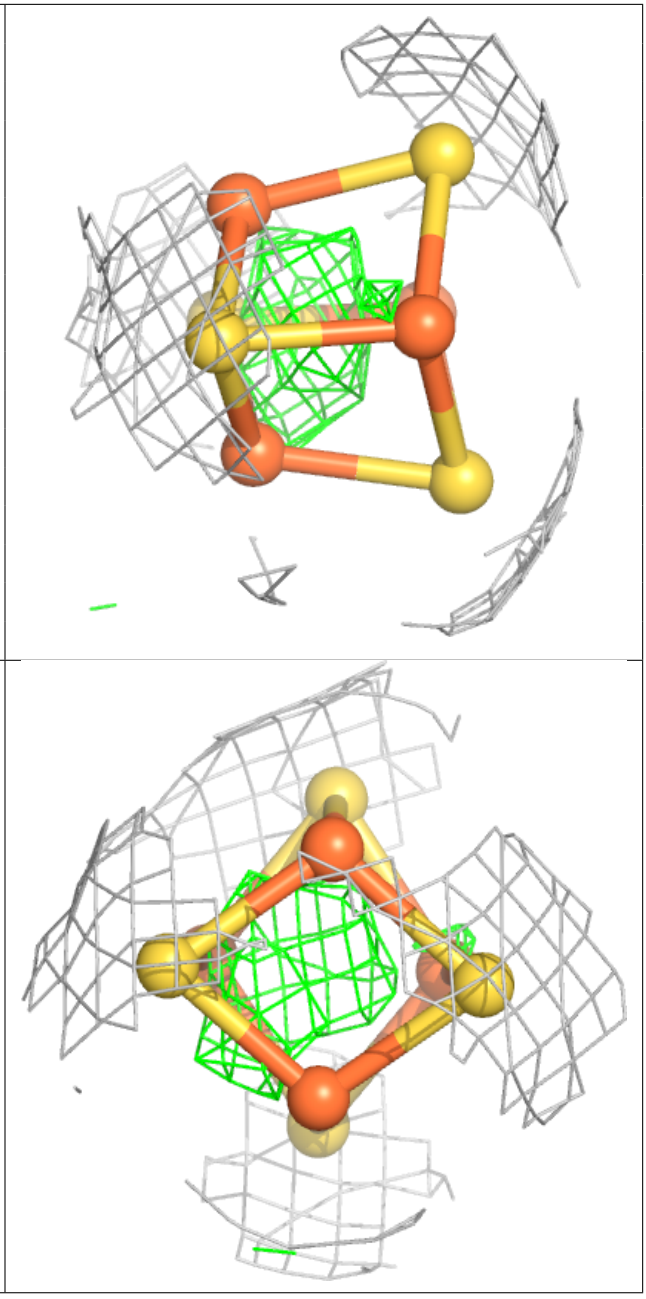
Electron density around SF4 H 5804:

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



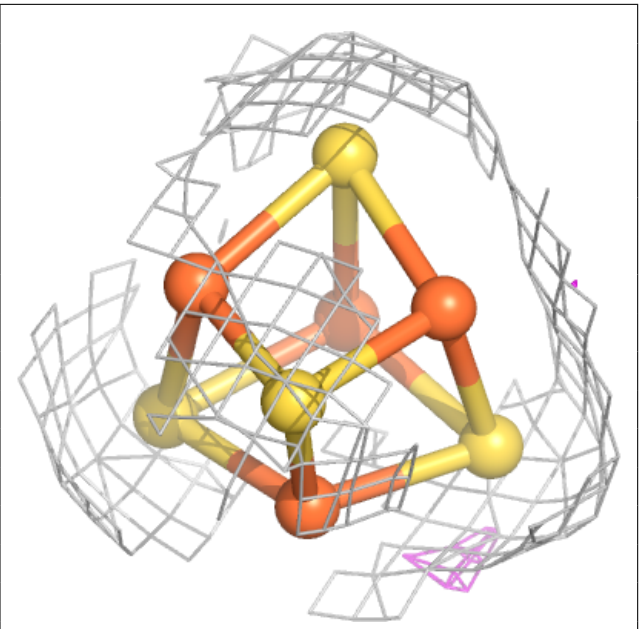
Electron density around SF4 V 503:

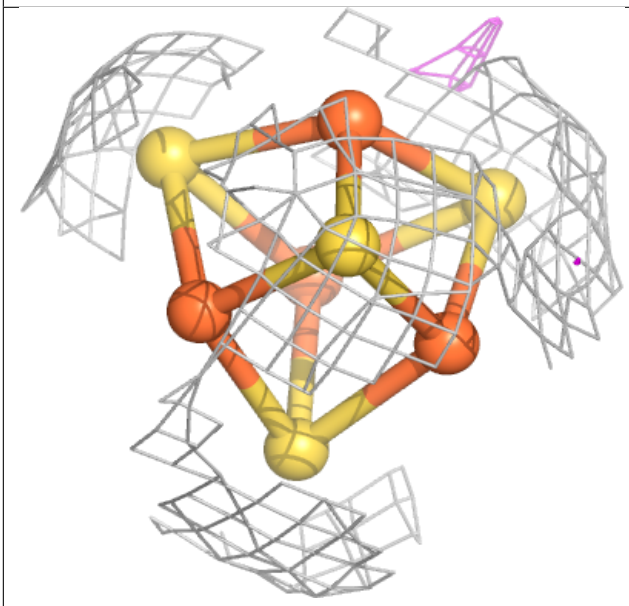
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

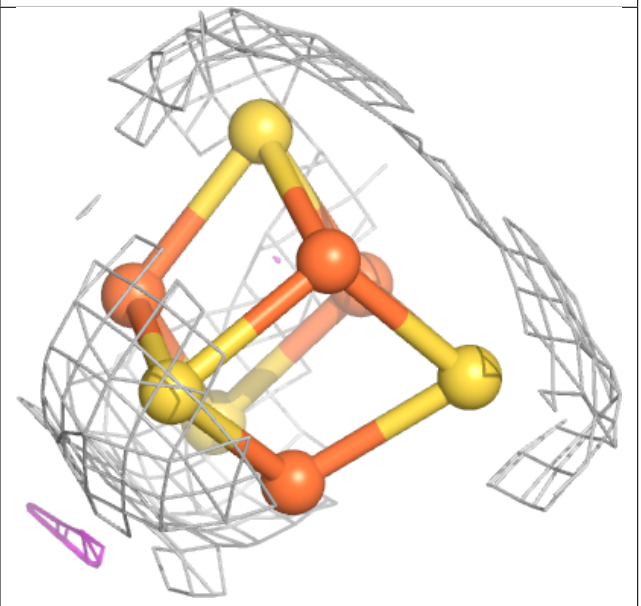


Electron density around SF4 M 502:

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

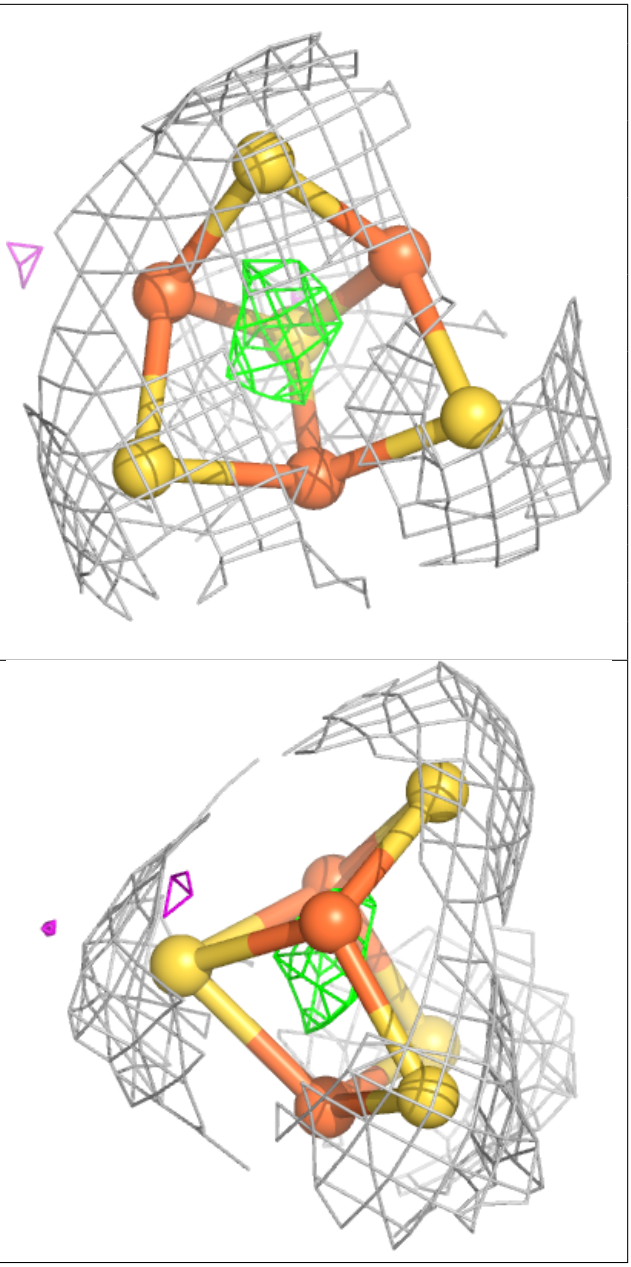






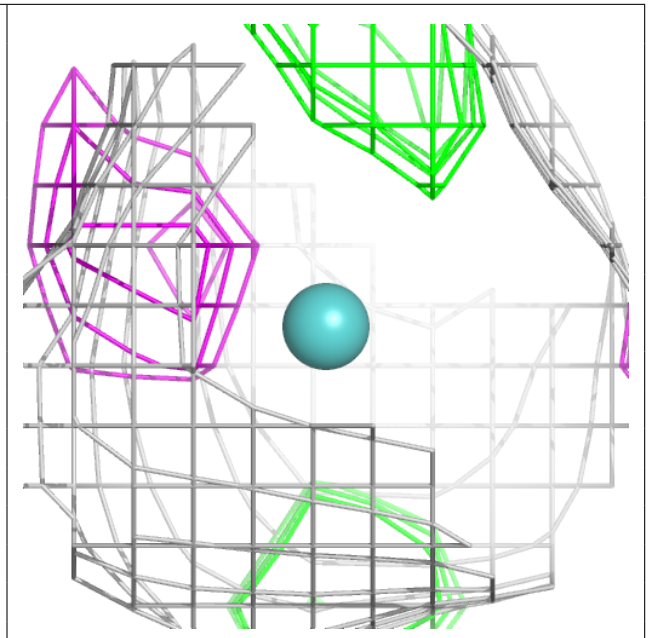
Electron density around F3S A 504:

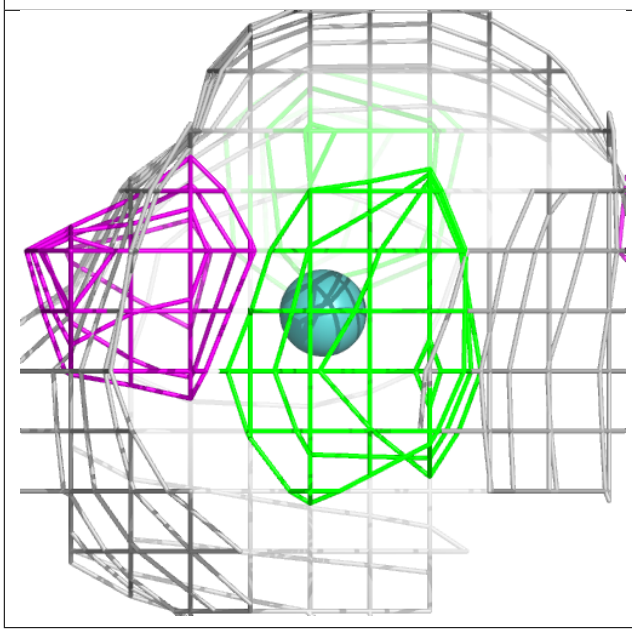
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

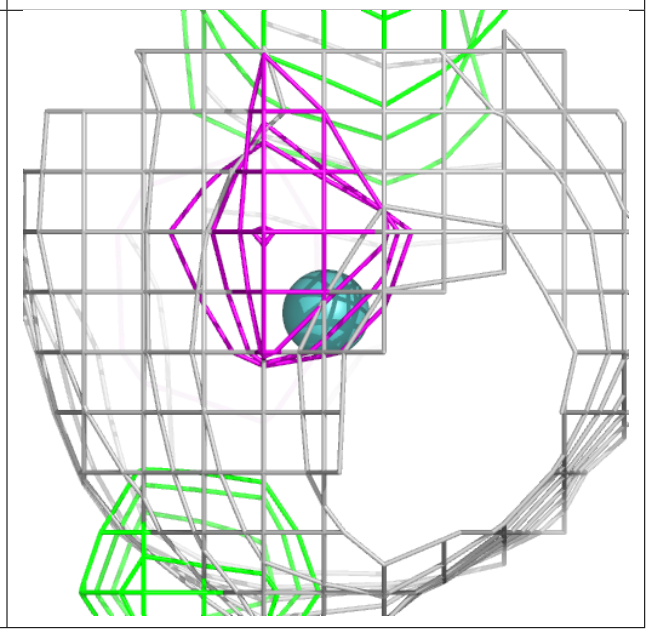


Electron density around MO Q 5803:

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

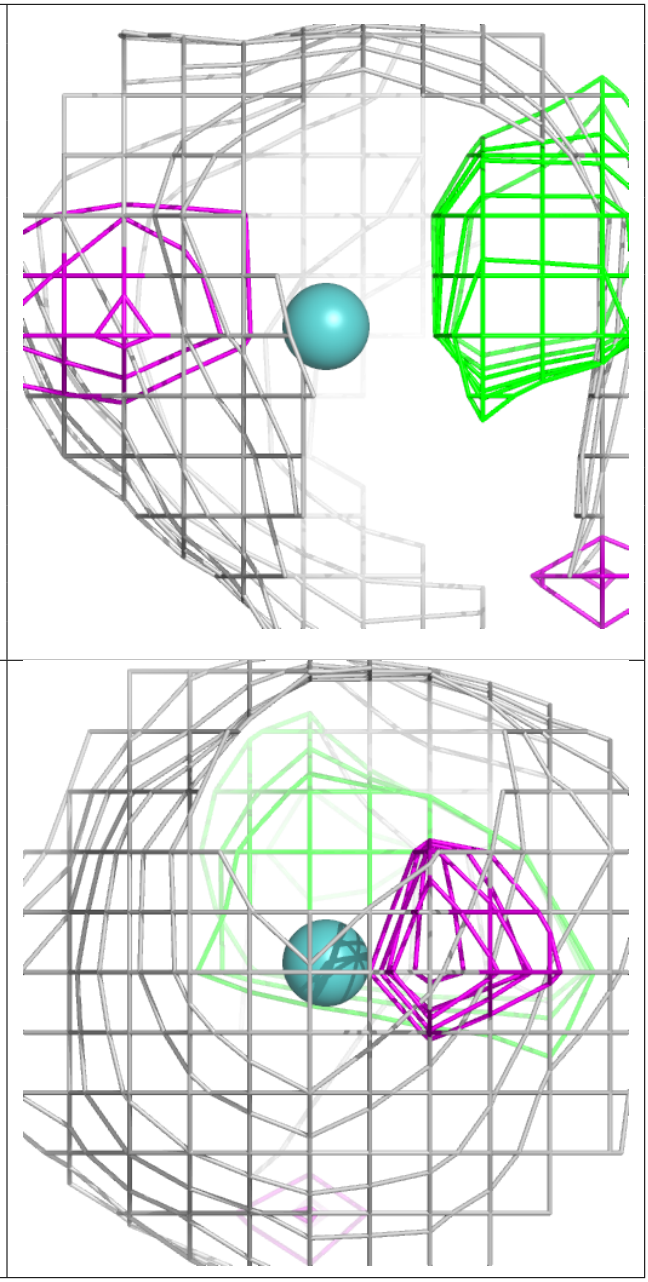






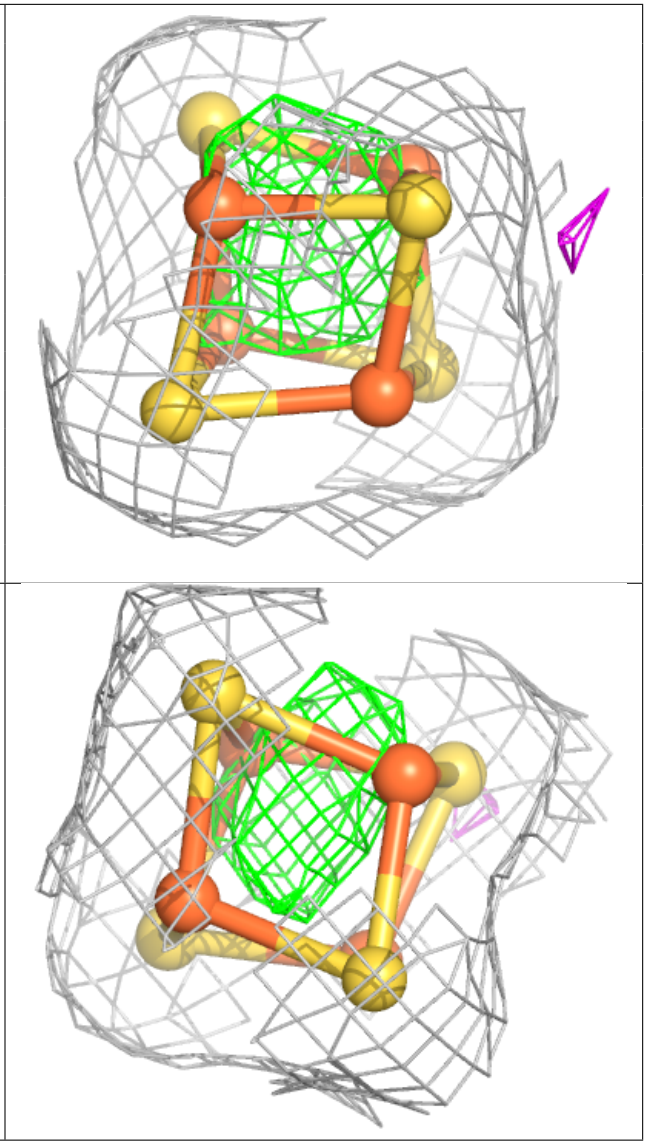
Electron density around MO T 5803:

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



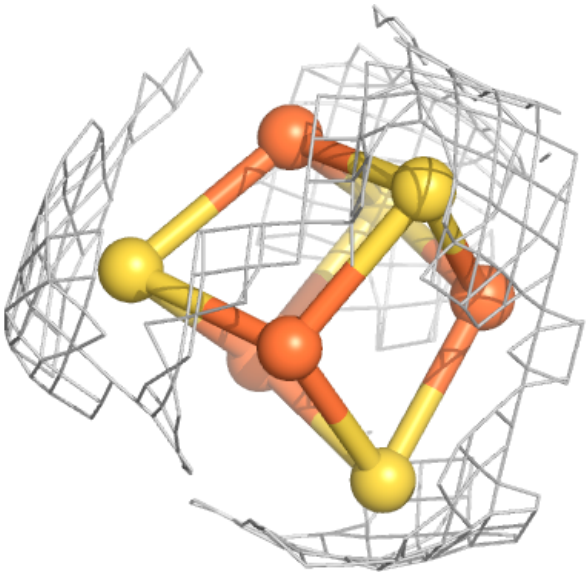
Electron density around SF4 J 501:

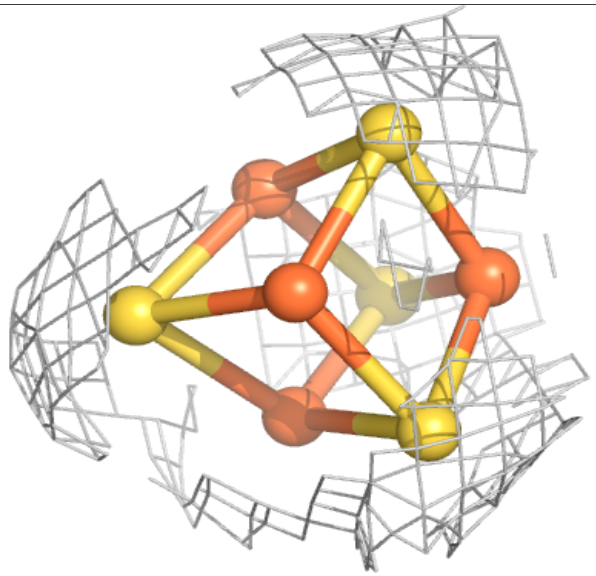
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

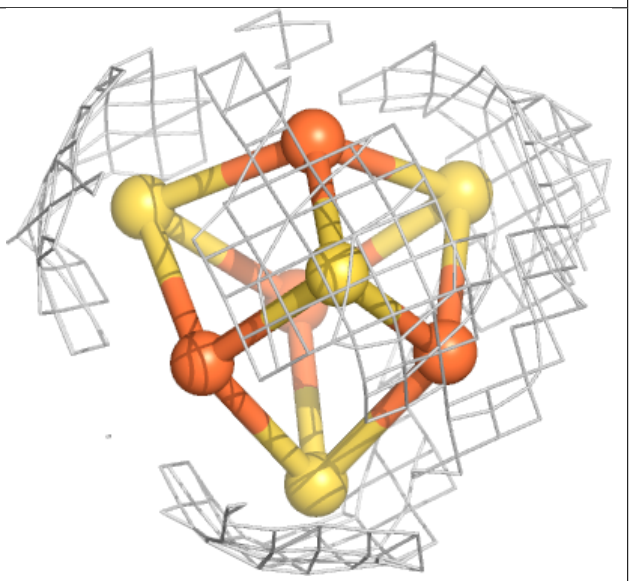


Electron density around SF4 P 503:

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

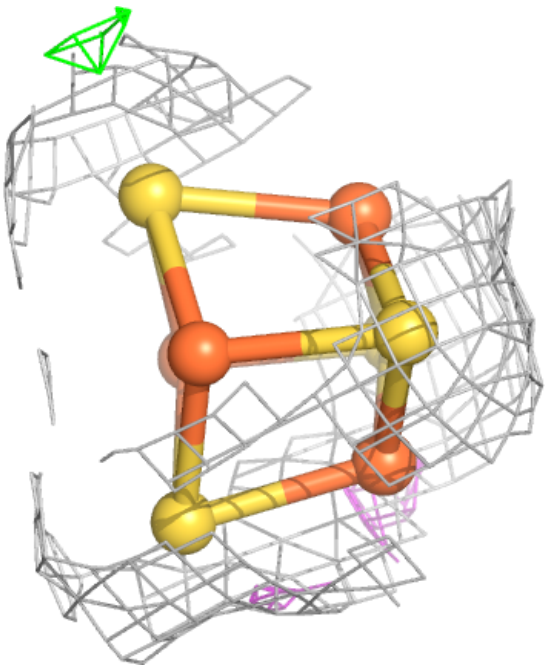


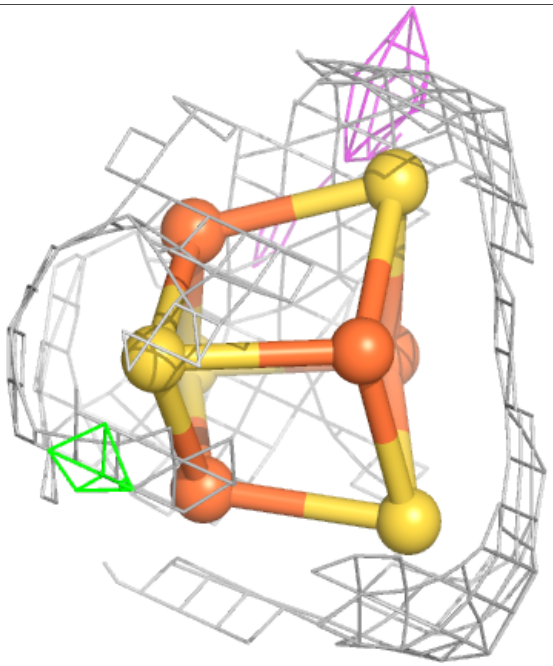


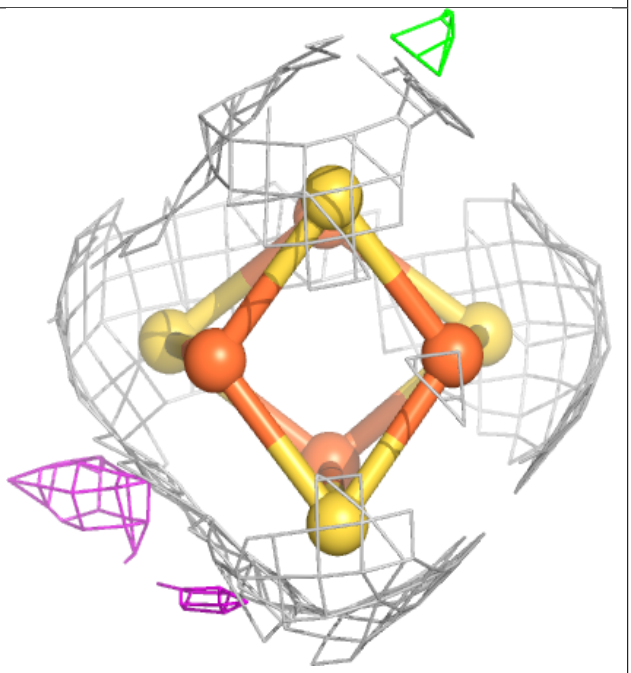


Electron density around SF4 J 502:

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

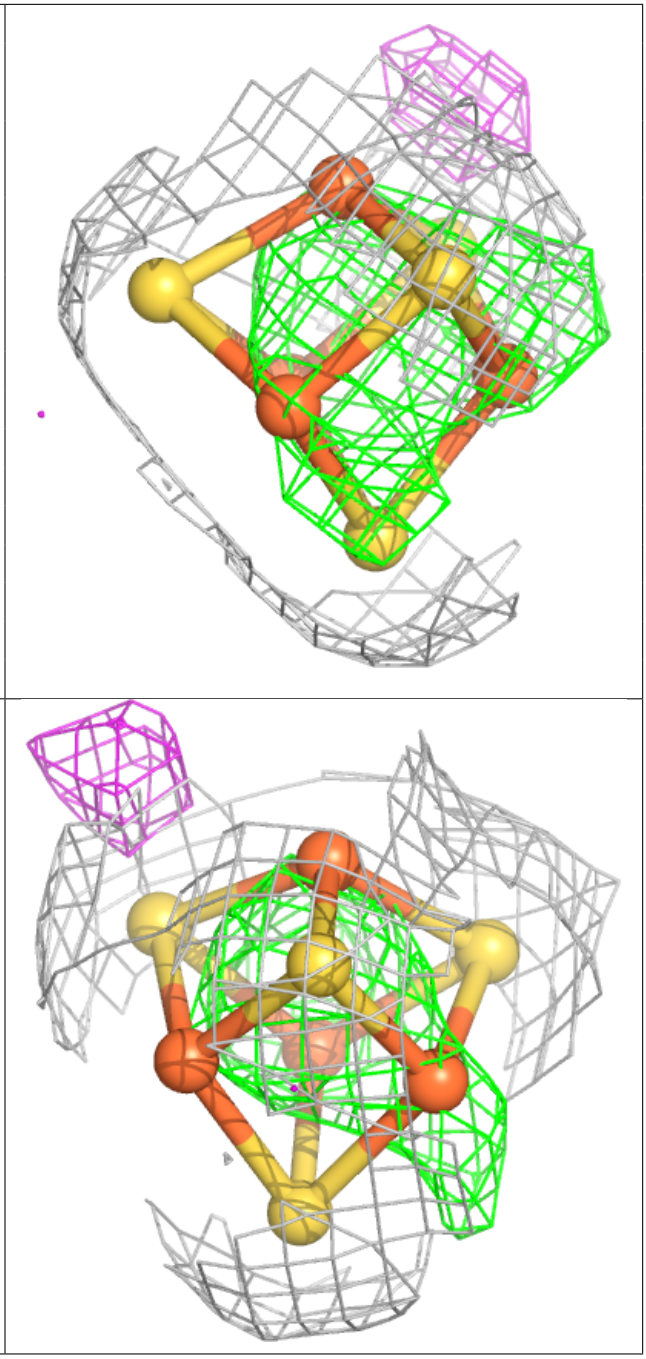






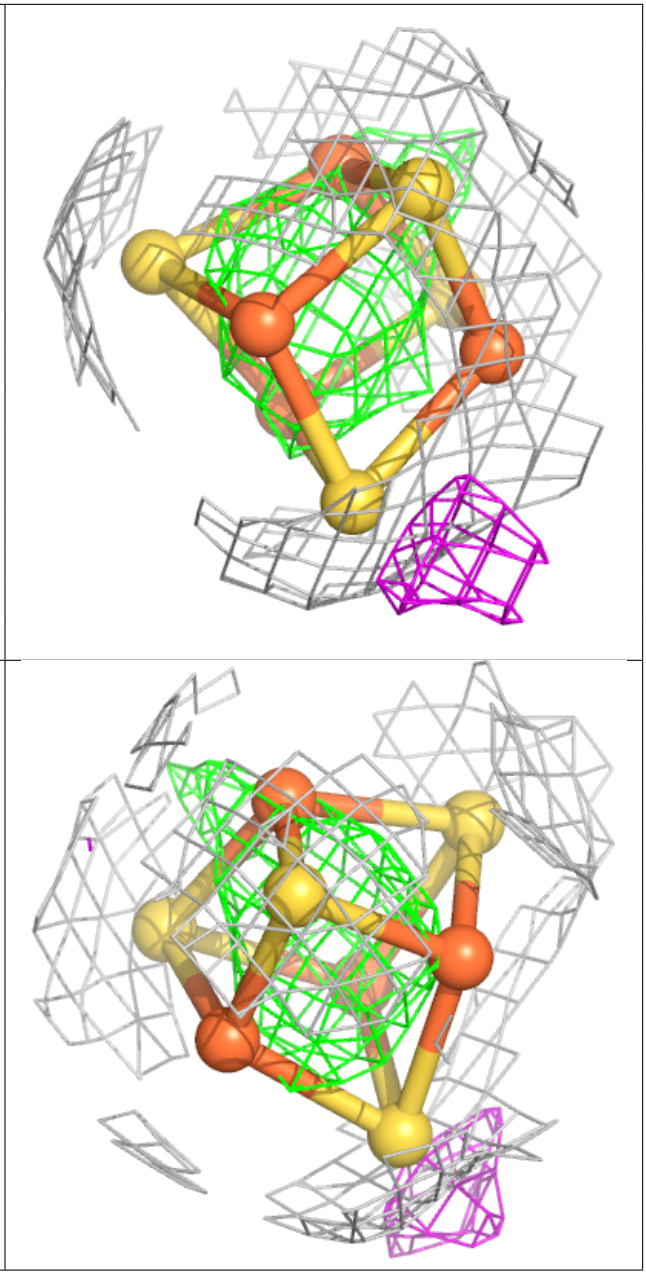
Electron density around SF4 S 501:

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



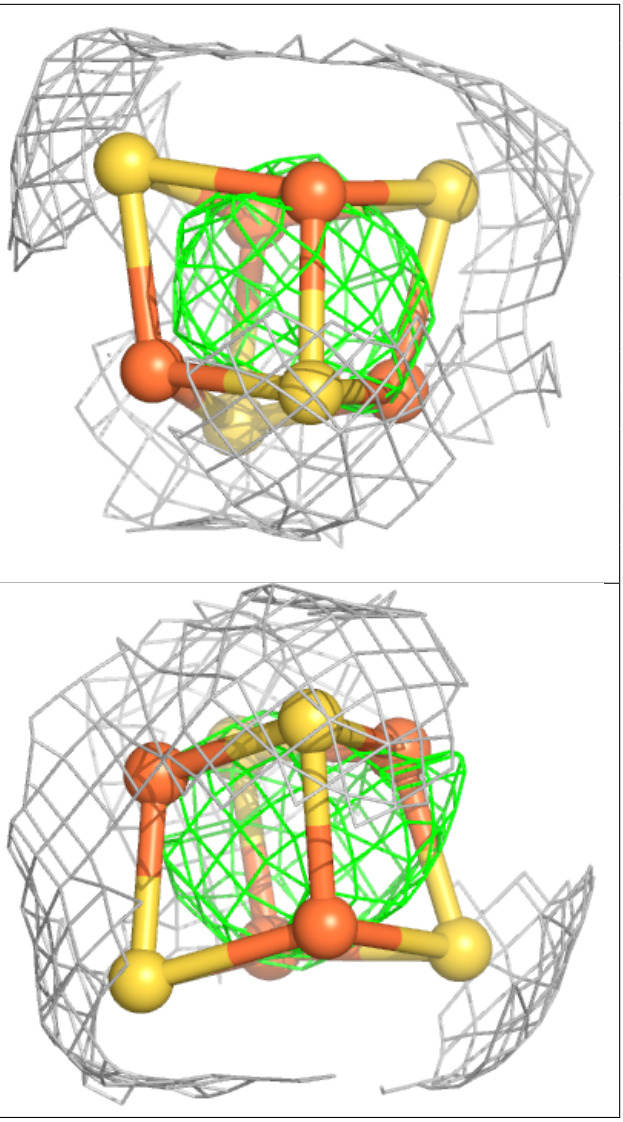
Electron density around SF4 T 5804:

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



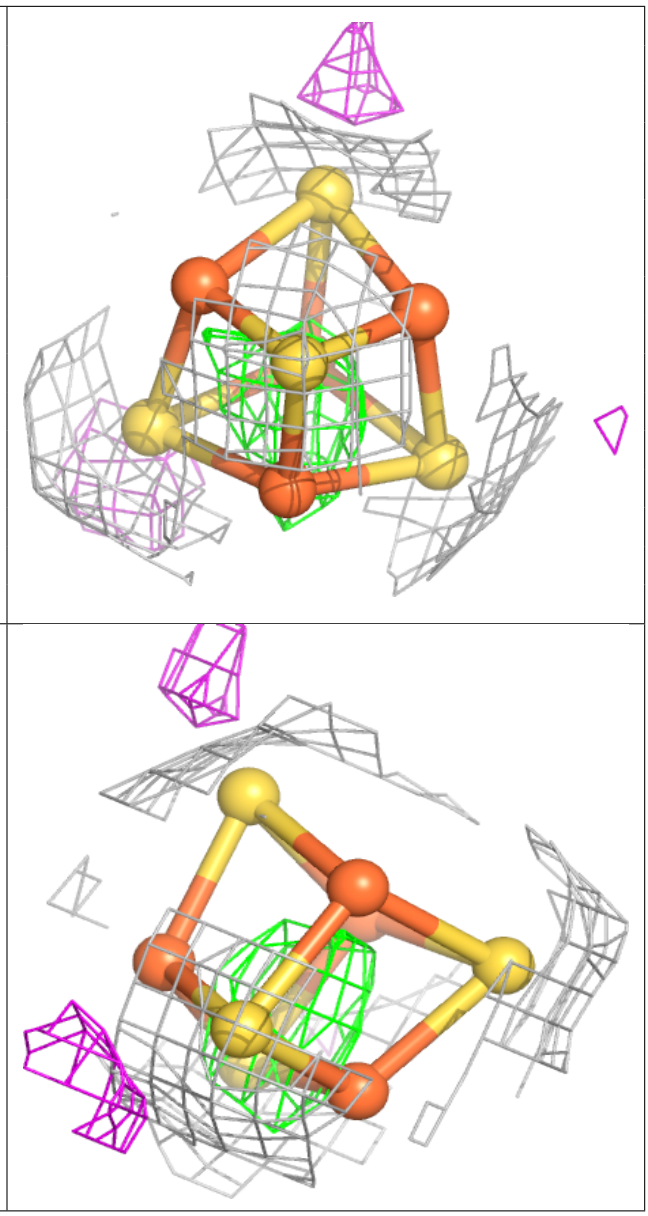
Electron density around SF4 A 501:

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



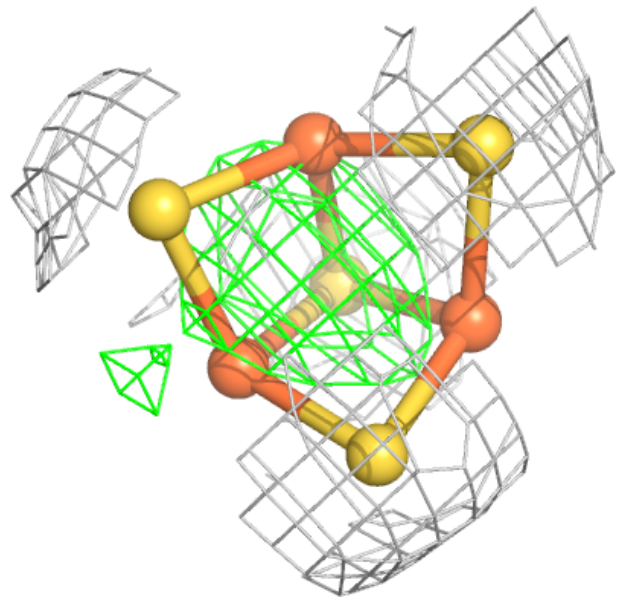
Electron density around SF4 M 501:

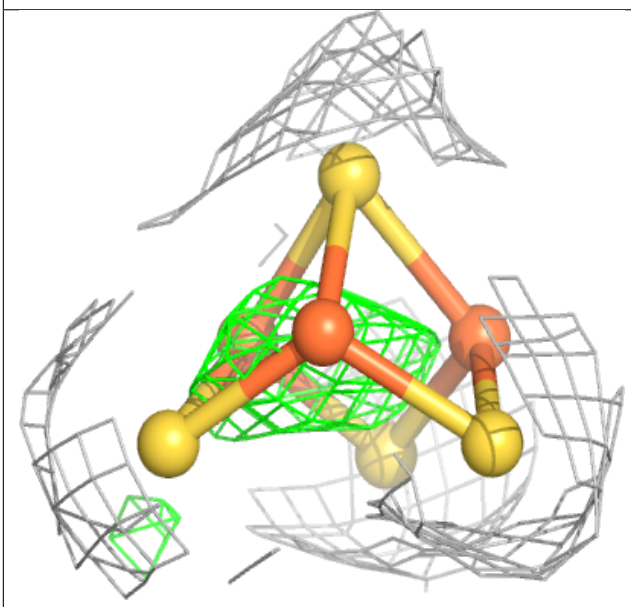
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

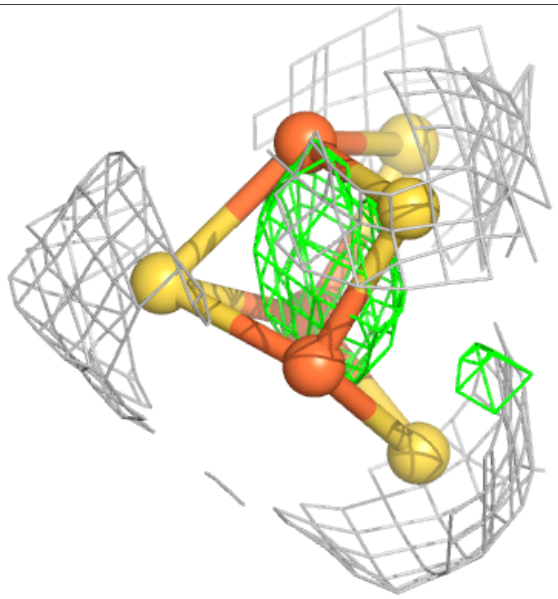


Electron density around F3S G 504:

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

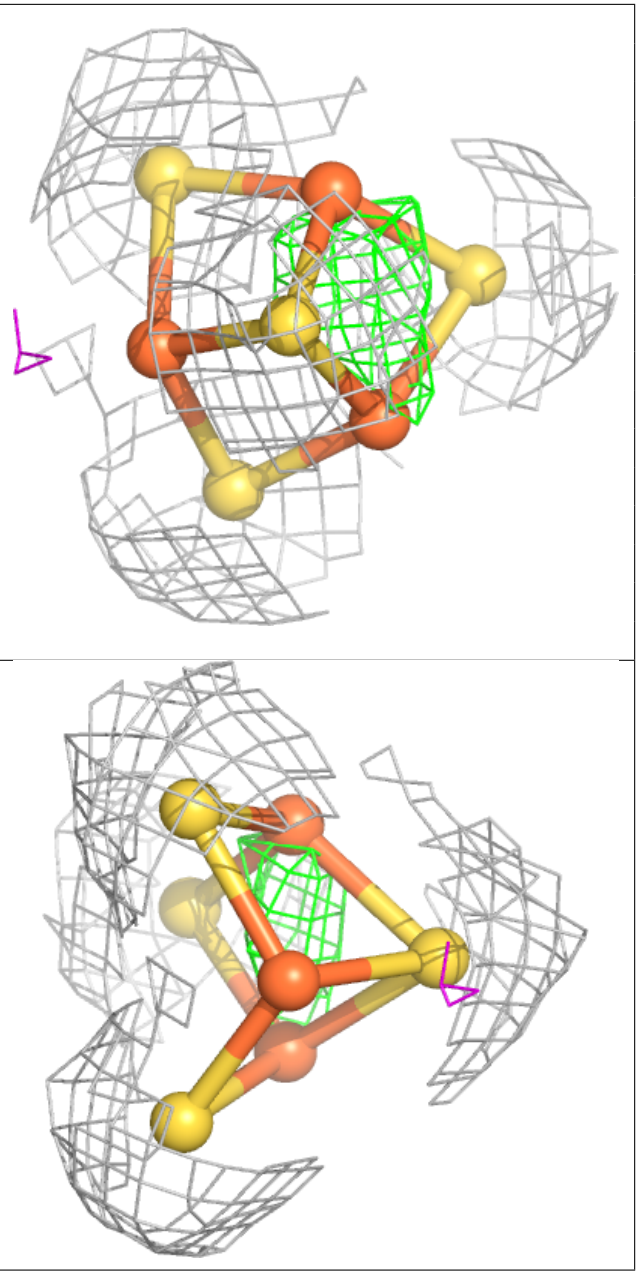






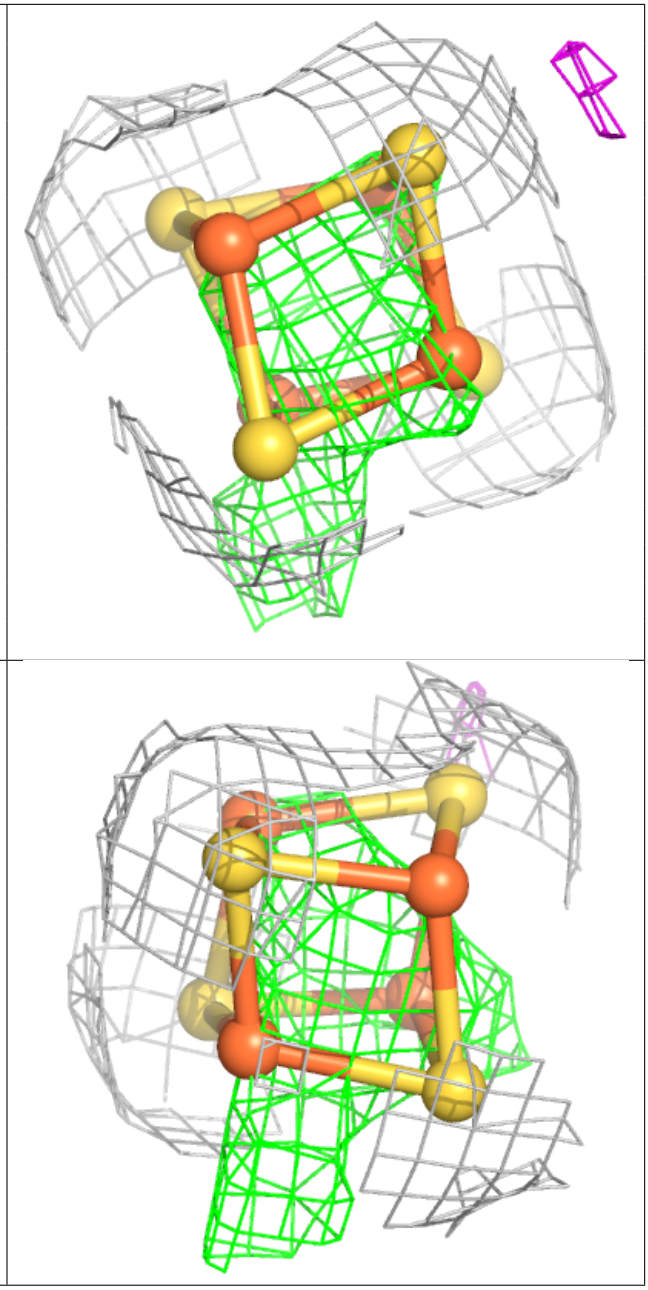
Electron density around F3S J 504:

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



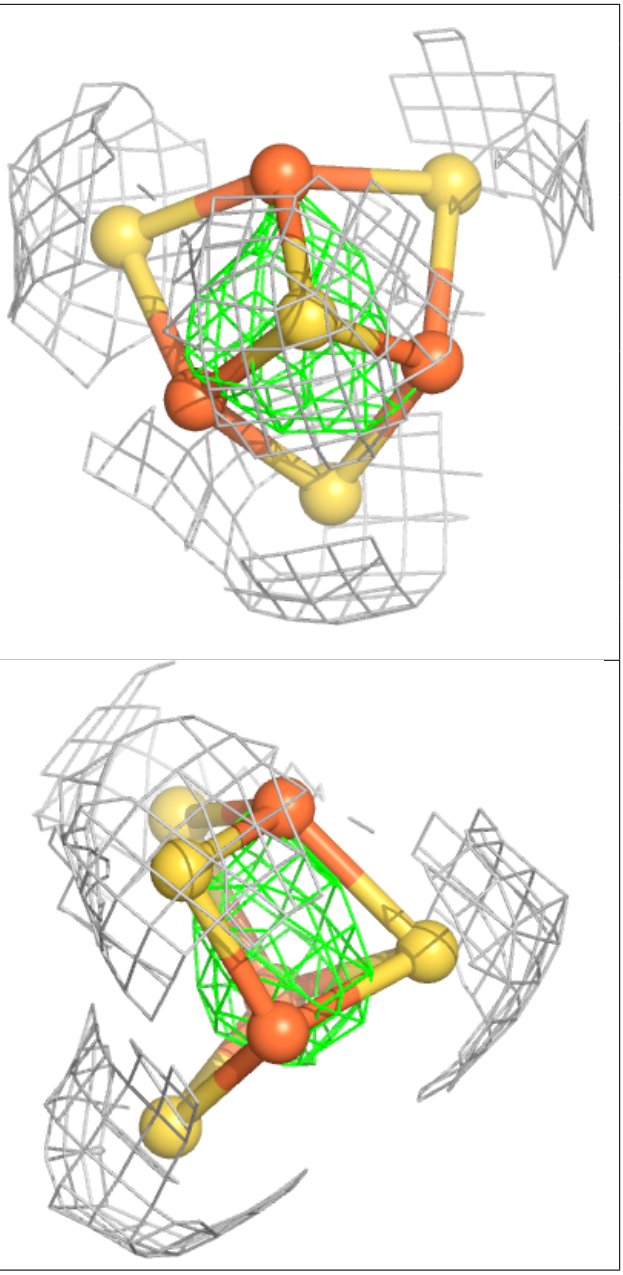
Electron density around SF4 G 501:

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



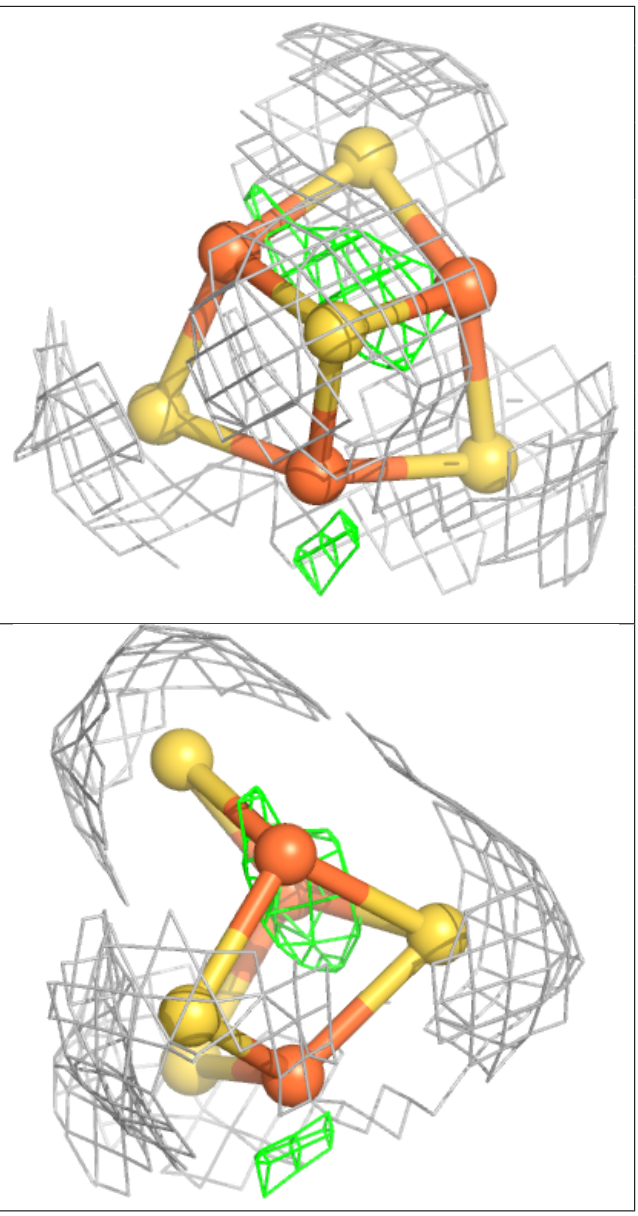
Electron density around F3S P 504:

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



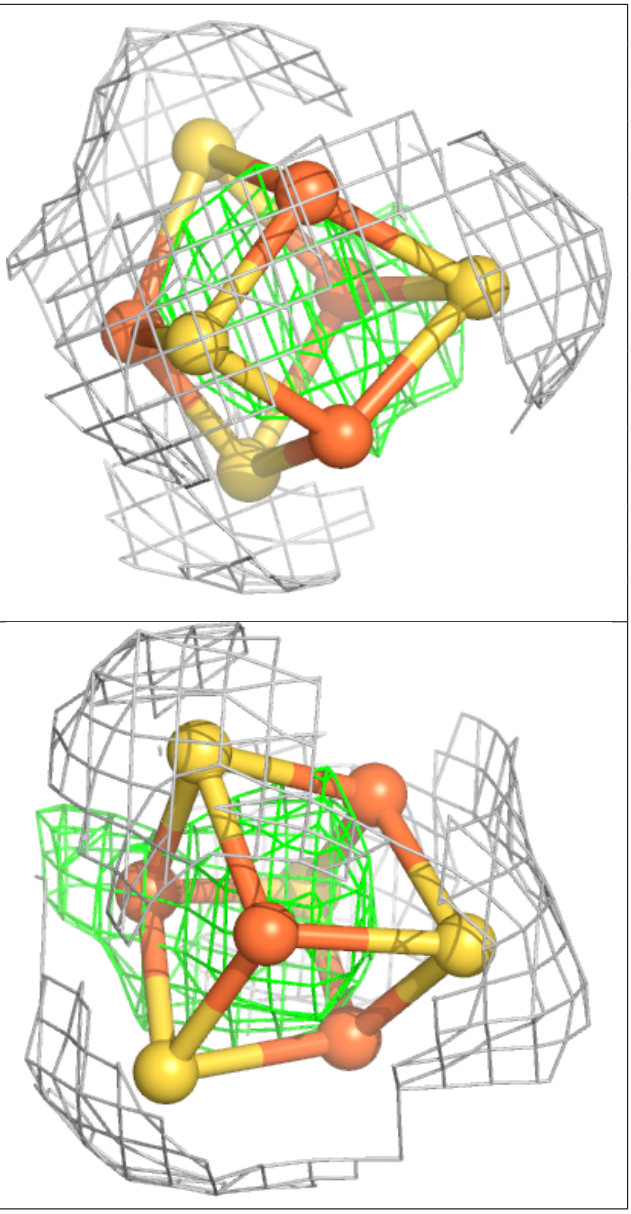
Electron density around F3S S 504:

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



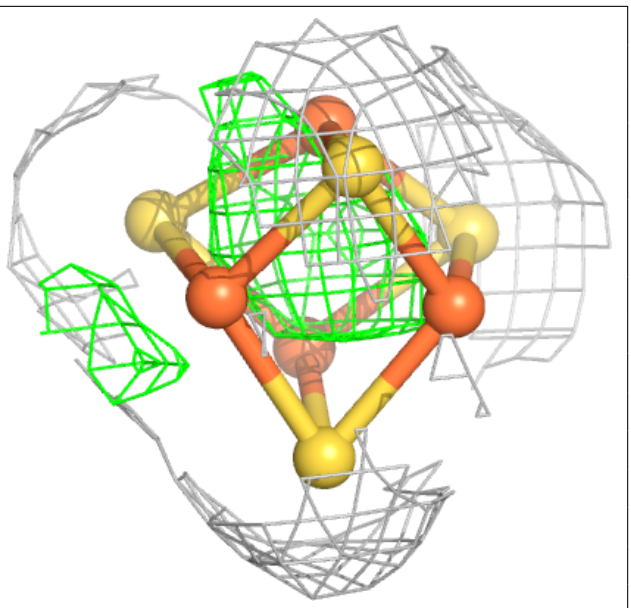
Electron density around SF4 P 501:

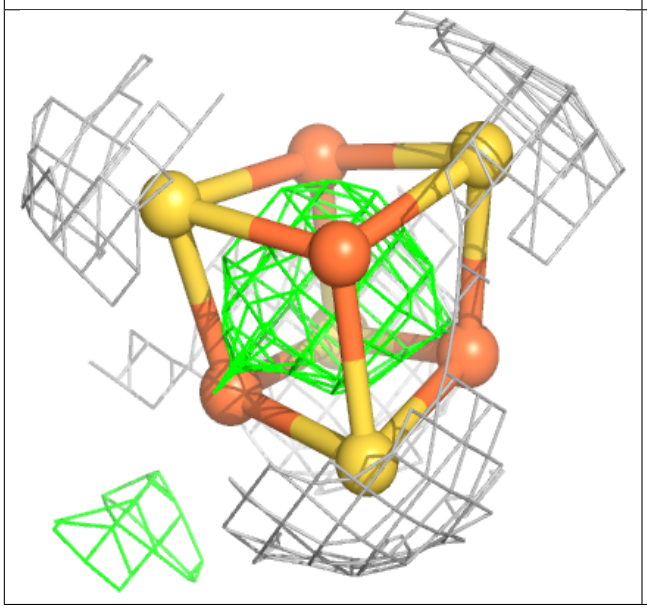
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

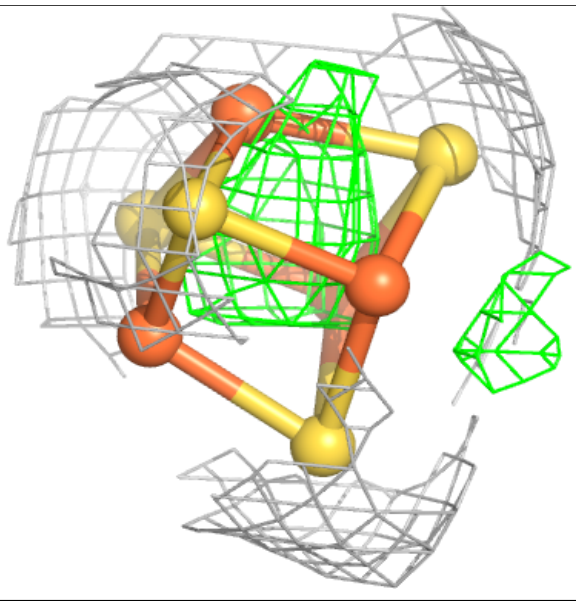


Electron density around SF4 P 502:

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

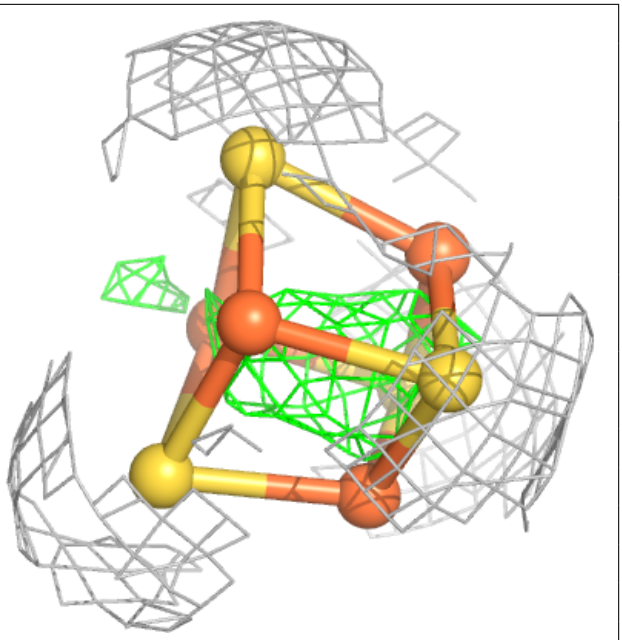


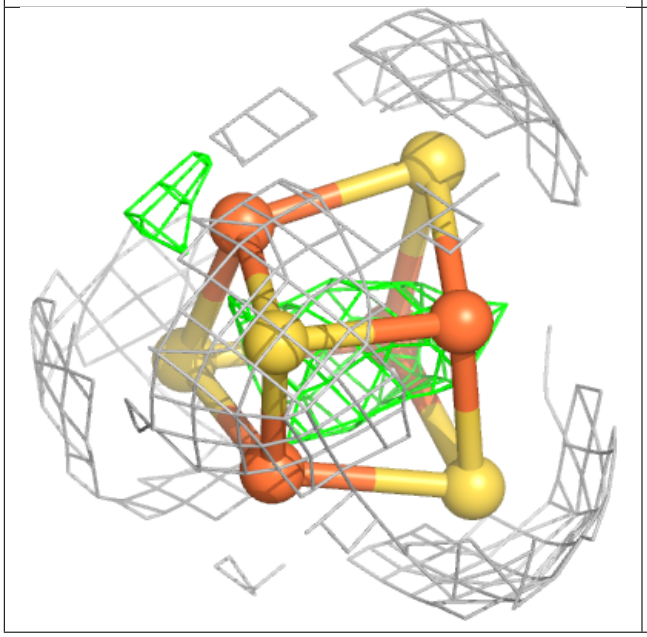


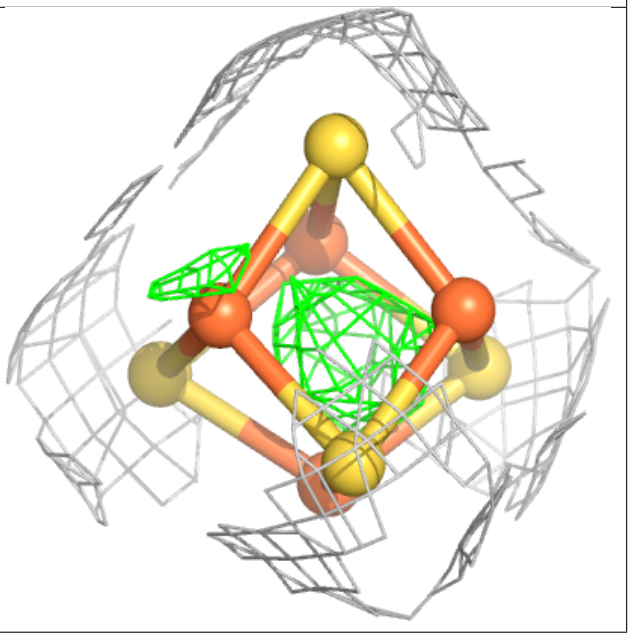


Electron density around SF4 G 502:

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

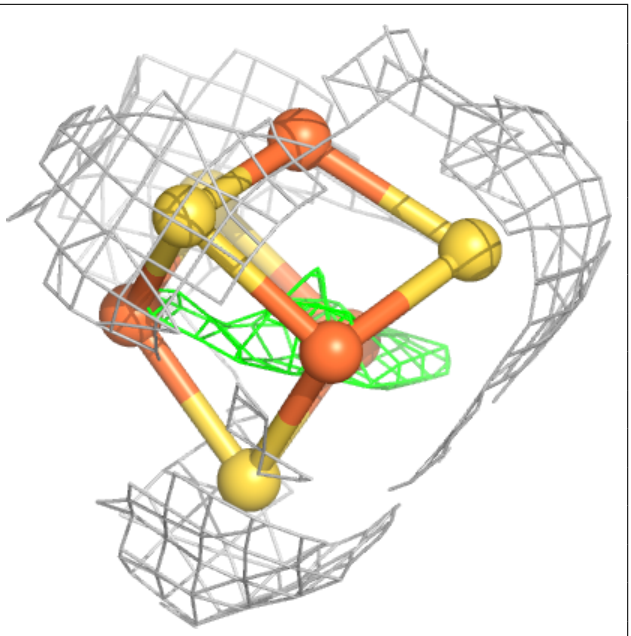


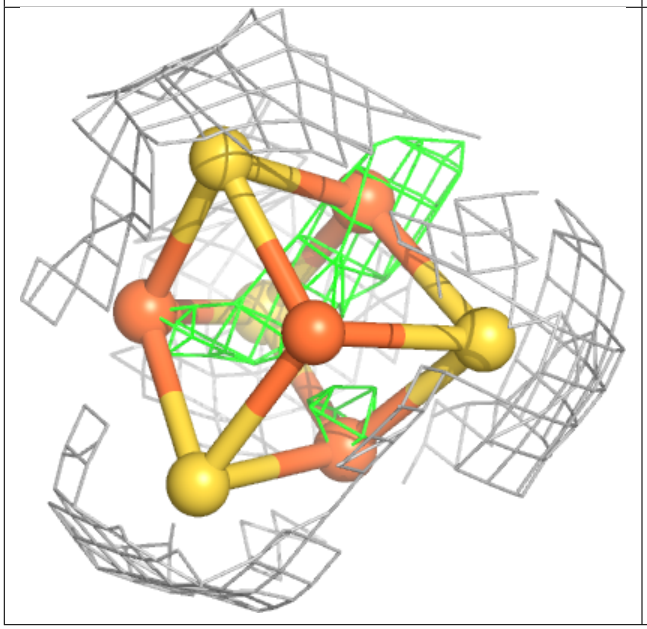


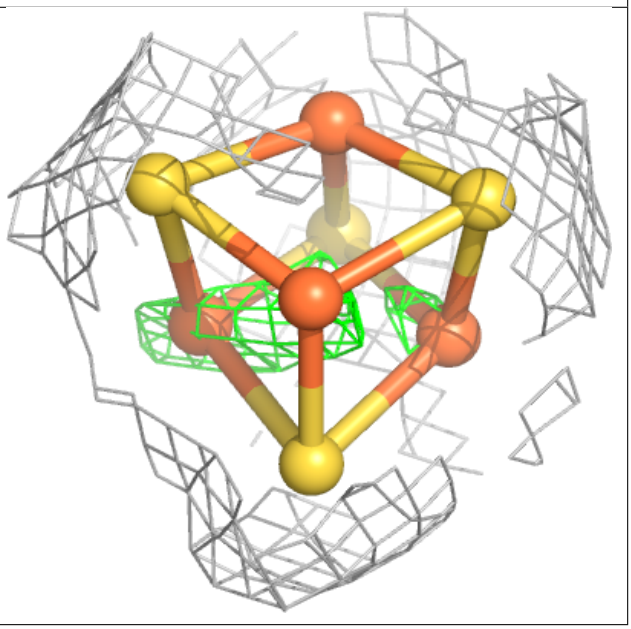


Electron density around SF4 G 503:

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

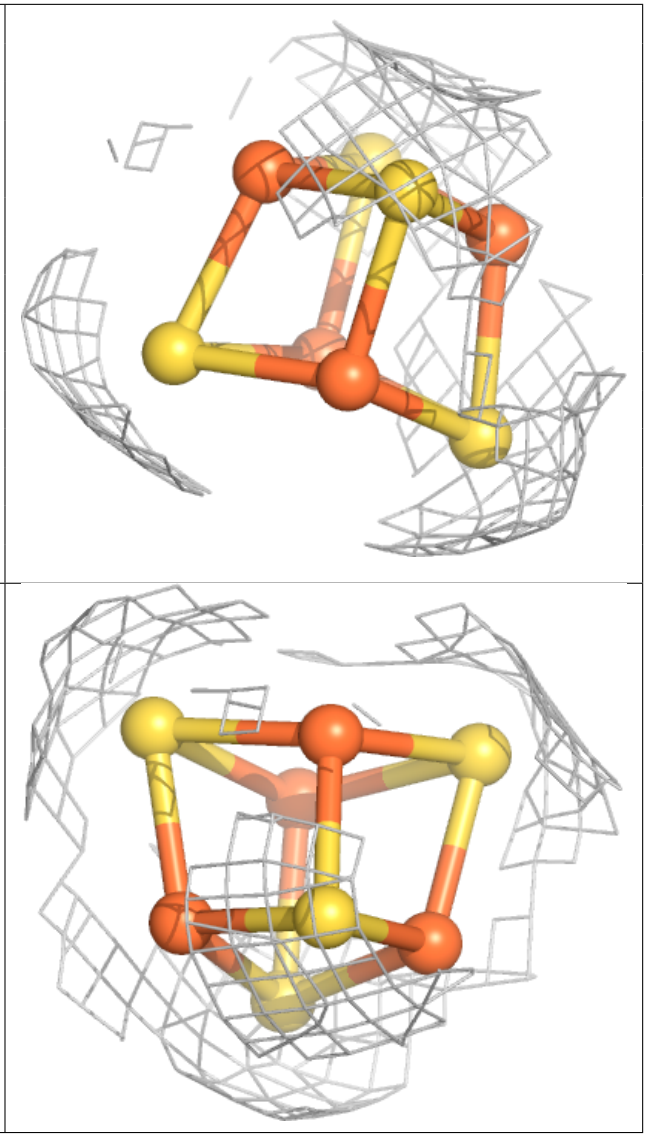






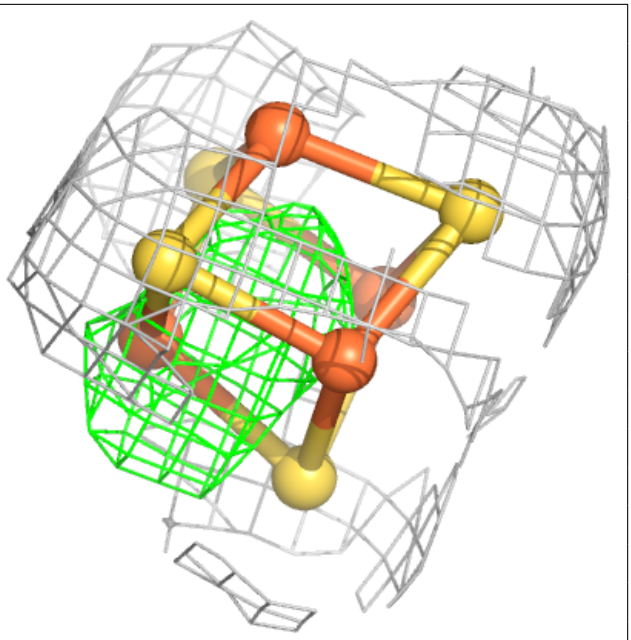
Electron density around SF4 M 503:

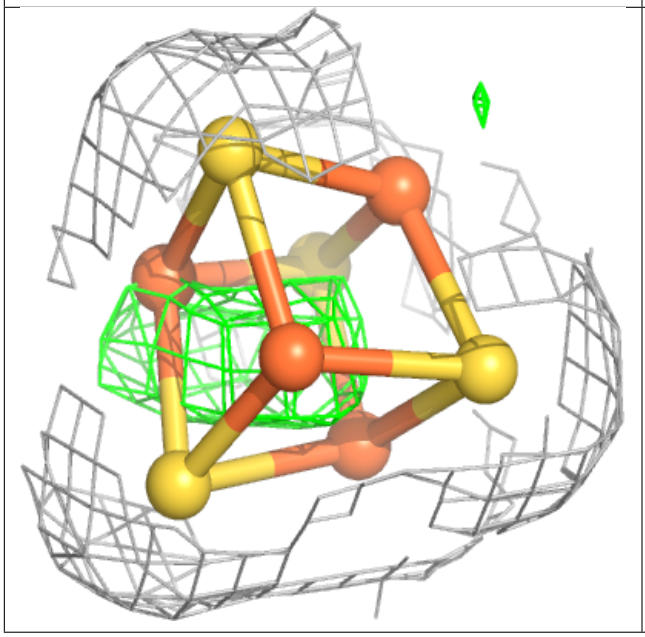
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

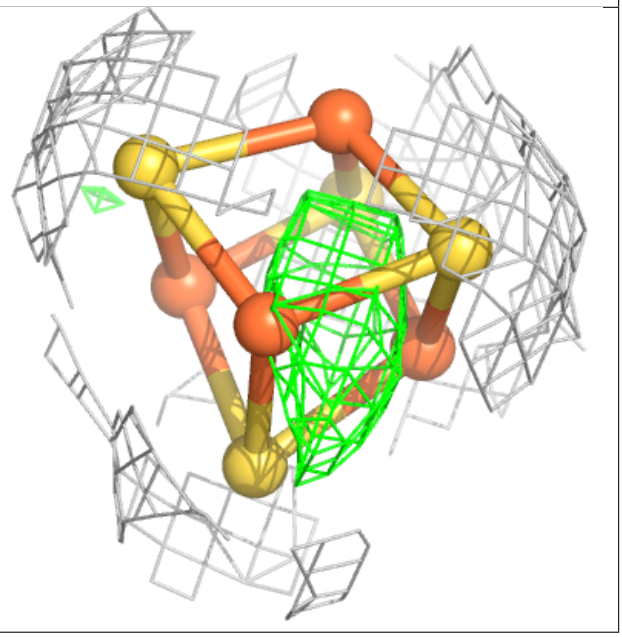


Electron density around SF4 S 502:

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

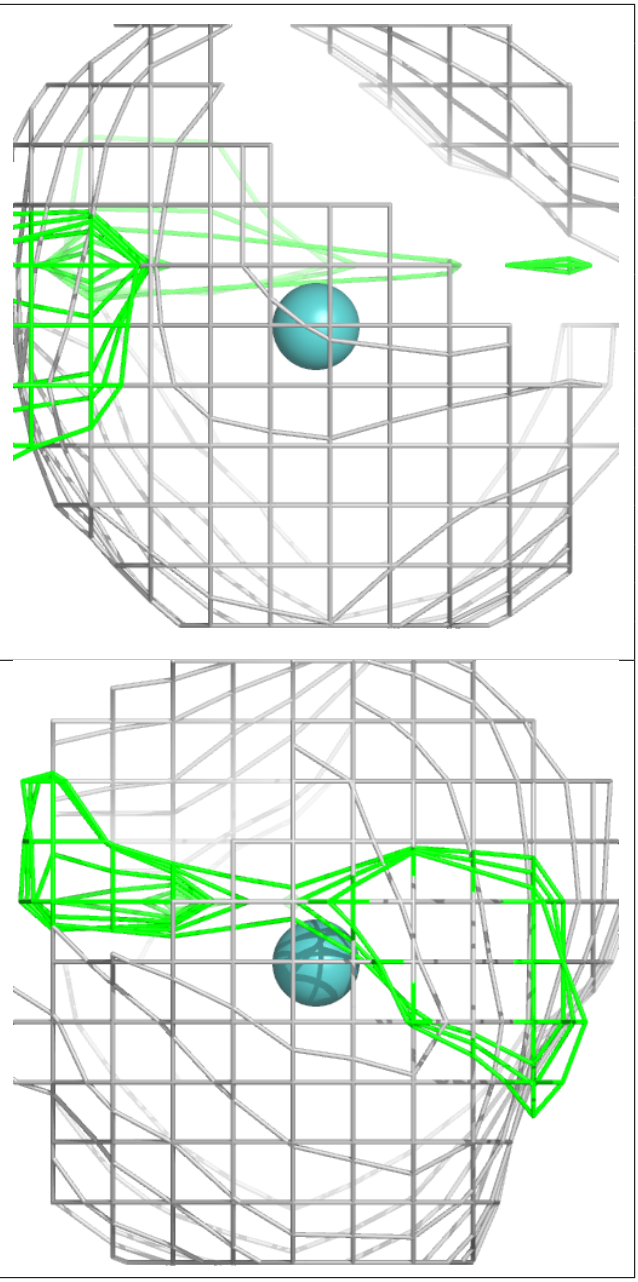






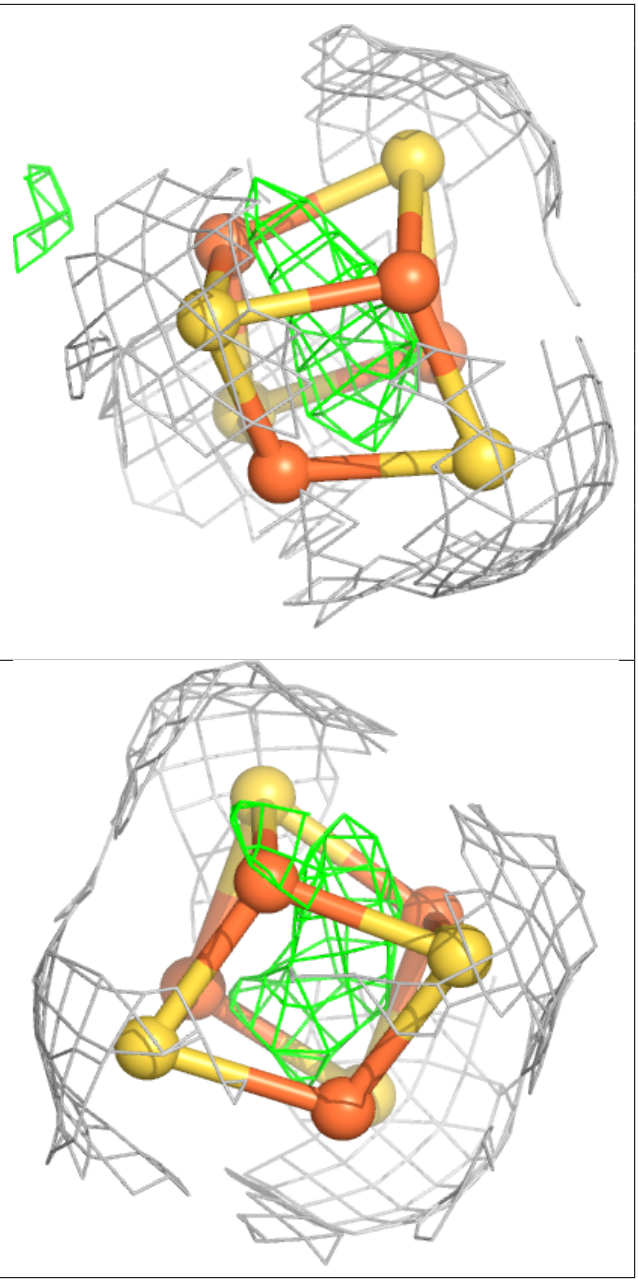
Electron density around MO B 5803:

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



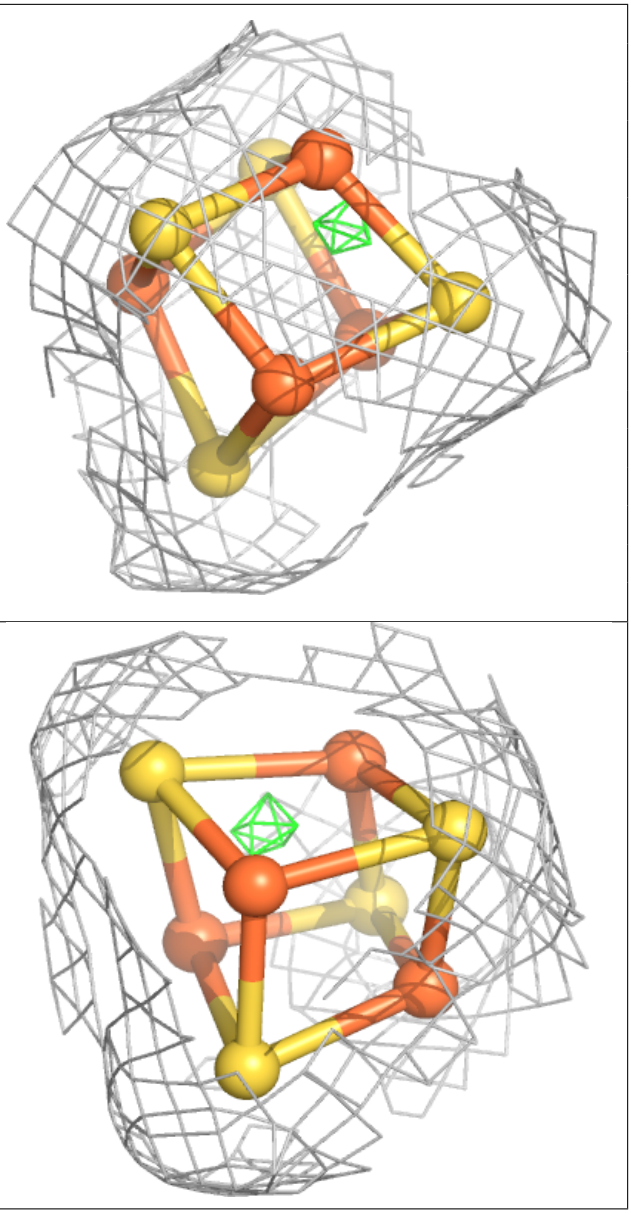
Electron density around SF4 A 503:

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



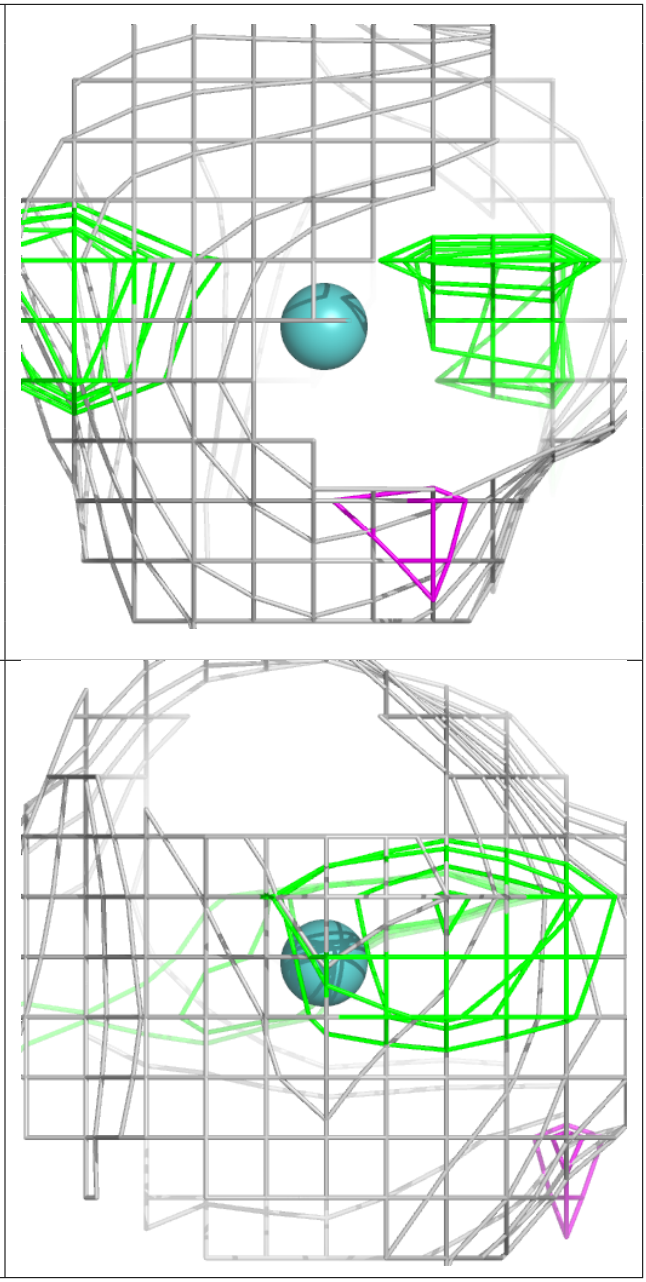
Electron density around SF4 A 502:

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



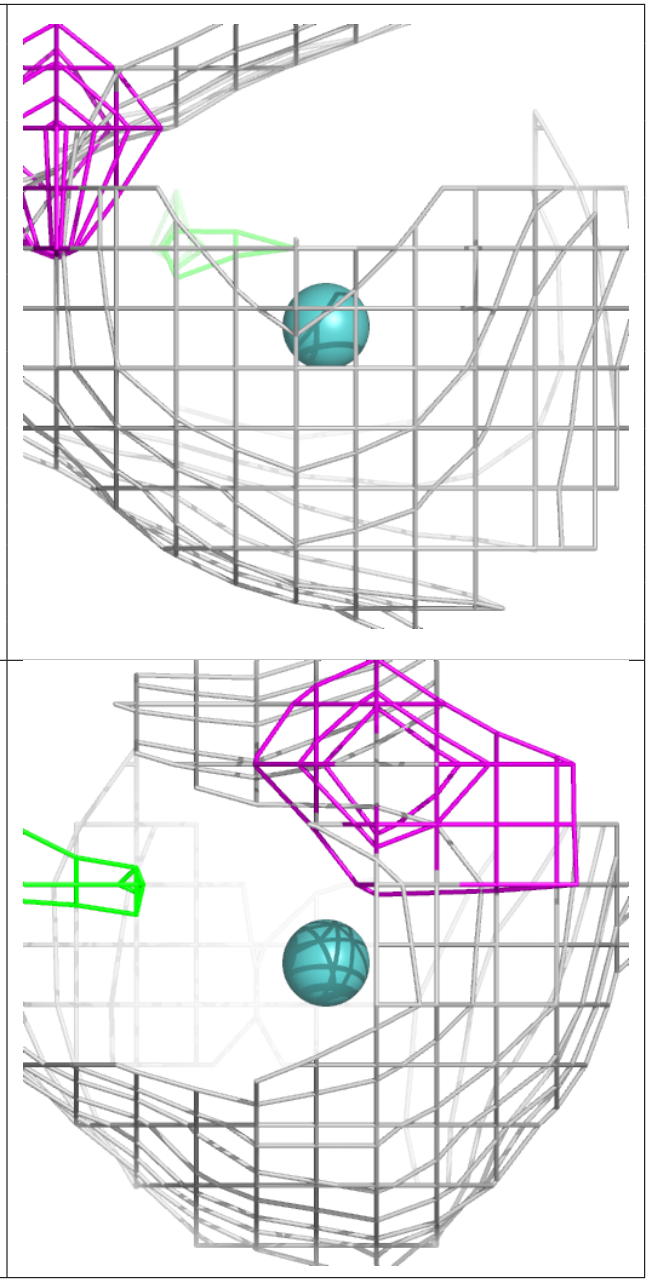
Electron density around MO H 5803:

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



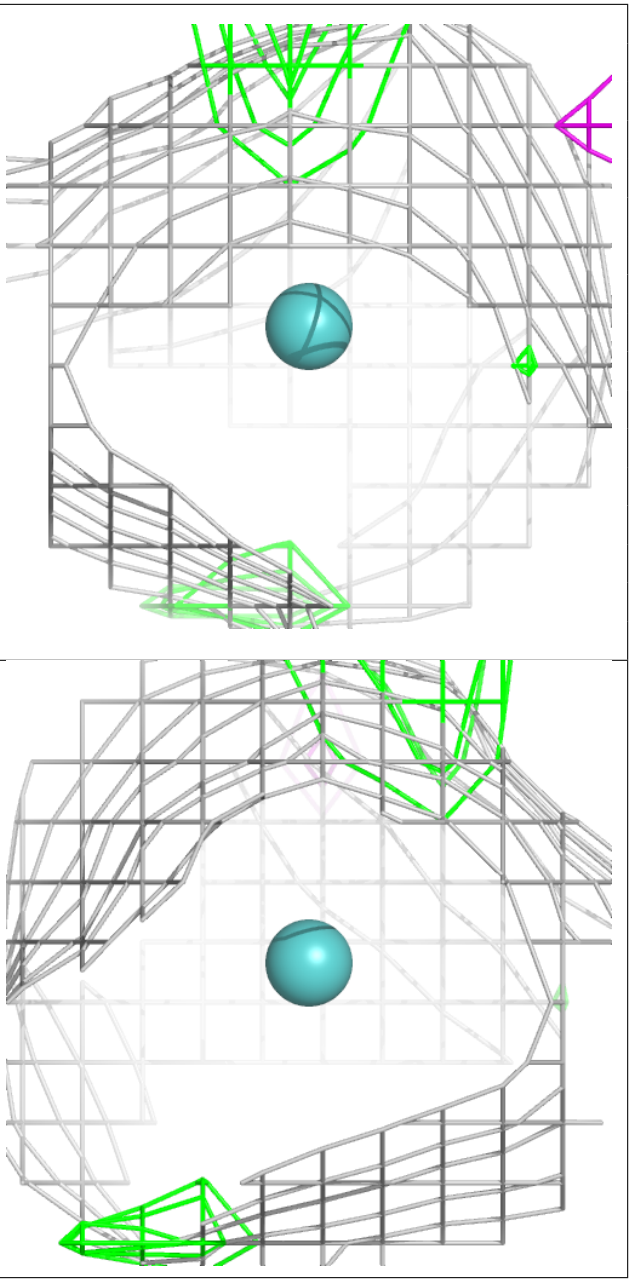
Electron density around MO K 5803:

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



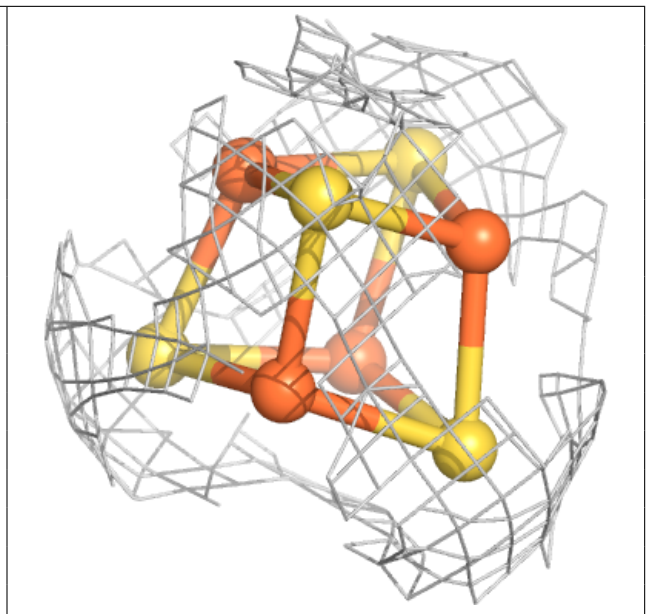
Electron density around MO N 5803:

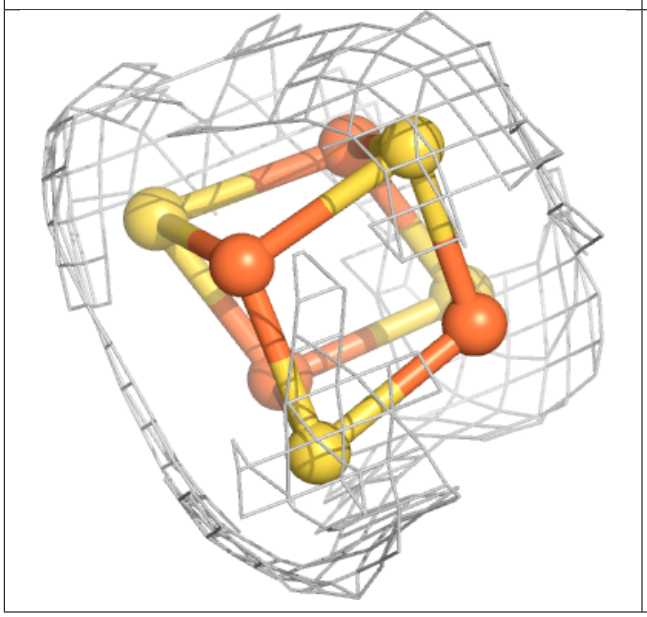
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

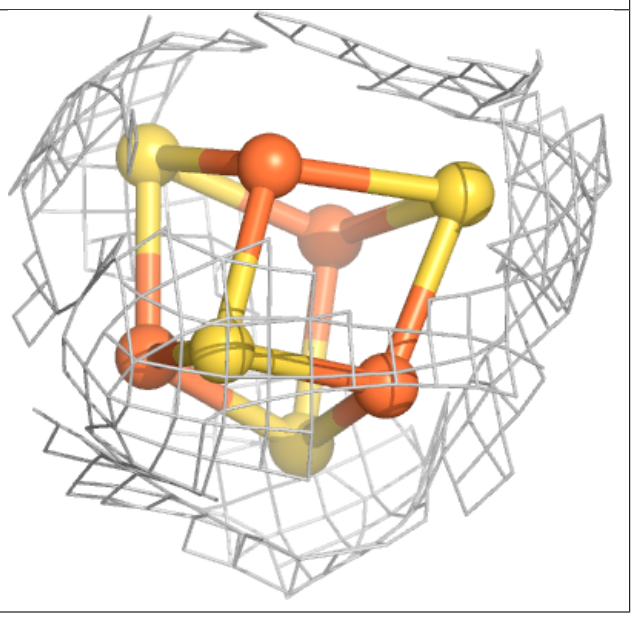


Electron density around SF4 S 503:

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

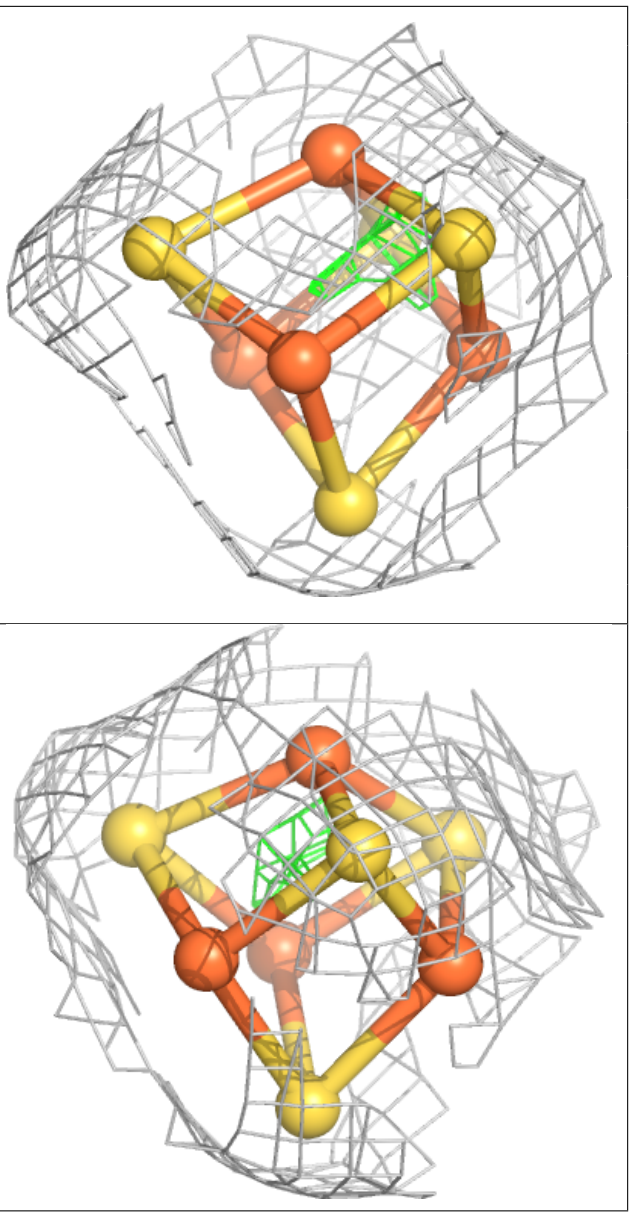






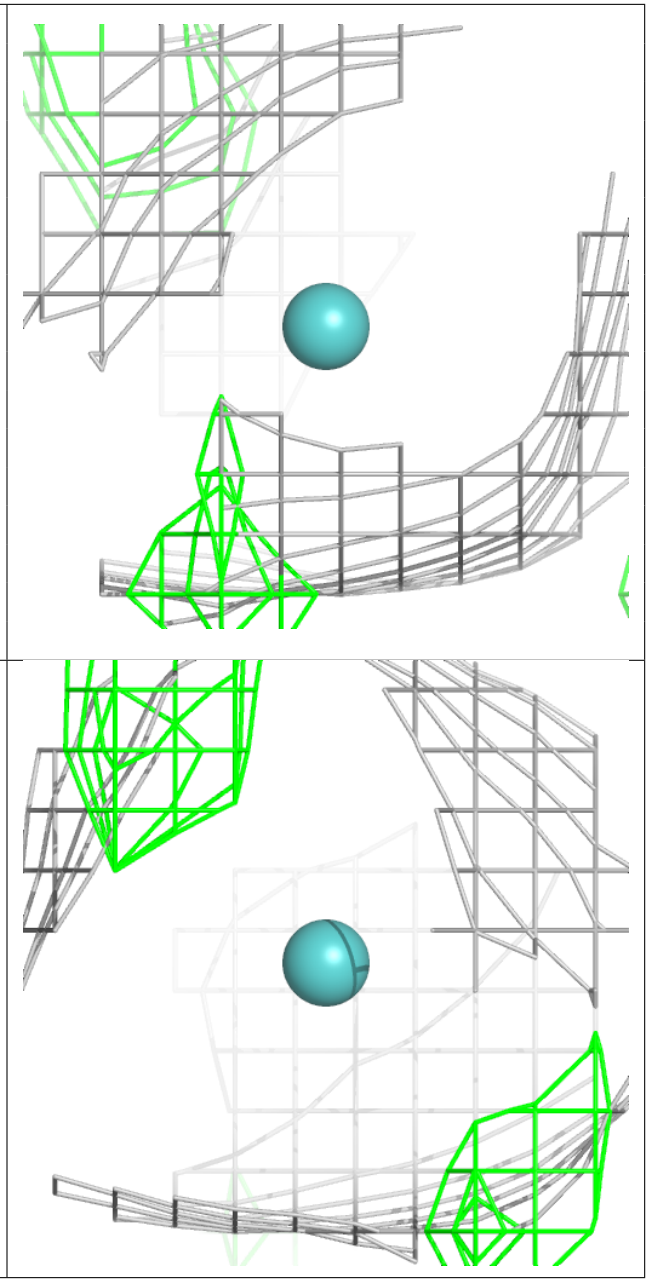
Electron density around SF4 J 503:

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



Electron density around MO W 5803:

$2mF_o$-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.