



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:55 PM UTC

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

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

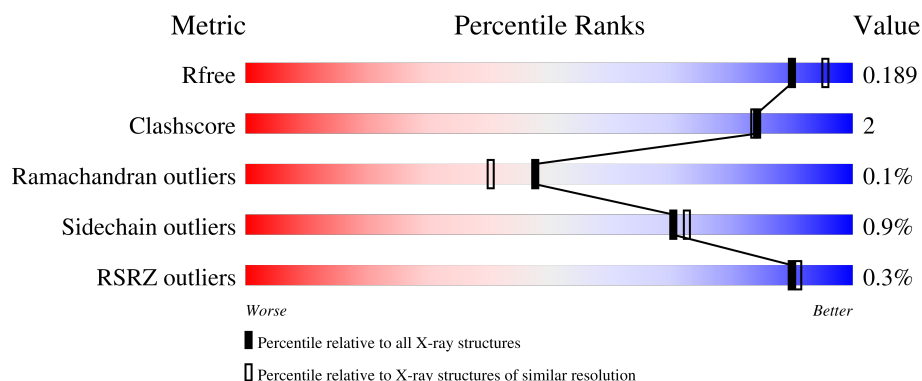
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

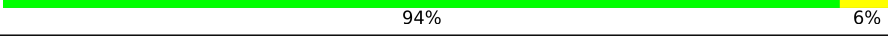
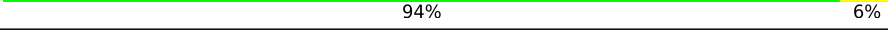
The reported resolution of this entry is 1.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



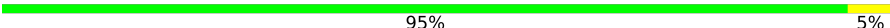
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	792	 89% 6% .
1	D	792	 89% 6% .
2	B	370	 94% 6%
2	E	370	 94% 6%
3	C	174	 89% 10% .

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

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21942 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acetyl-CoA decarboxylase/synthase complex subunit alpha.

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

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

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

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

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

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



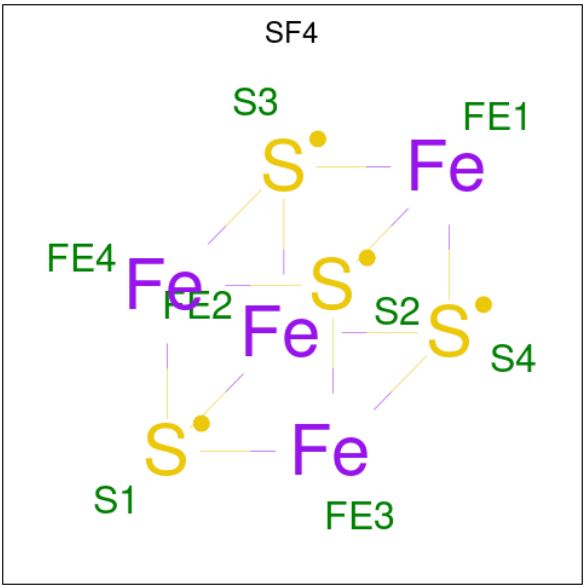
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



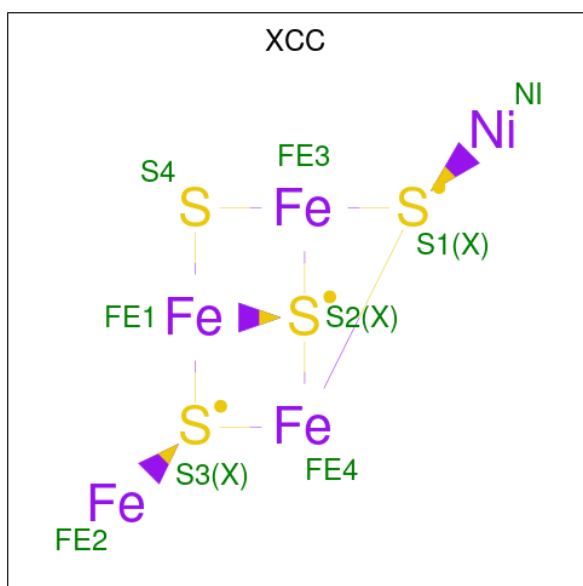
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	D	1	Total	Fe	S	0	0
			8	4	4		
6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

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

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

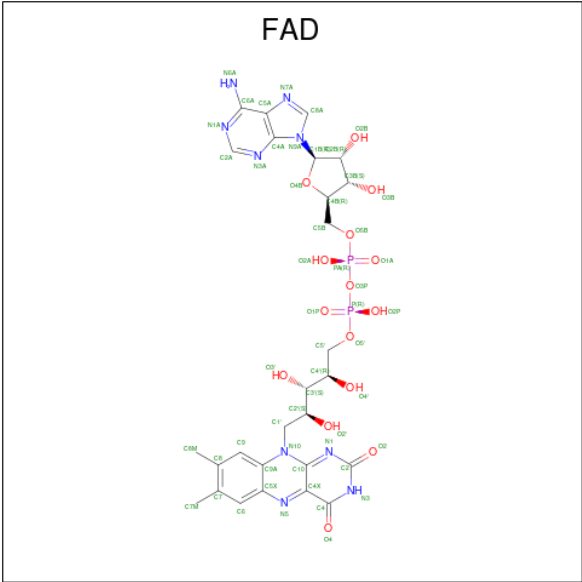


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
7	D	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

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

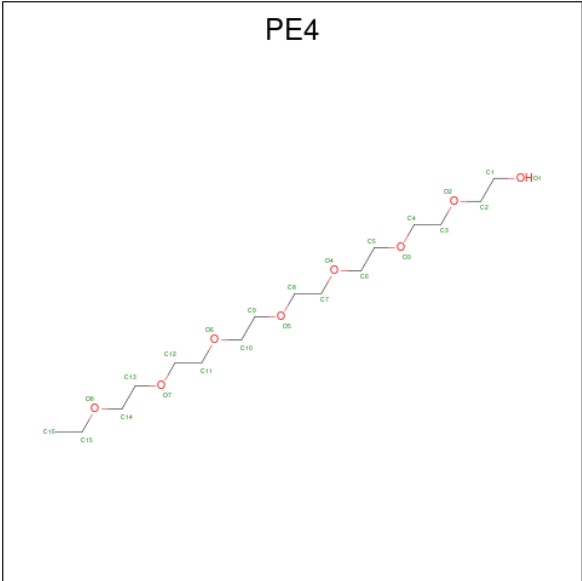
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	K	0	0
			1	1		
8	D	1	Total	K	0	0
			1	1		

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: PE4) (formula: C₁₆H₃₄O₈).



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

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

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

- Molecule 12 is water.

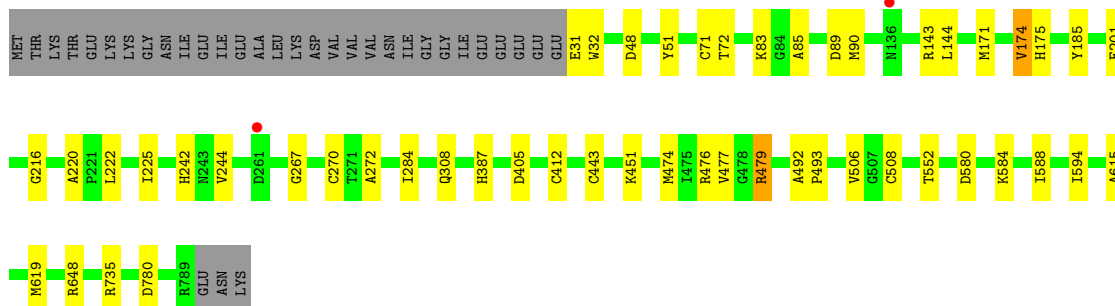
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	455	Total O 455 455	0	0
12	B	140	Total O 140 140	0	0
12	C	160	Total O 160 160	0	1
12	D	351	Total O 351 351	0	0
12	E	179	Total O 179 179	0	0
12	F	133	Total O 133 133	0	1

3 Residue-property plots

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

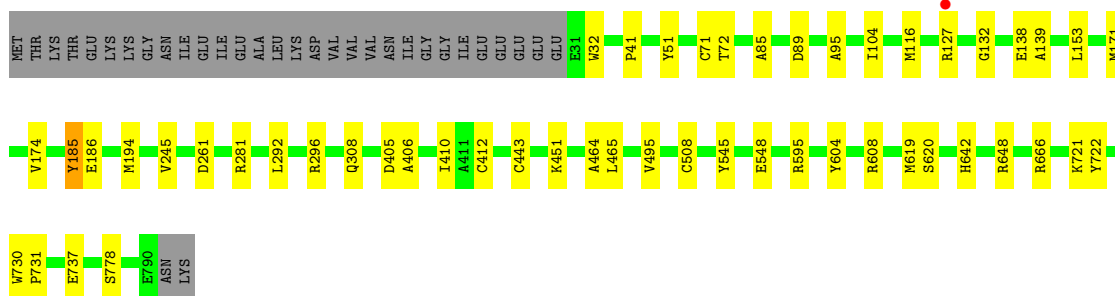
- Molecule 1: Acetyl-CoA decarboxylase/synthase complex subunit alpha

Chain A: 

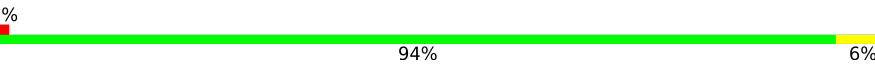


- Molecule 1: Acetyl-CoA decarboxylase/synthase complex subunit alpha

Chain D: 

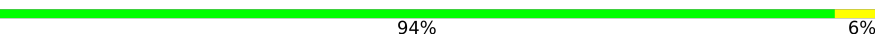


- Molecule 2: Coenzyme F420 hydrogenase/dehydrogenase, beta subunit C terminus

Chain B: 

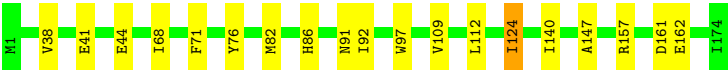
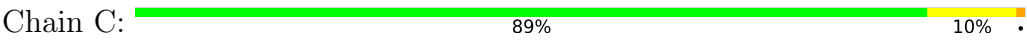


- Molecule 2: Coenzyme F420 hydrogenase/dehydrogenase, beta subunit C terminus

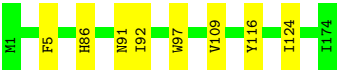
Chain E: 



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



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



4 Data and refinement statistics

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

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.59	0/5972	0.81	2/8088 (0.0%)
1	D	0.54	0/6021	0.74	1/8152 (0.0%)
2	B	0.56	0/2886	0.81	1/3885 (0.0%)
2	E	0.50	0/2897	0.72	1/3899 (0.0%)
3	C	0.56	0/1379	0.79	1/1861 (0.1%)
3	F	0.53	0/1370	0.73	0/1848
All	All	0.55	0/20525	0.77	6/27733 (0.0%)

There are no bond length outliers.

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

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 96 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:812:XCC:FE4	7:A:812:XCC:S2	1.86	0.66
1:D:292:LEU:O	1:D:296[B]:ARG:HG3	2.04	0.57
3:C:41:GLU:O	3:C:44:GLU:HG2	2.10	0.51
1:A:51:TYR:CD2	4:A:813:GOL:H31	2.45	0.51
1:A:267:GLY:C	1:A:272:ALA:HB2	2.37	0.49

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

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

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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

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

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

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

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 3 are monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	D	801	-	5,5,5	0.08	0	5,5,5	0.32	0
6	SF4	D	803	1	0,12,12	-	-	-		
5	EDO	A	807	-	3,3,3	0.14	0	2,2,2	0.29	0
6	SF4	E	401	2	0,12,12	-	-	-		
6	SF4	D	804	1	0,12,12	-	-	-		
5	EDO	A	806	-	3,3,3	0.07	0	2,2,2	0.09	0
5	EDO	A	818	-	3,3,3	0.06	0	2,2,2	0.15	0
7	XCC	D	806	1	0,11,11	-	-	-		
6	SF4	A	810	1	0,12,12	-	-	-		
4	GOL	A	801	-	5,5,5	0.89	0	5,5,5	1.10	0
5	EDO	A	804	-	3,3,3	0.12	0	2,2,2	0.09	0
5	EDO	A	803	-	3,3,3	0.09	0	2,2,2	0.11	0
10	PE4	D	807	-	5,5,23	0.33	0	4,4,22	0.40	0
4	GOL	F	403	-	5,5,5	1.05	0	5,5,5	0.91	0
6	SF4	D	805	1	0,12,12	-	-	-		
6	SF4	B	405	2	0,12,12	-	-	-		
6	SF4	B	402	2	0,12,12	-	-	-		
4	GOL	B	406	-	5,5,5	0.08	0	5,5,5	0.36	0
9	FAD	E	403	-	58,58,58	0.59	0	85,89,89	0.57	1 (1%)
9	FAD	B	404	-	58,58,58	0.57	0	85,89,89	0.57	1 (1%)
5	EDO	A	802	-	3,3,3	0.11	0	2,2,2	0.04	0
4	GOL	C	203	-	5,5,5	0.99	0	5,5,5	0.95	0
4	GOL	A	816	-	5,5,5	0.08	0	5,5,5	0.34	0
4	GOL	A	815	-	5,5,5	0.10	0	5,5,5	0.35	0
4	GOL	E	405	-	5,5,5	0.97	0	5,5,5	0.98	0
4	GOL	C	201	-	5,5,5	0.08	0	5,5,5	0.38	0
4	GOL	F	401	-	5,5,5	0.08	0	5,5,5	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	813	-	5,5,5	0.07	0	5,5,5	0.33	0
5	EDO	F	402	-	3,3,3	0.14	0	2,2,2	0.18	0
5	EDO	B	401	-	3,3,3	0.12	0	2,2,2	0.13	0
6	SF4	E	404	2	0,12,12	-	-	-		
6	SF4	A	819	1	0,12,12	-	-	-		
6	SF4	A	809	1	0,12,12	-	-	-		
4	GOL	A	814	-	5,5,5	1.06	0	5,5,5	0.92	0
5	EDO	A	808	-	3,3,3	0.08	0	2,2,2	0.15	0
7	XCC	A	812	1	0,11,11	-	-	-		
4	GOL	A	817	-	5,5,5	1.00	0	5,5,5	1.02	0
4	GOL	C	202	-	5,5,5	0.85	0	5,5,5	1.04	0
5	EDO	A	805	-	3,3,3	0.16	0	2,2,2	0.16	0
5	EDO	D	802	-	3,3,3	0.06	0	2,2,2	0.12	0
6	SF4	B	403	2	0,12,12	-	-	-		
6	SF4	A	811	1	0,12,12	-	-	-		
4	GOL	A	820	-	5,5,5	0.08	0	5,5,5	0.41	0
6	SF4	E	402	2	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
4	GOL	D	801	-	-	3/4/4/4	-
6	SF4	D	803	1	-	-	0/6/5/5
5	EDO	A	807	-	-	0/1/1/1	-
6	SF4	E	401	2	-	-	0/6/5/5
6	SF4	D	804	1	-	-	0/6/5/5
5	EDO	A	806	-	-	1/1/1/1	-
5	EDO	A	818	-	-	1/1/1/1	-
7	XCC	D	806	1	-	-	0/3/3/3
6	SF4	A	810	1	-	-	0/6/5/5
4	GOL	A	801	-	-	0/4/4/4	-
5	EDO	A	804	-	-	0/1/1/1	-
5	EDO	A	803	-	-	1/1/1/1	-
10	PE4	D	807	-	-	2/3/3/21	-
4	GOL	F	403	-	-	3/4/4/4	-
6	SF4	D	805	1	-	-	0/6/5/5
6	SF4	B	405	2	-	-	0/6/5/5
6	SF4	B	402	2	-	-	0/6/5/5
4	GOL	B	406	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FAD	E	403	-	-	1/34/50/50	0/6/6/6
5	EDO	A	802	-	-	1/1/1/1	-
4	GOL	C	203	-	-	0/4/4/4	-
4	GOL	A	816	-	-	3/4/4/4	-
4	GOL	A	815	-	-	2/4/4/4	-
4	GOL	E	405	-	-	3/4/4/4	-
4	GOL	C	201	-	-	2/4/4/4	-
4	GOL	F	401	-	-	0/4/4/4	-
4	GOL	A	813	-	-	3/4/4/4	-
5	EDO	F	402	-	-	0/1/1/1	-
5	EDO	B	401	-	-	0/1/1/1	-
6	SF4	E	404	2	-	-	0/6/5/5
6	SF4	A	819	1	-	-	0/6/5/5
6	SF4	A	809	1	-	-	0/6/5/5
4	GOL	A	814	-	-	0/4/4/4	-
5	EDO	A	808	-	-	0/1/1/1	-
7	XCC	A	812	1	-	-	0/3/3/3
4	GOL	A	817	-	-	2/4/4/4	-
4	GOL	C	202	-	-	2/4/4/4	-
5	EDO	A	805	-	-	0/1/1/1	-
5	EDO	D	802	-	-	1/1/1/1	-
6	SF4	A	811	1	-	-	0/6/5/5
6	SF4	B	403	2	-	-	0/6/5/5
9	FAD	B	404	-	-	0/34/50/50	0/6/6/6
4	GOL	A	820	-	-	3/4/4/4	-
6	SF4	E	402	2	-	-	0/6/5/5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	404	FAD	C4-N3-C2	-2.06	121.98	125.64
9	E	403	FAD	C4-N3-C2	-2.03	122.04	125.64

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	813	GOL	C1-C2-C3-O3

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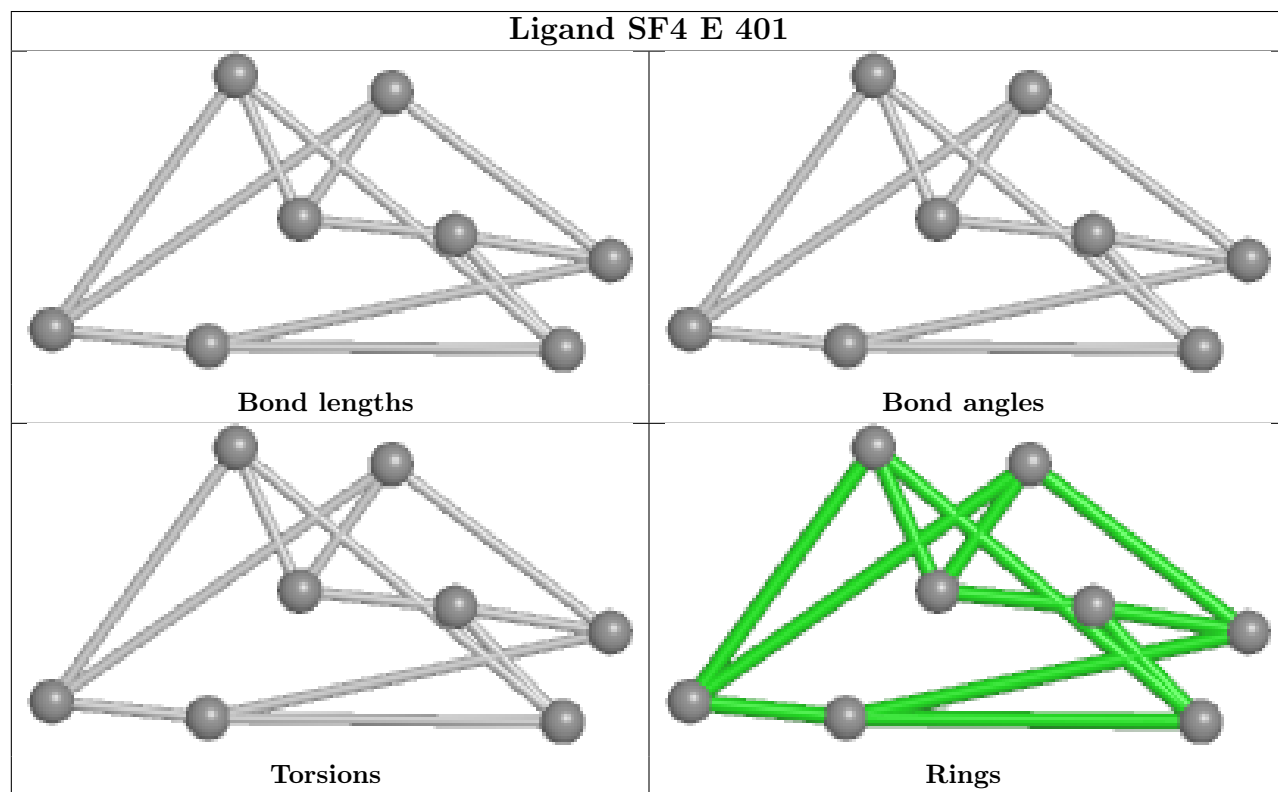
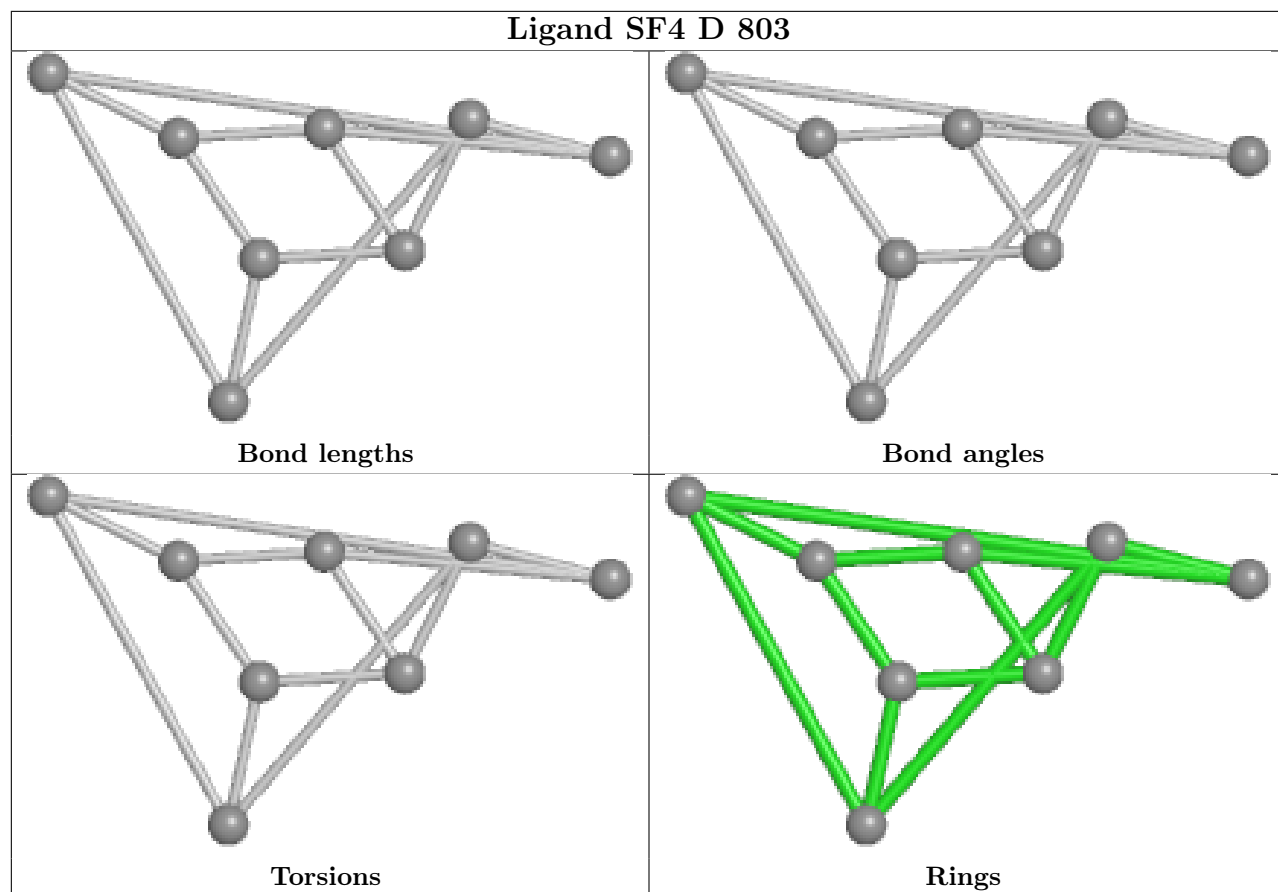
Mol	Chain	Res	Type	Atoms
4	A	816	GOL	C1-C2-C3-O3
4	A	817	GOL	O1-C1-C2-C3
4	C	201	GOL	O1-C1-C2-C3
4	E	405	GOL	O1-C1-C2-C3

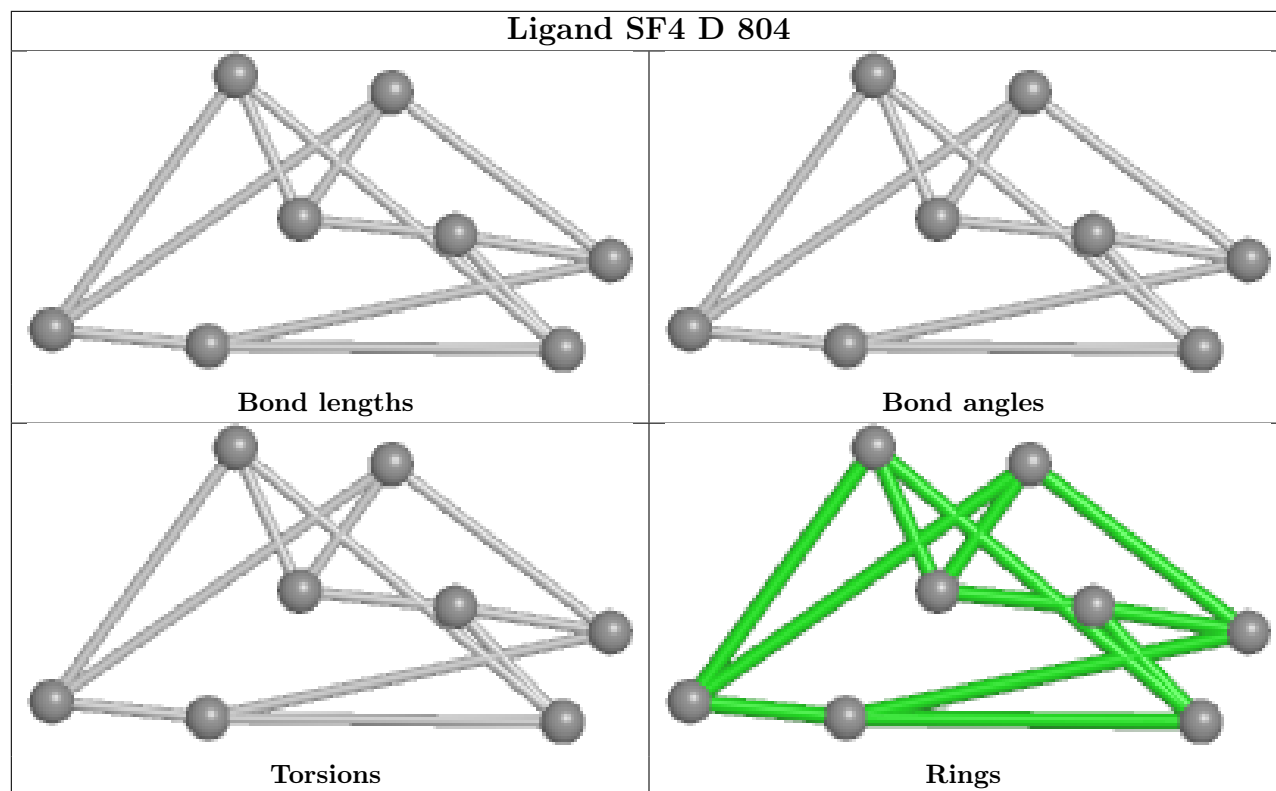
There are no ring outliers.

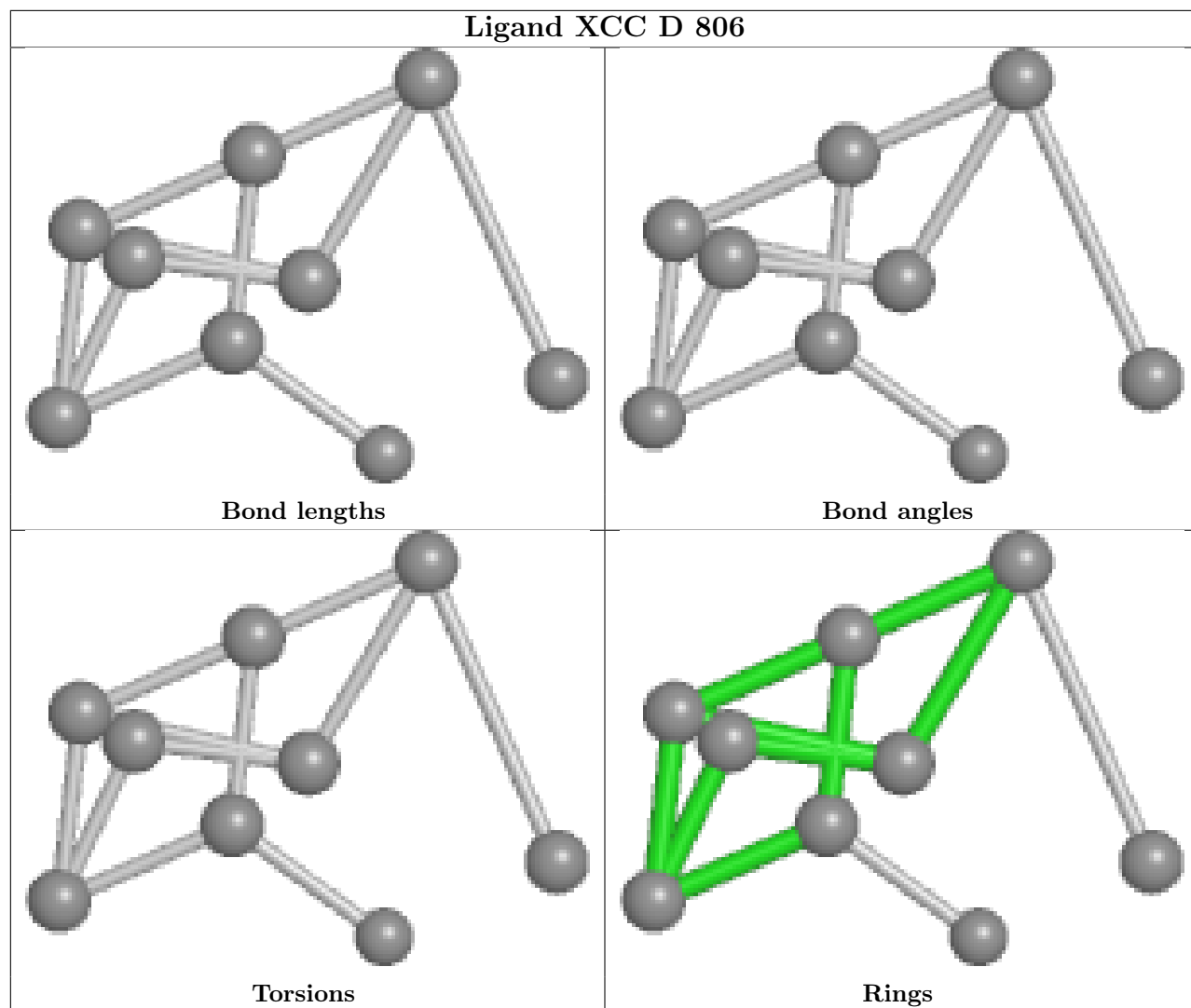
8 monomers are involved in 8 short contacts:

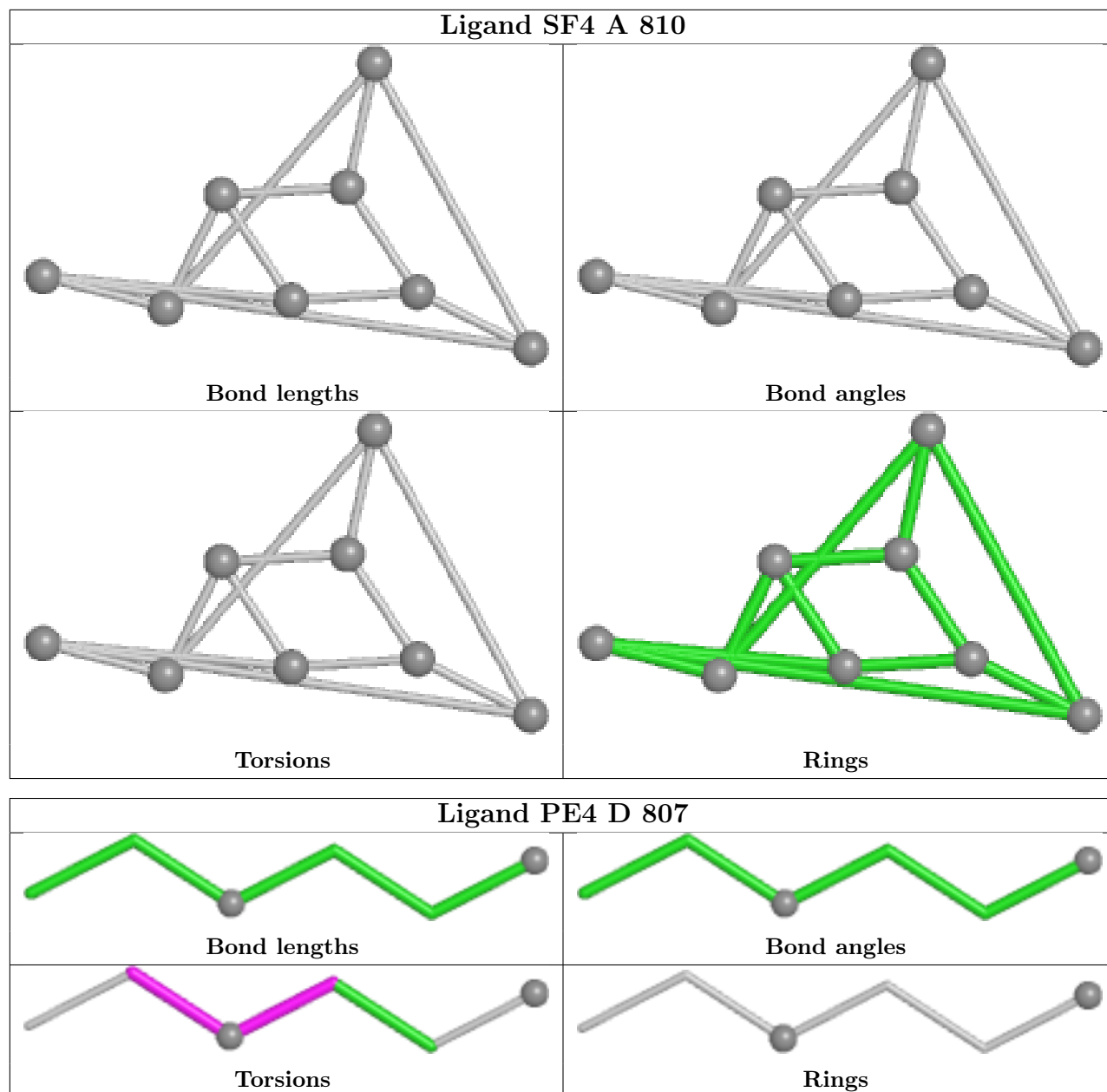
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	801	GOL	1	0
6	D	804	SF4	1	0
6	A	810	SF4	1	0
9	E	403	FAD	1	0
4	A	816	GOL	1	0
4	A	813	GOL	1	0
7	A	812	XCC	1	0
4	A	820	GOL	1	0

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

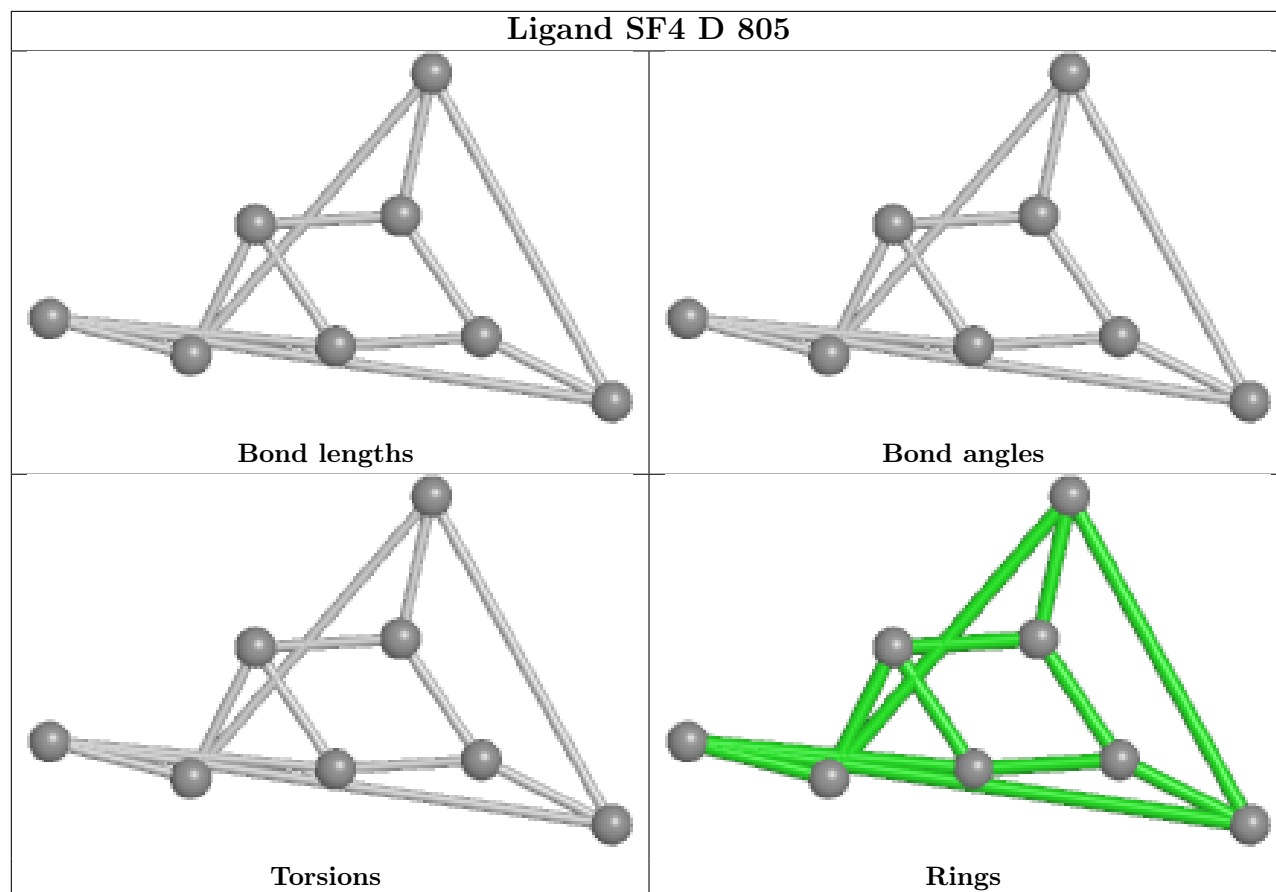




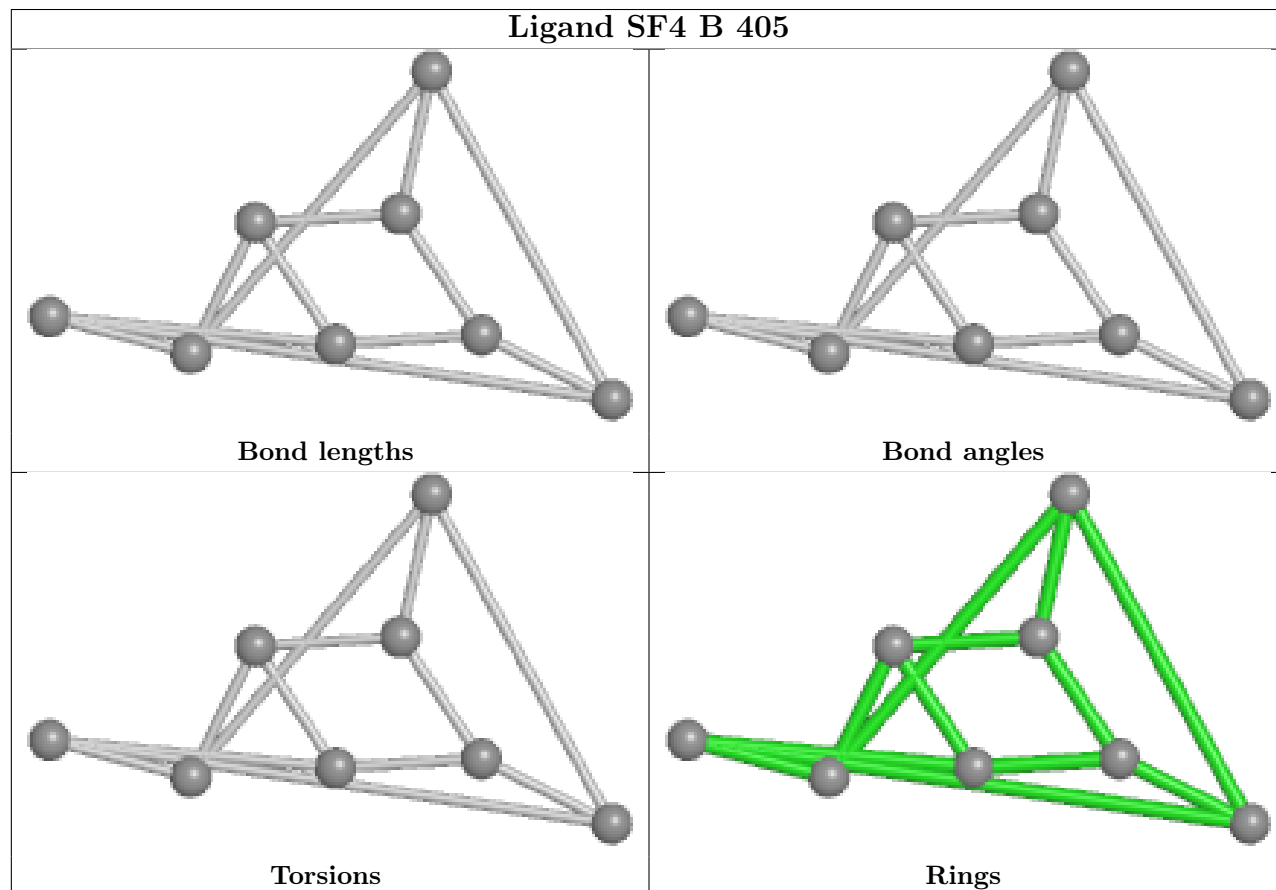


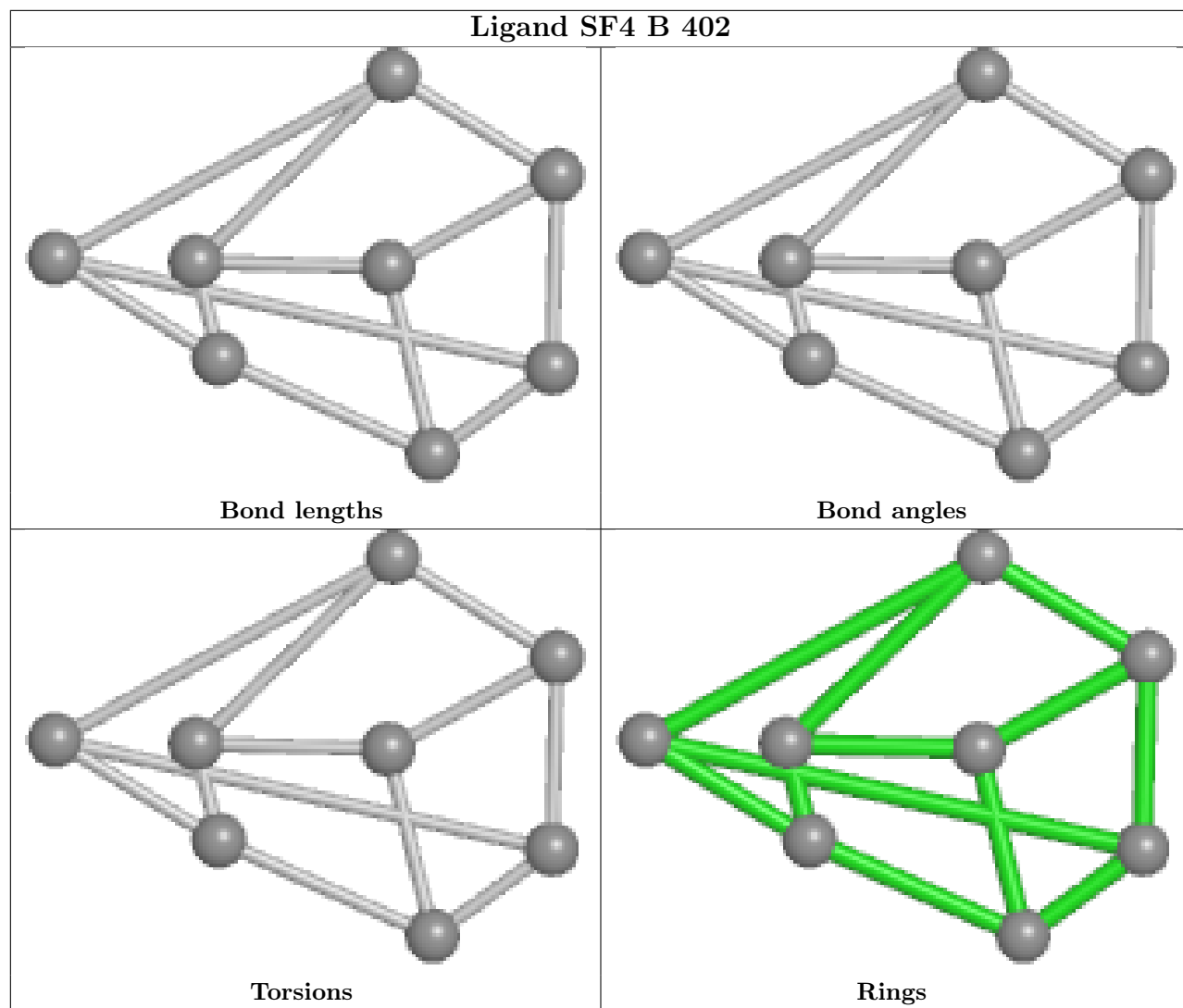


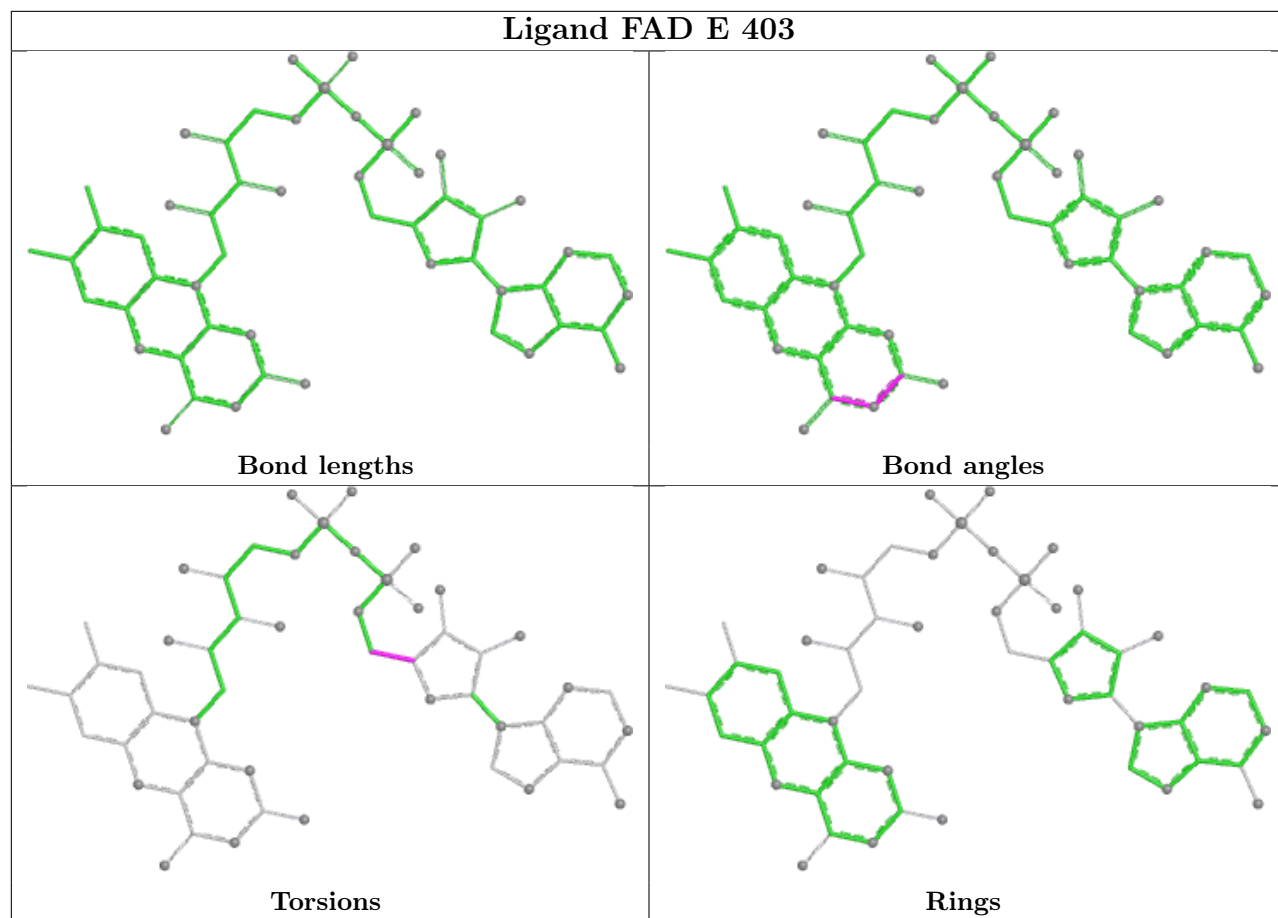
Ligand SF4 D 805

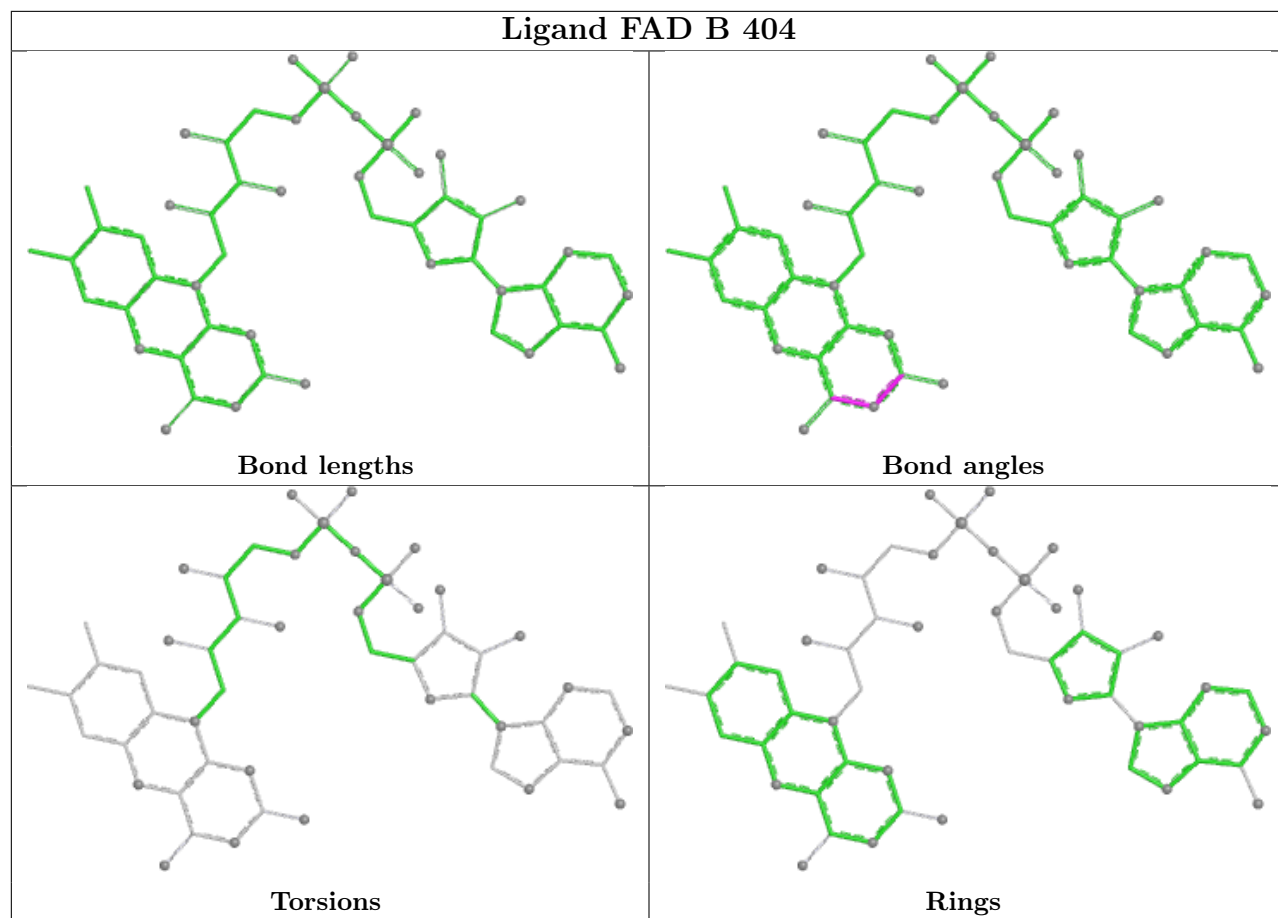


Ligand SF4 B 405

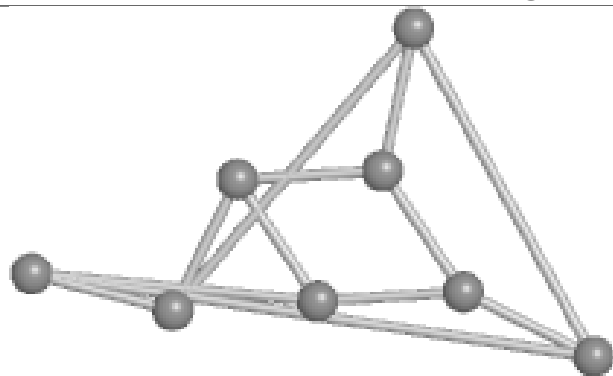




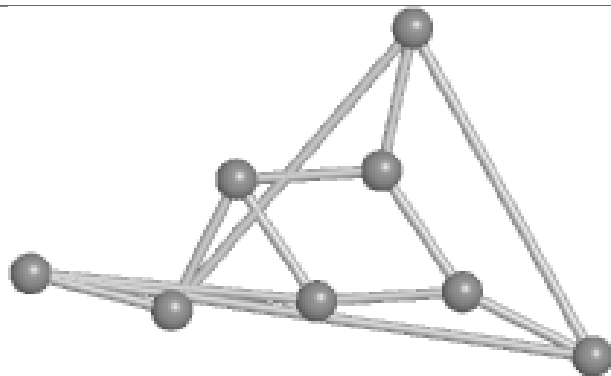




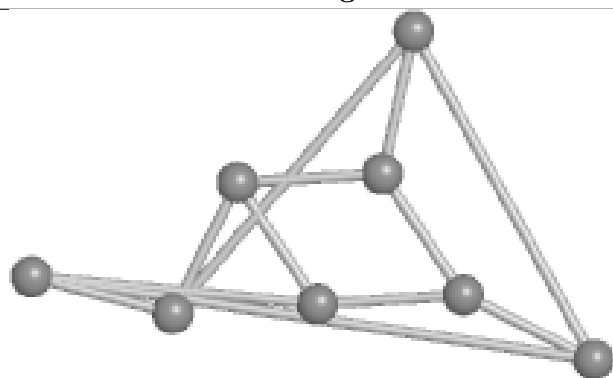
Ligand SF4 E 404



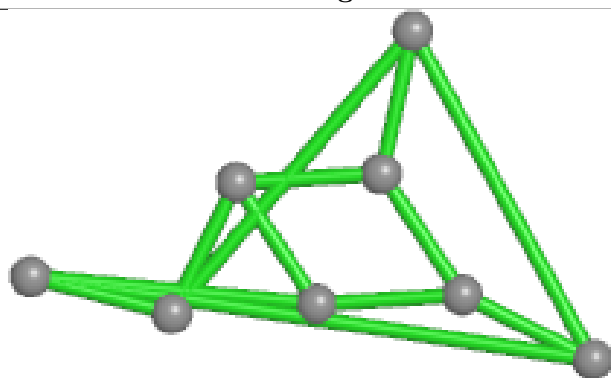
Bond lengths



Bond angles

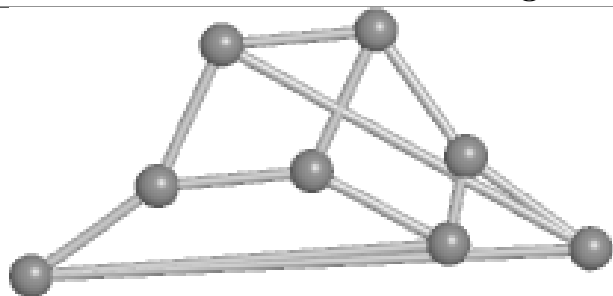


Torsions

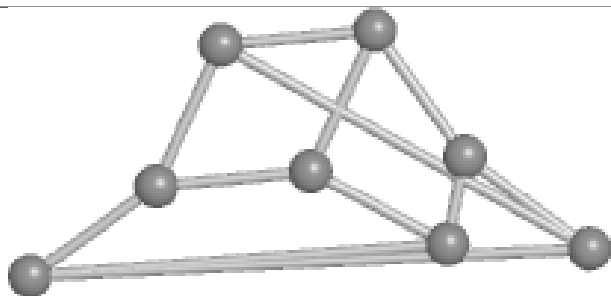


Rings

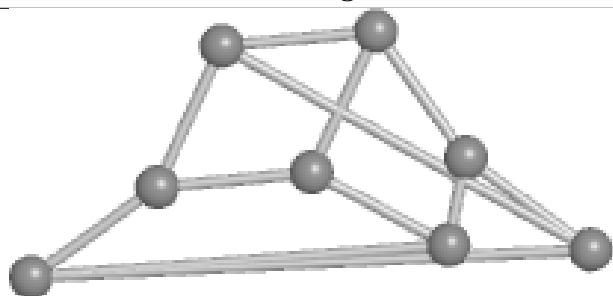
Ligand SF4 A 819



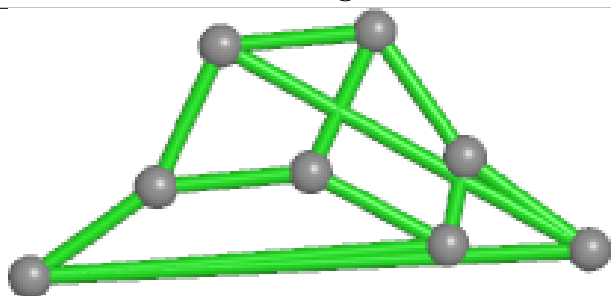
Bond lengths



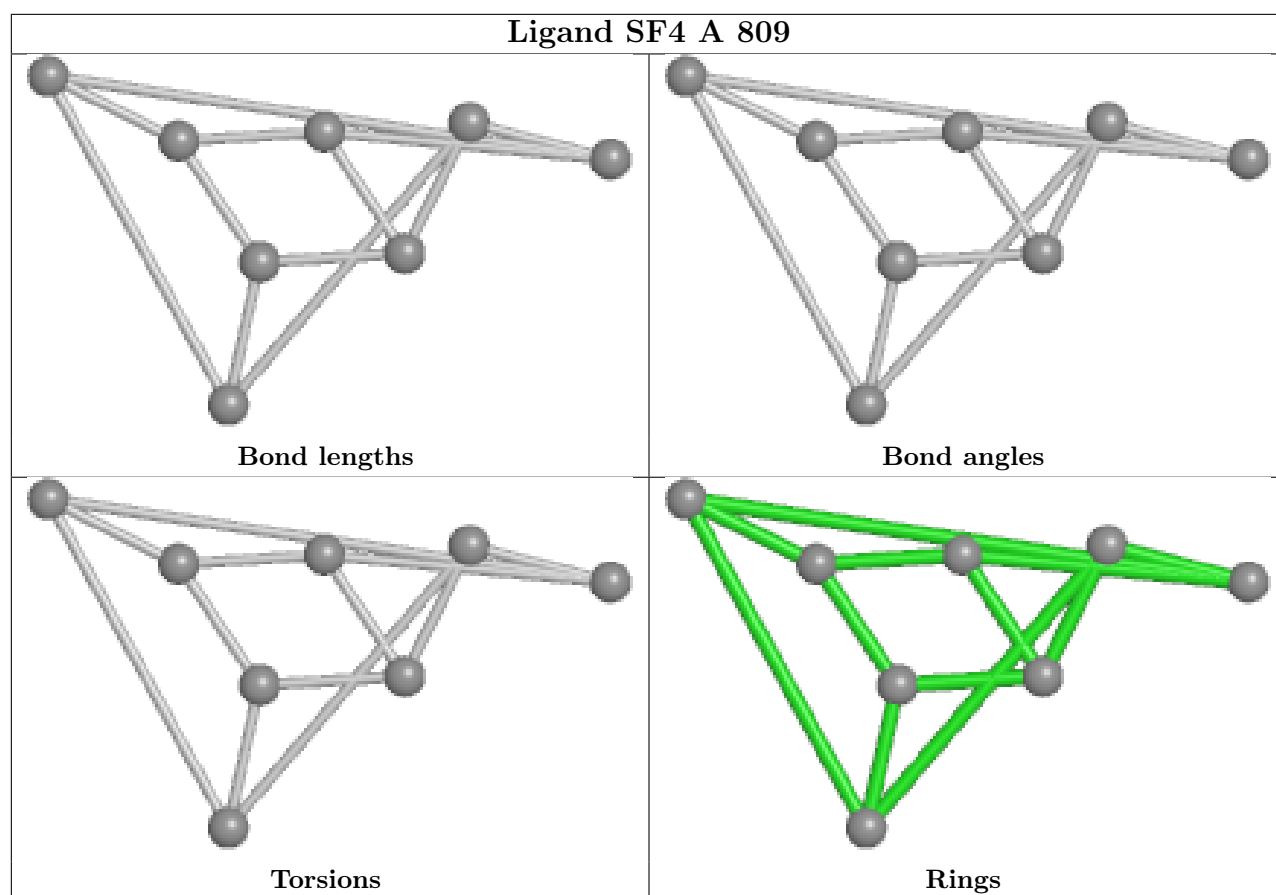
Bond angles

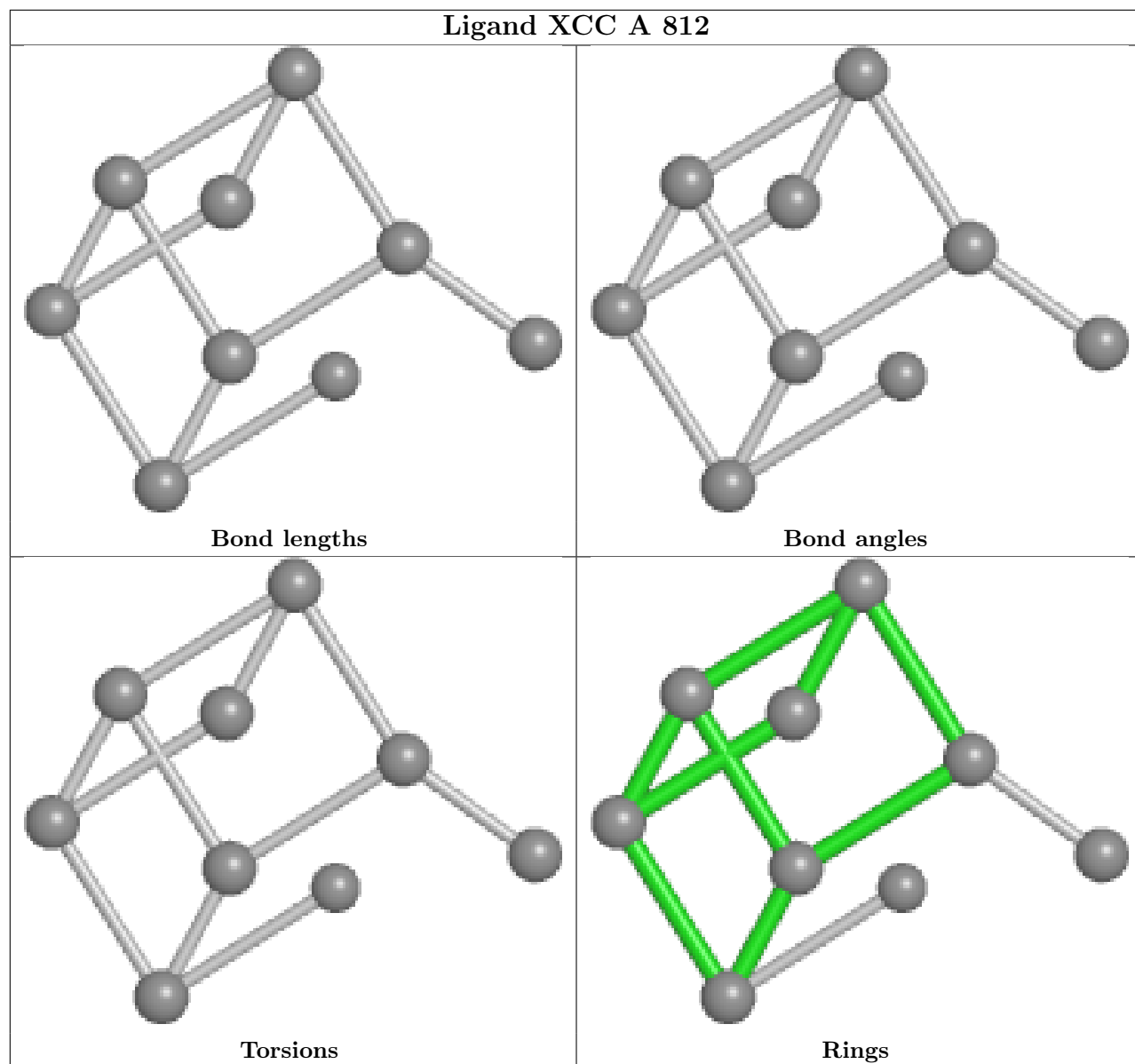


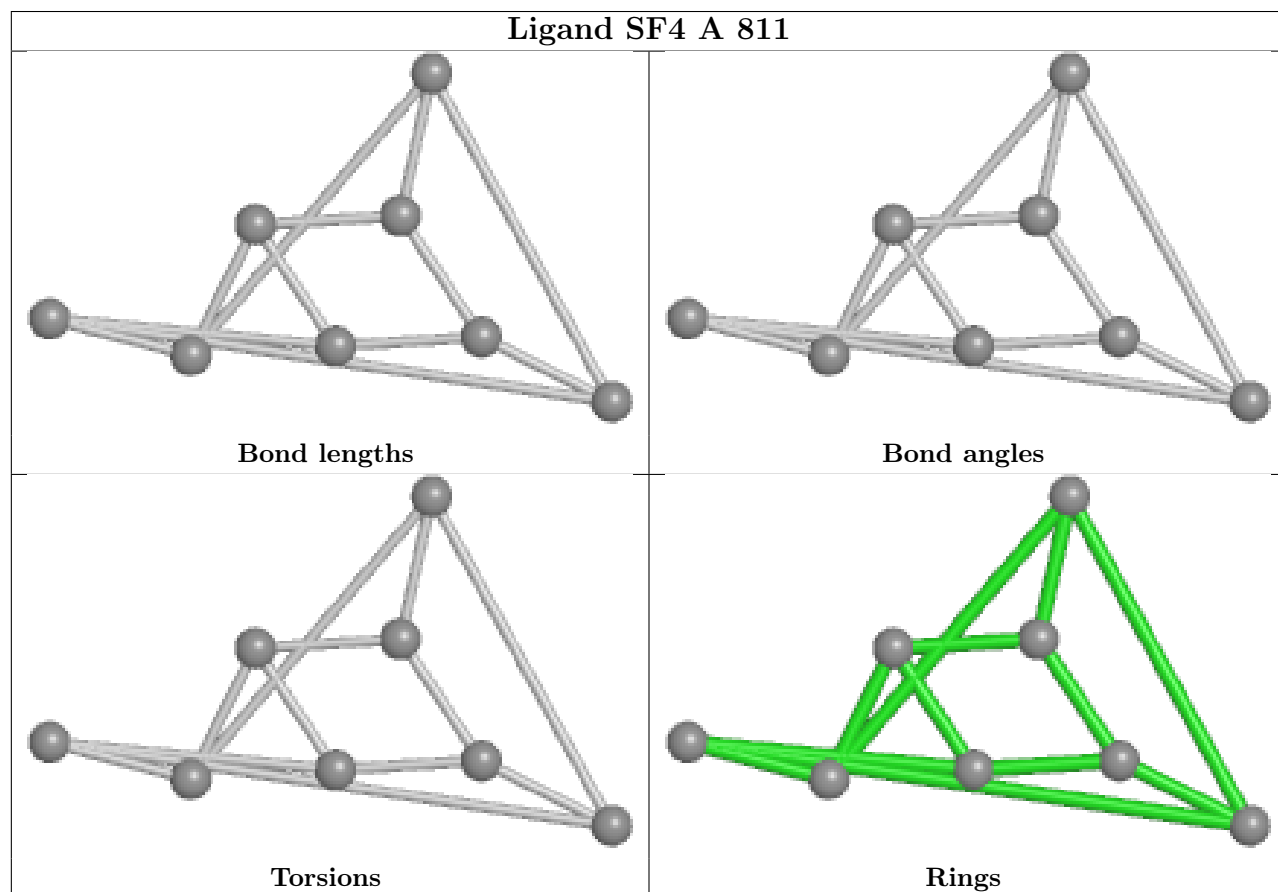
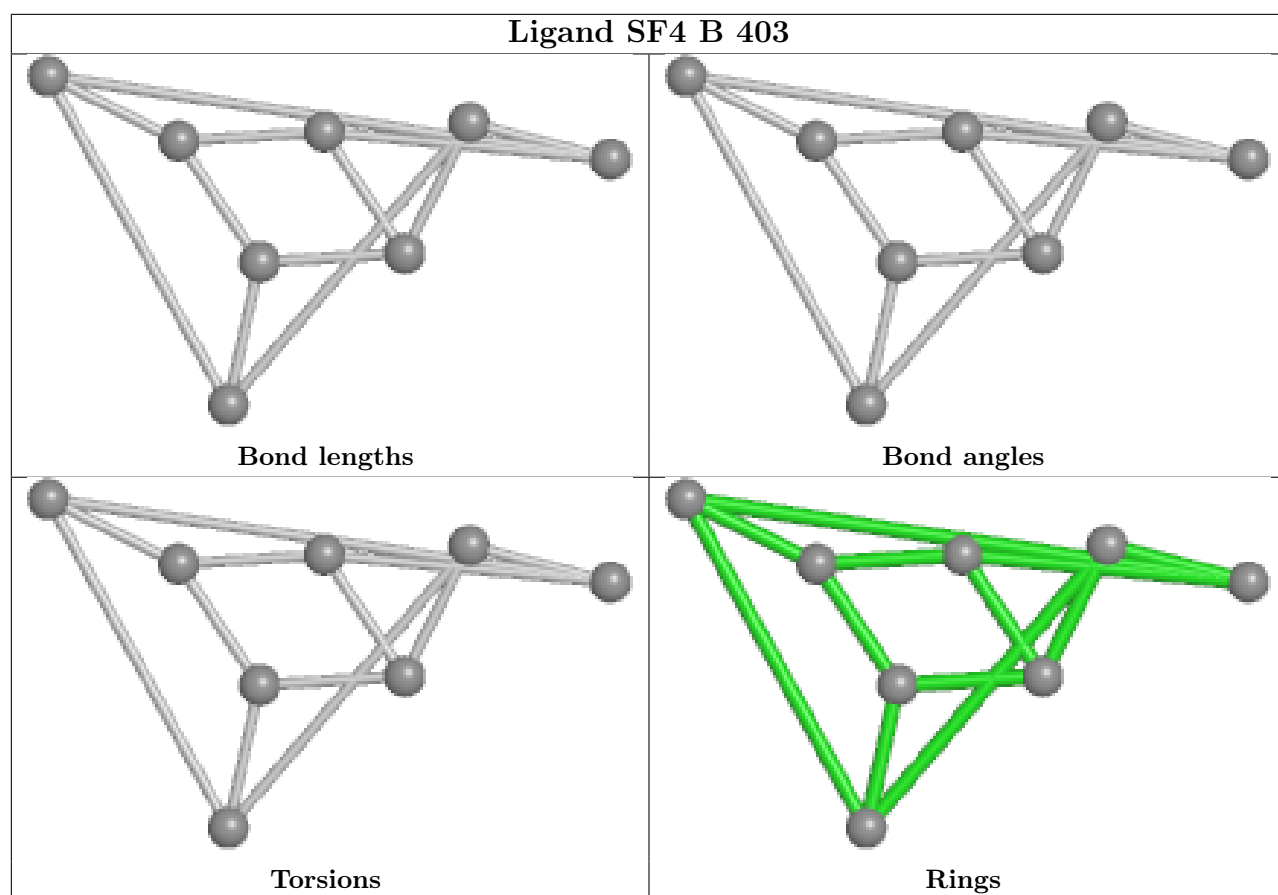
Torsions

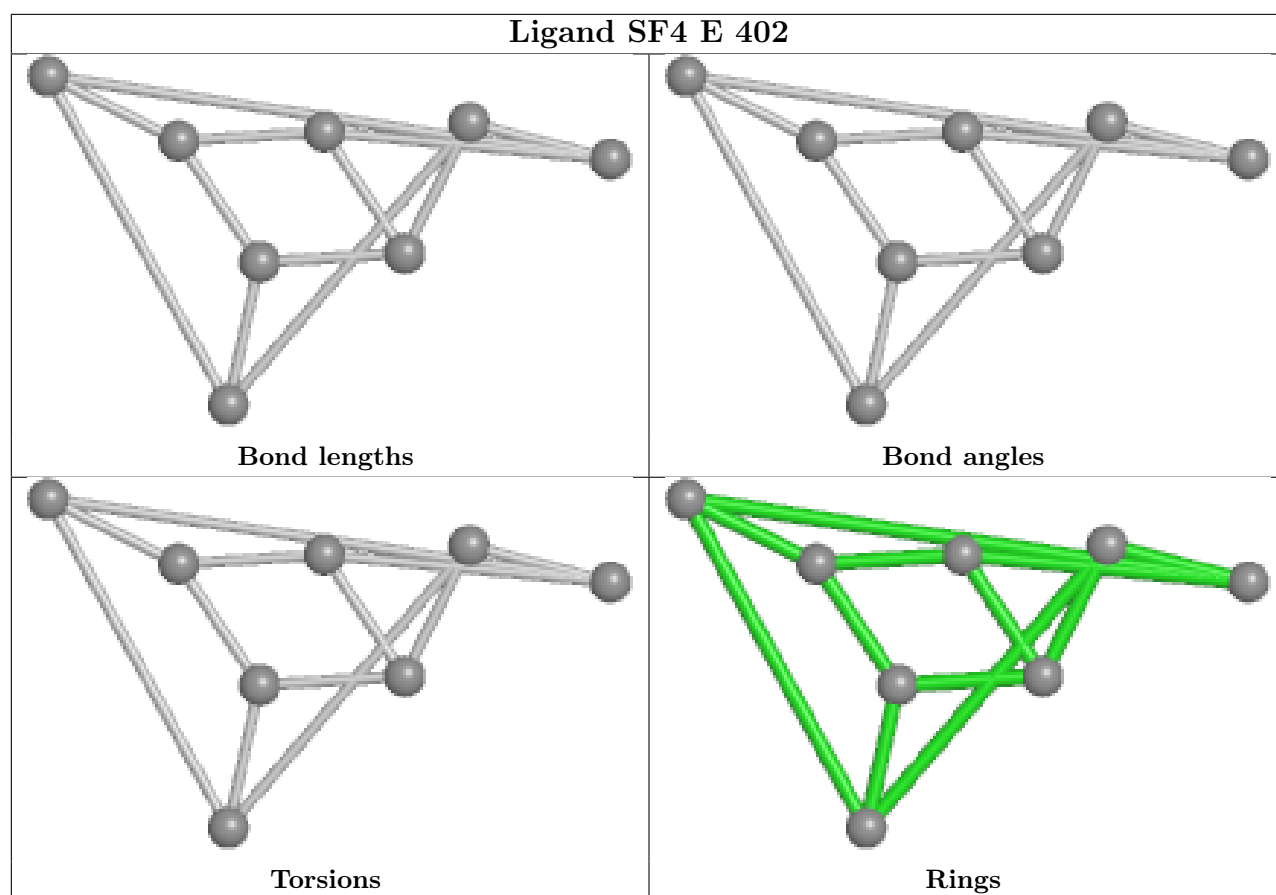


Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

The worst 5 of 8 RSRZ outliers are listed below:

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

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

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

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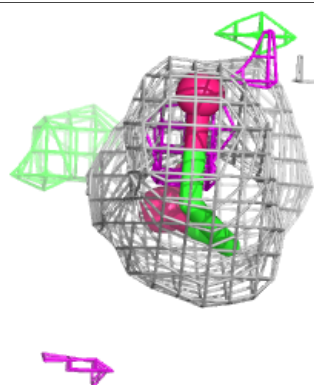
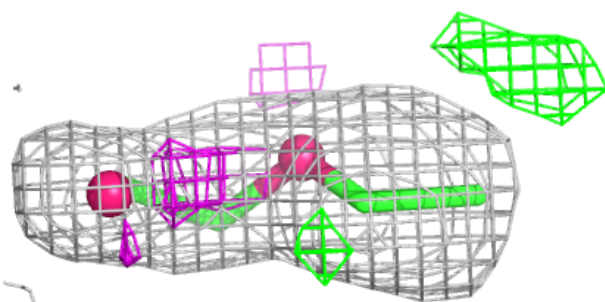
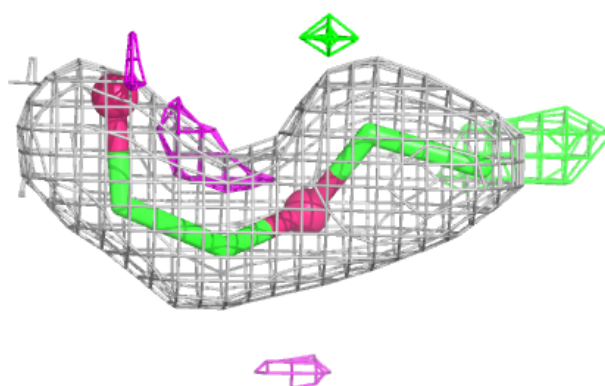
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SF4	E	402	8/8	0.99	0.03	29,31,31,33	0
6	SF4	E	404	8/8	0.99	0.03	33,34,35,37	0
6	SF4	A	810	8/8	0.99	0.02	27,29,29,30	0
6	SF4	A	811	8/8	0.99	0.03	28,30,31,31	0
6	SF4	A	819	8/8	0.99	0.03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

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

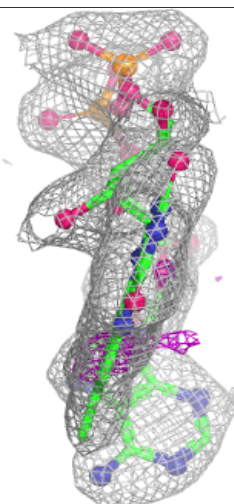
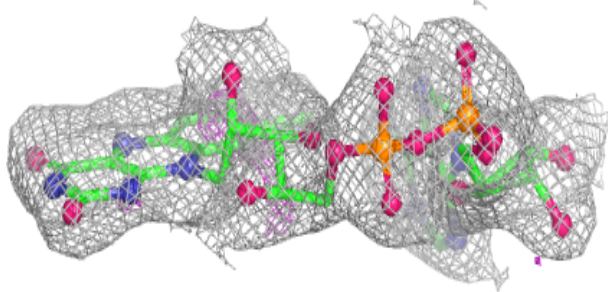
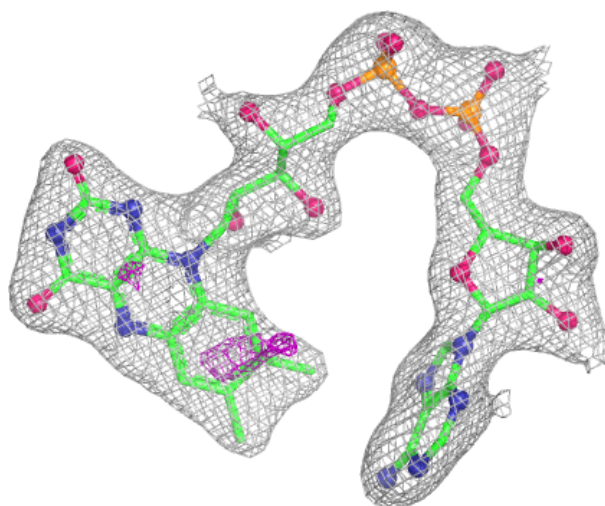
Electron density around PE4 D 807:

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



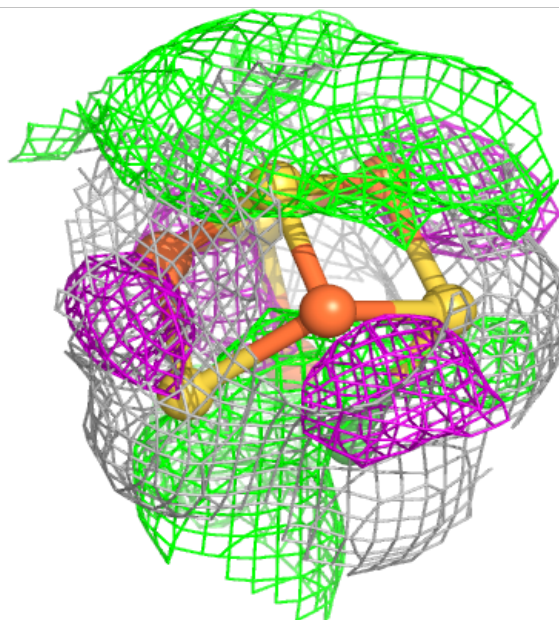
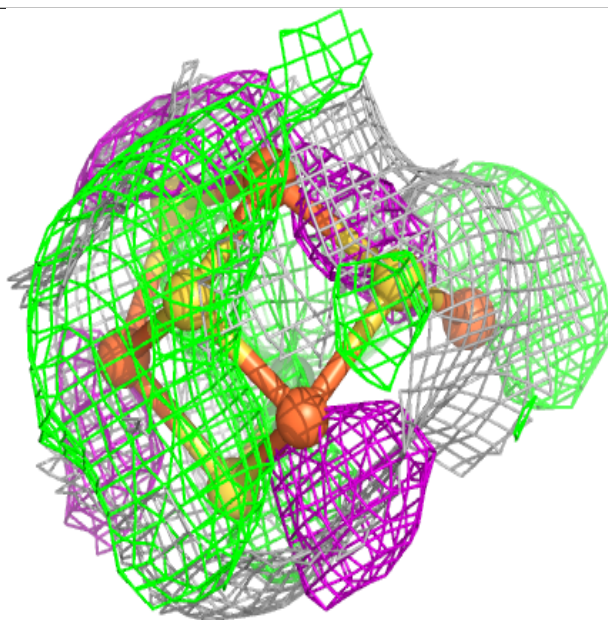
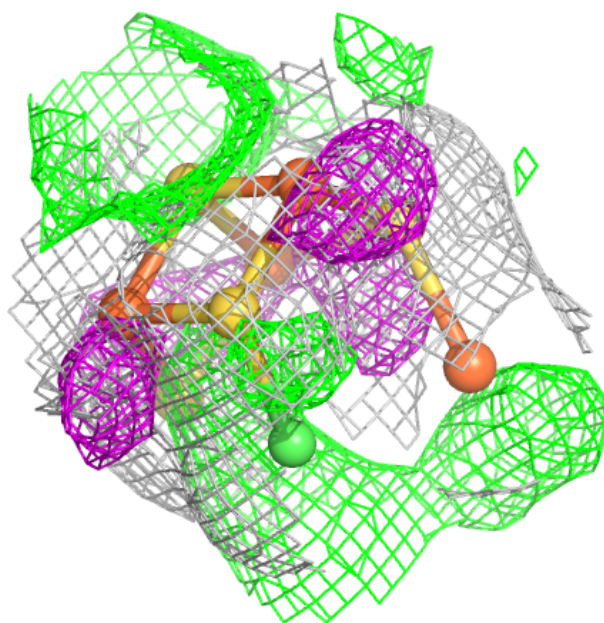
Electron density around FAD B 404:

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



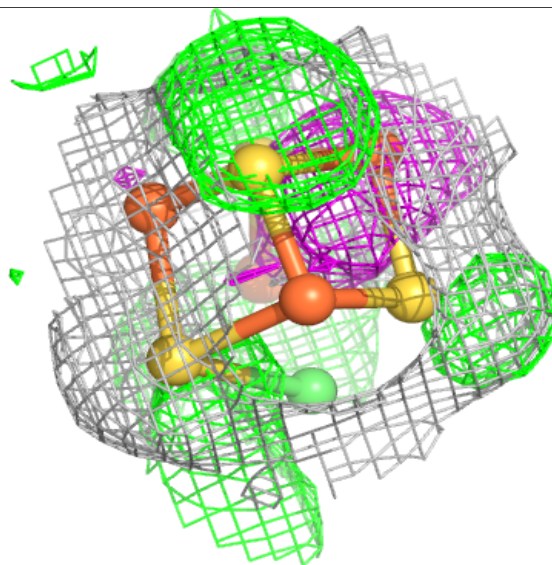
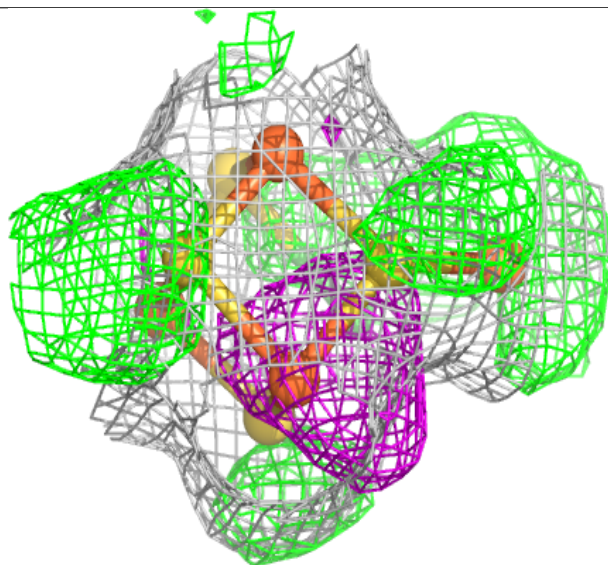
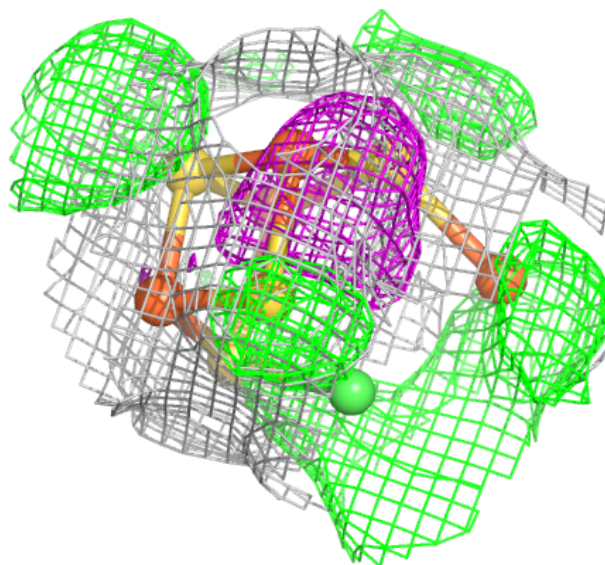
Electron density around XCC D 806:

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



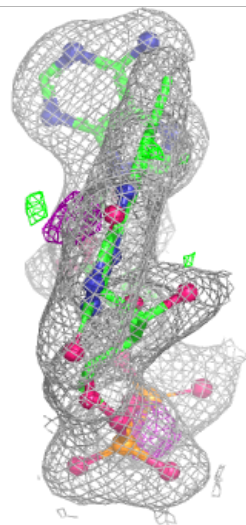
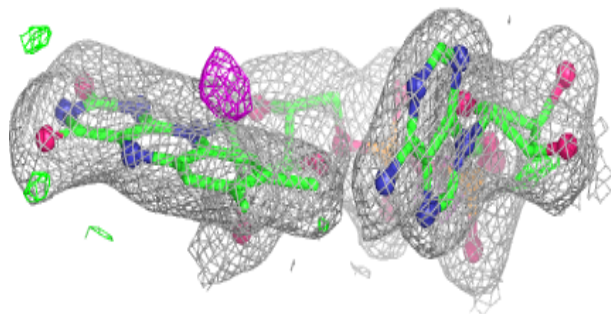
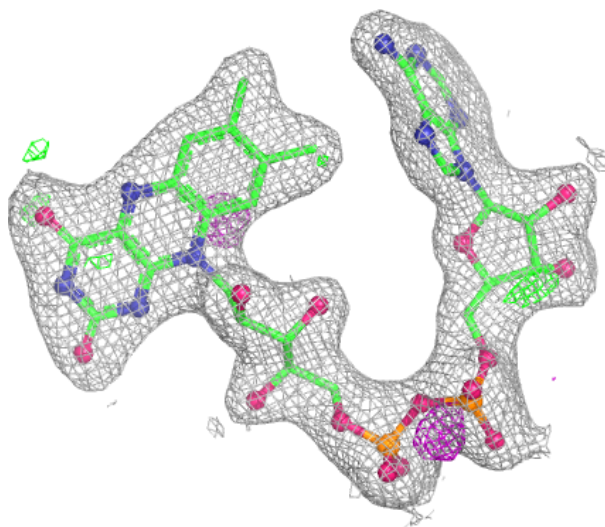
Electron density around XCC A 812:

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



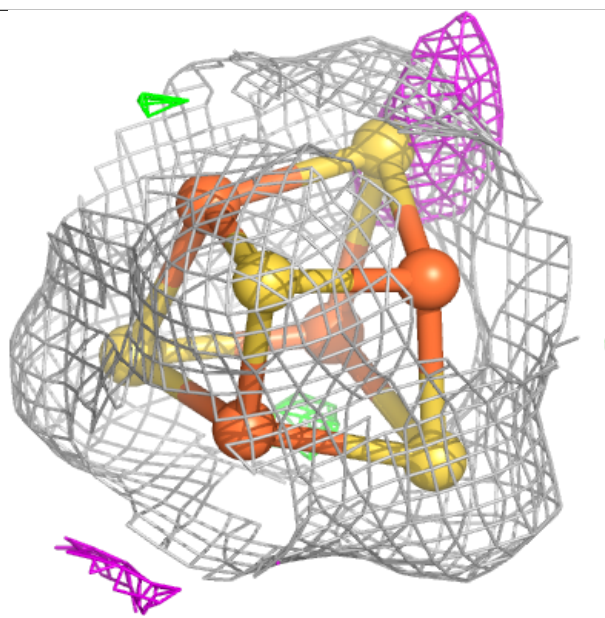
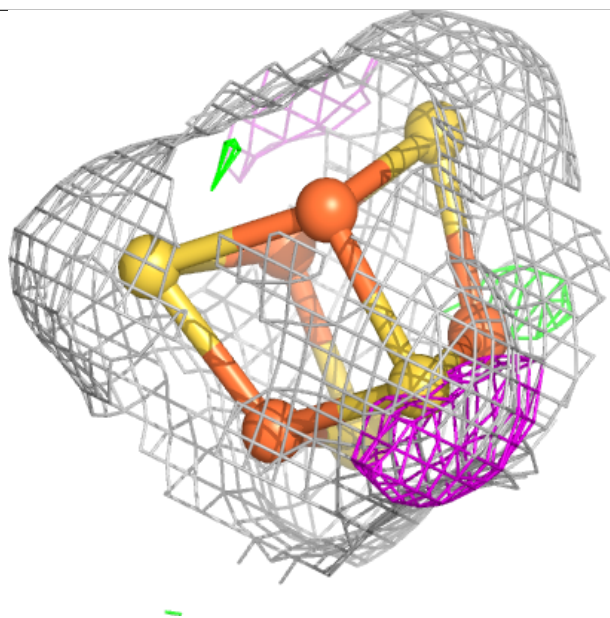
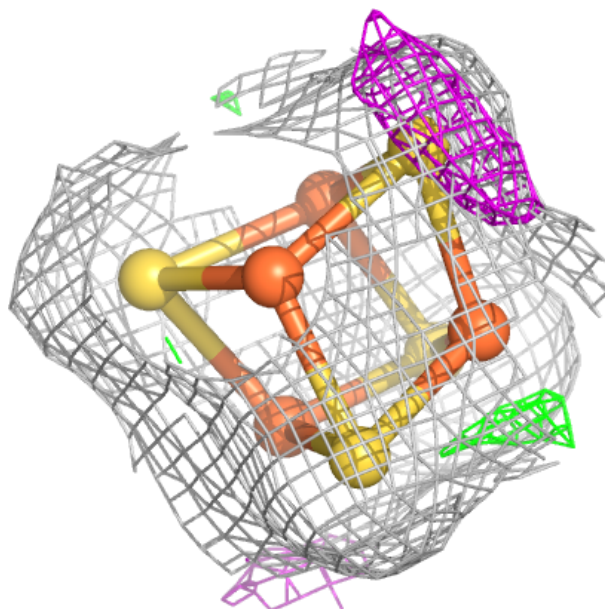
Electron density around FAD E 403:

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



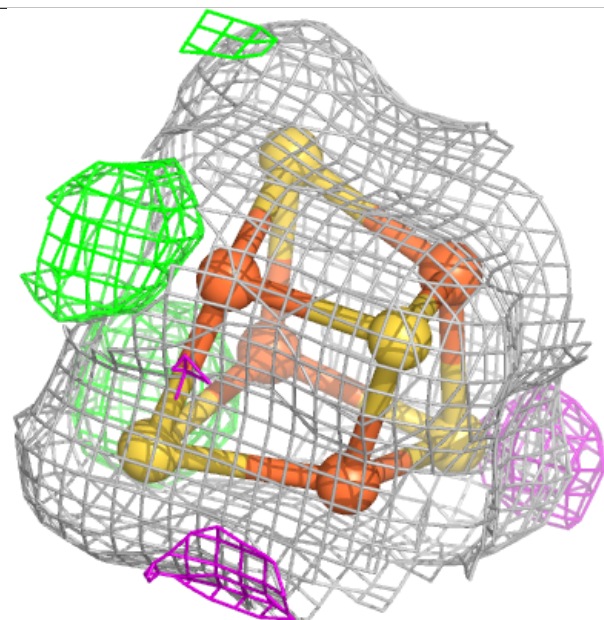
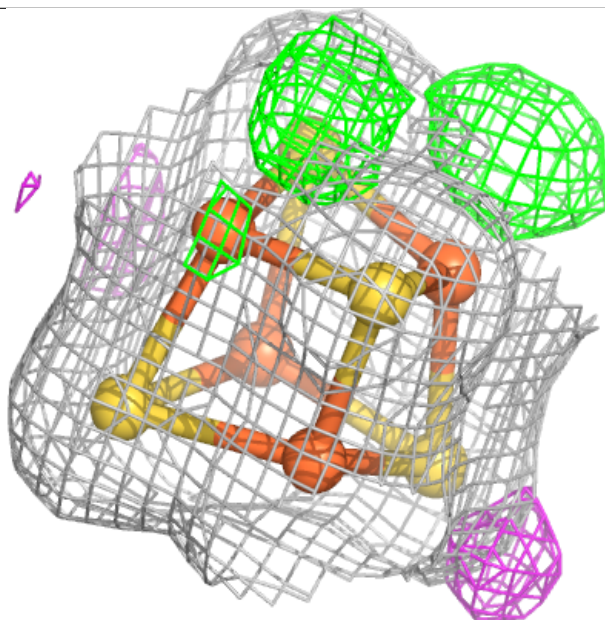
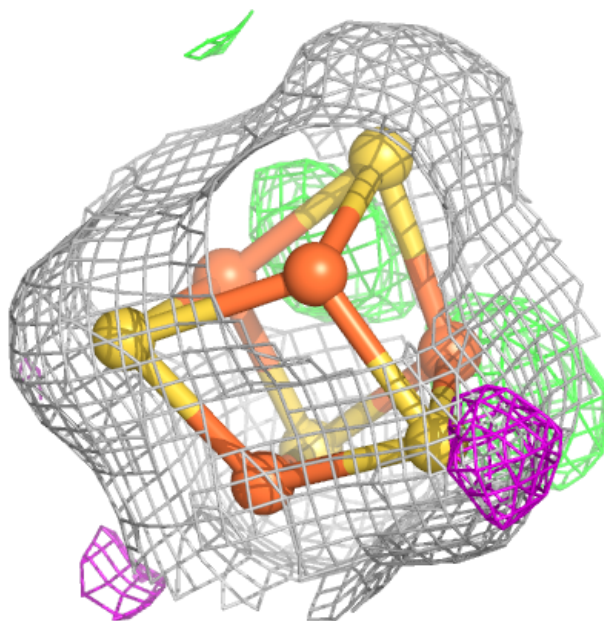
Electron density around SF4 B 405:

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



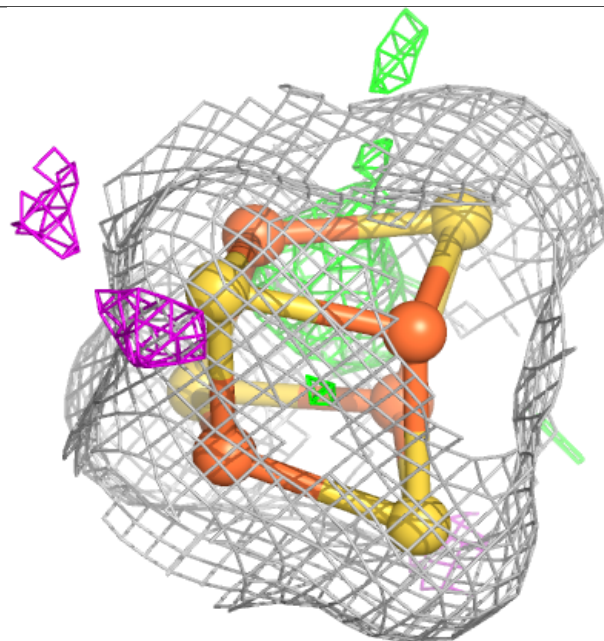
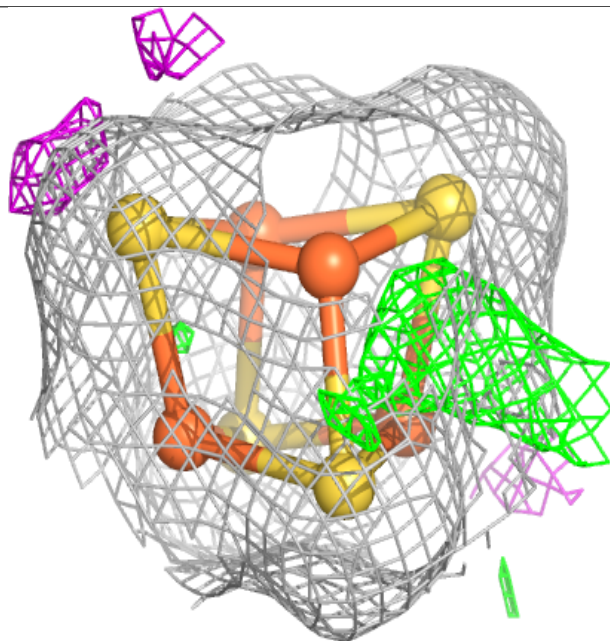
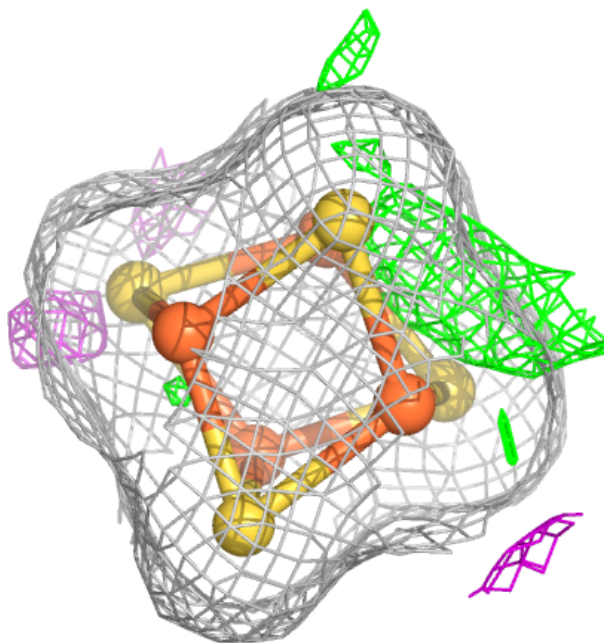
Electron density around SF4 D 805:

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



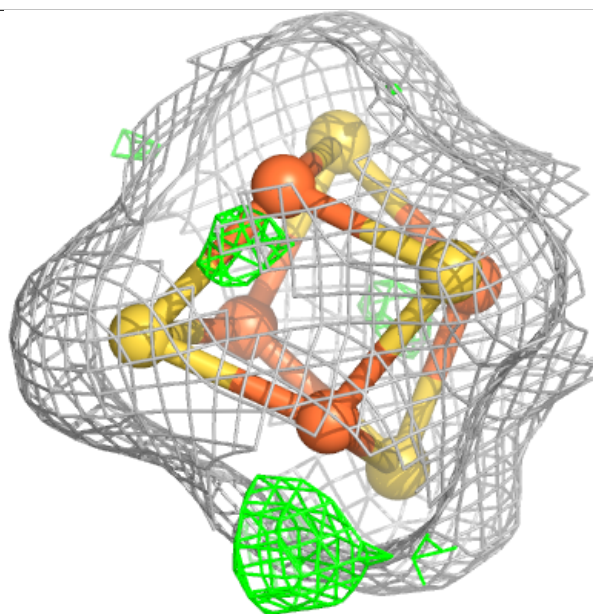
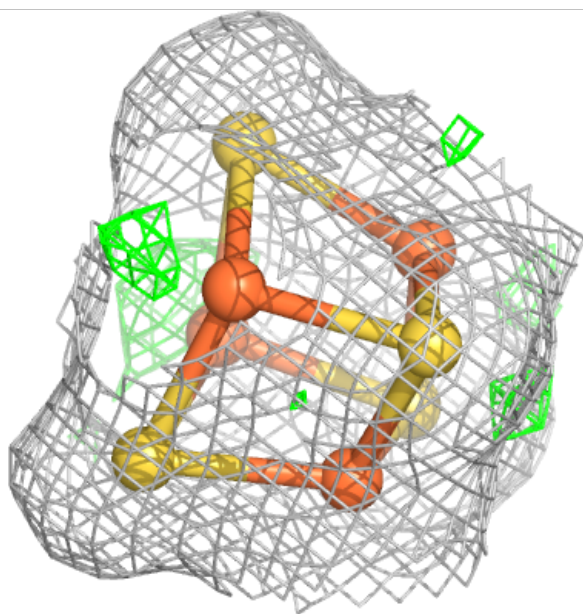
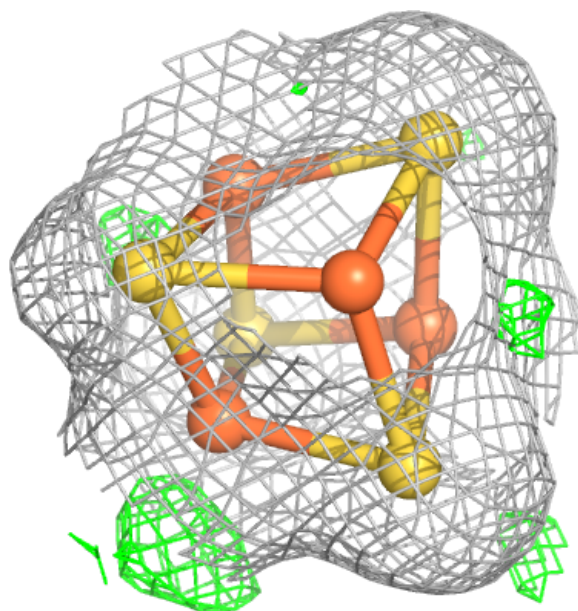
Electron density around SF4 E 401:

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



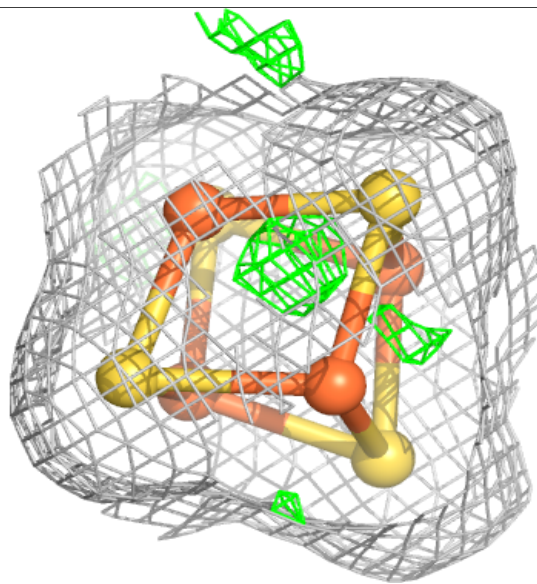
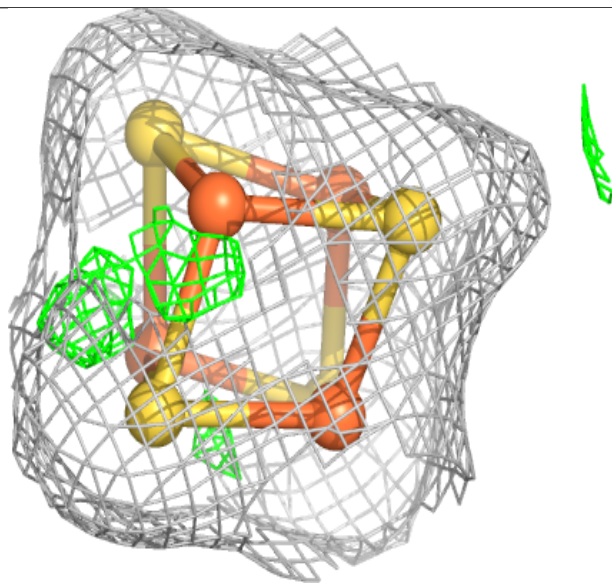
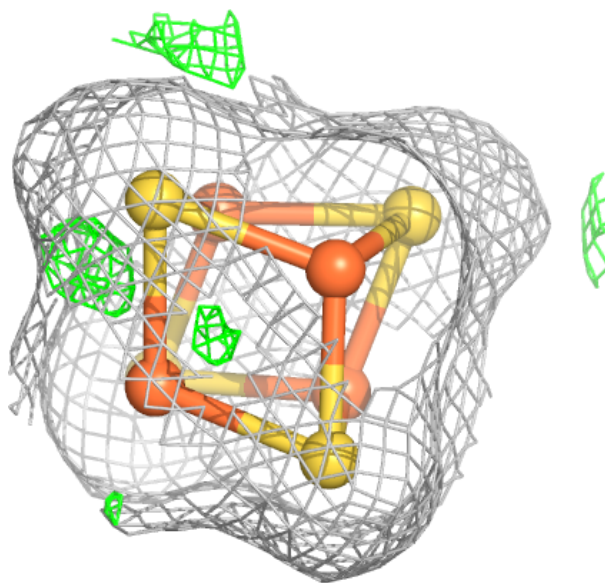
Electron density around SF4 E 402:

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



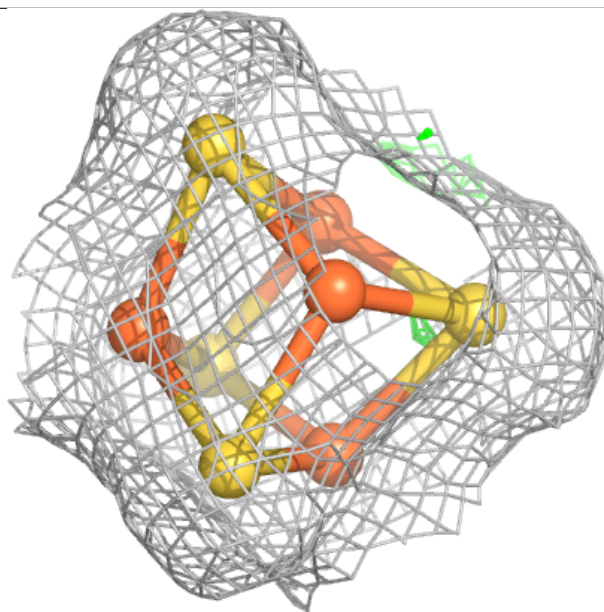
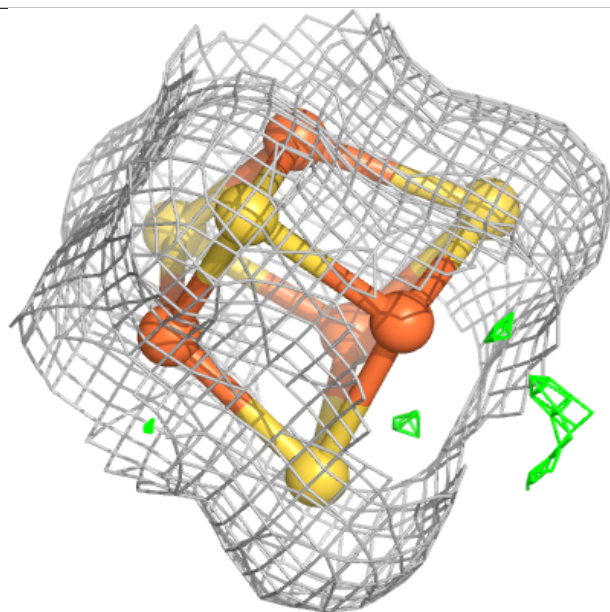
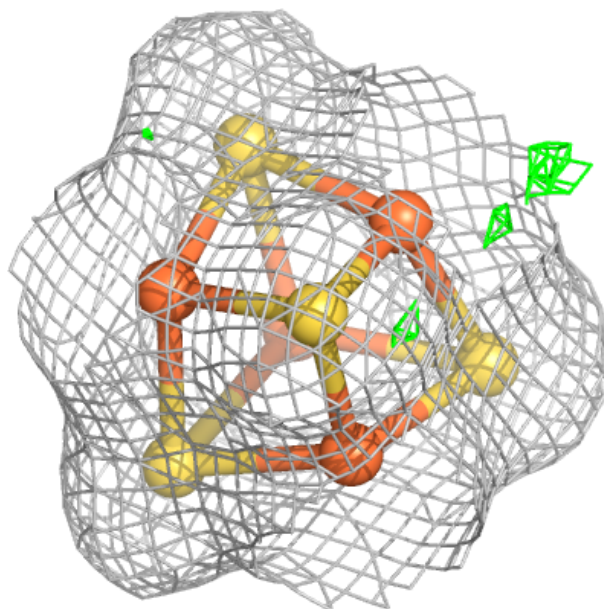
Electron density around SF4 E 404:

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



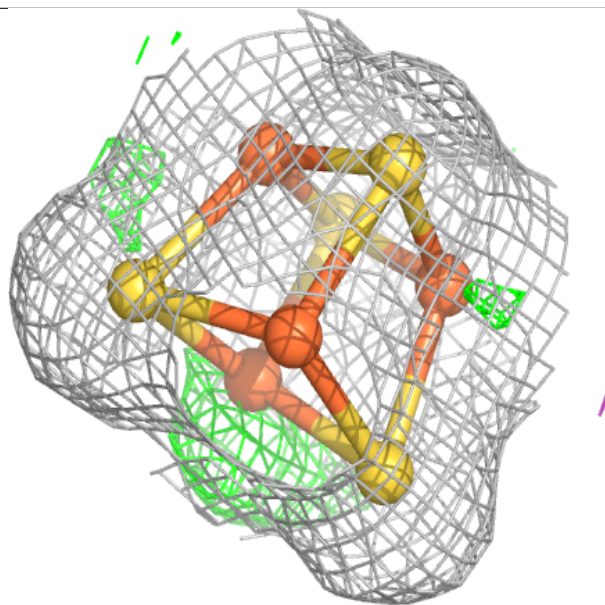
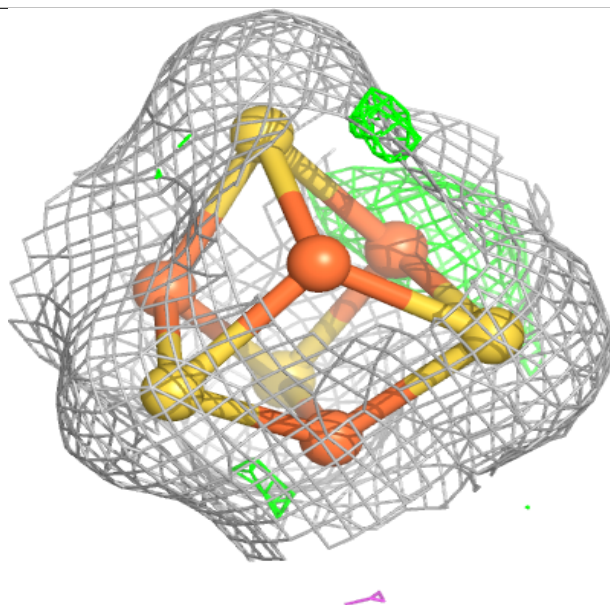
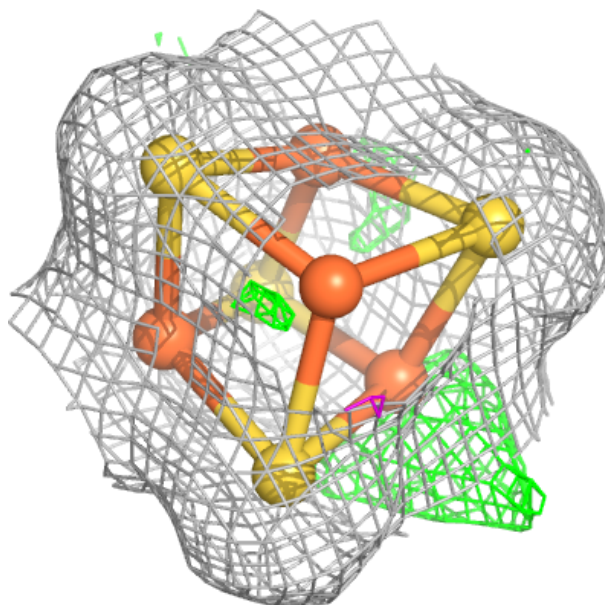
Electron density around SF4 A 810:

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



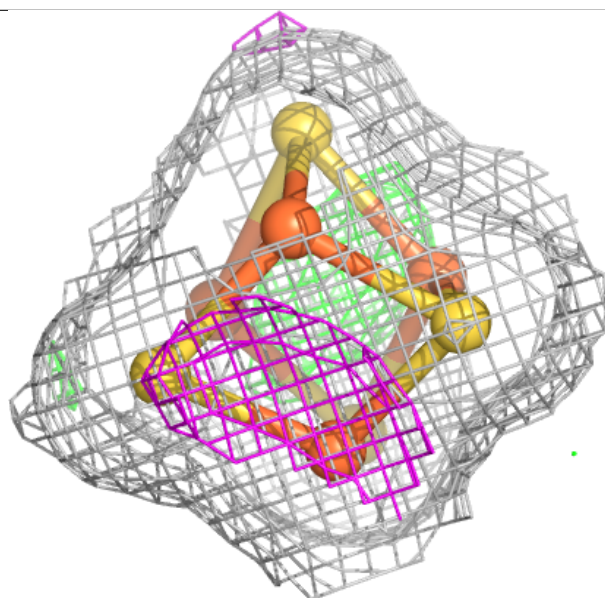
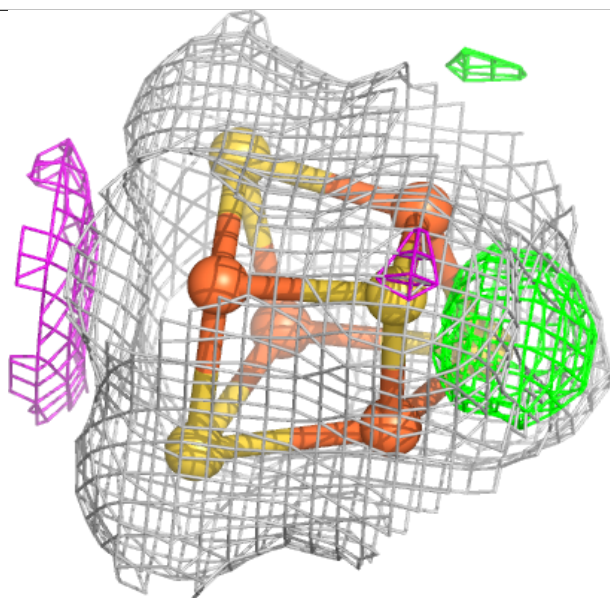
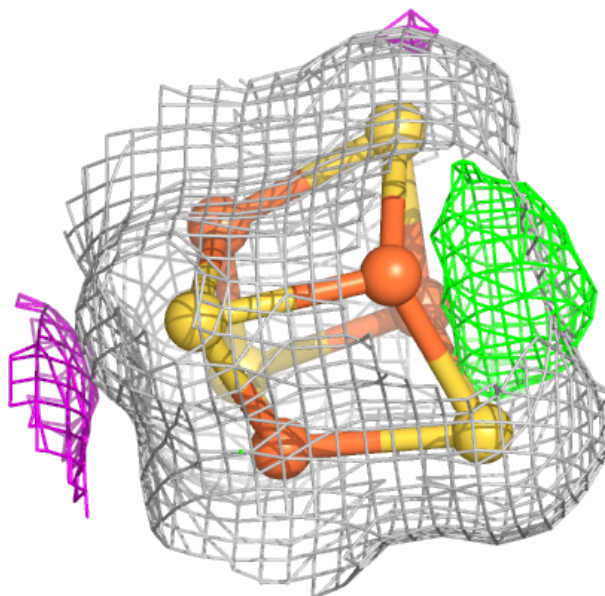
Electron density around SF4 A 811:

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



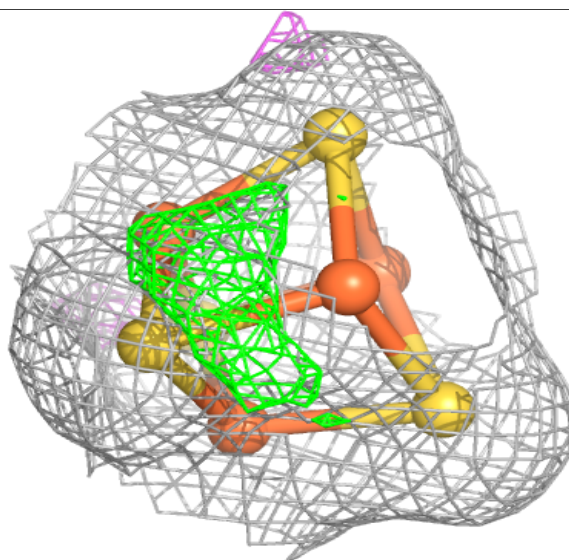
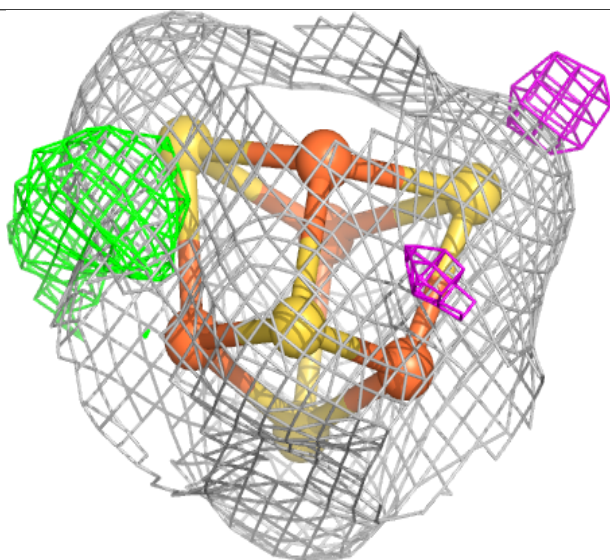
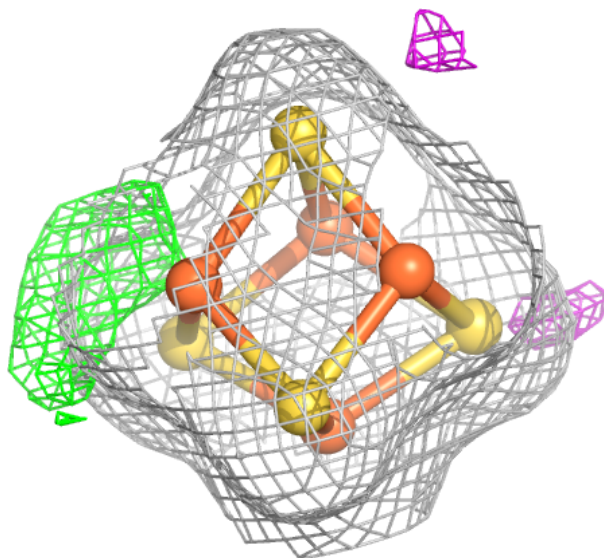
Electron density around SF4 A 819:

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



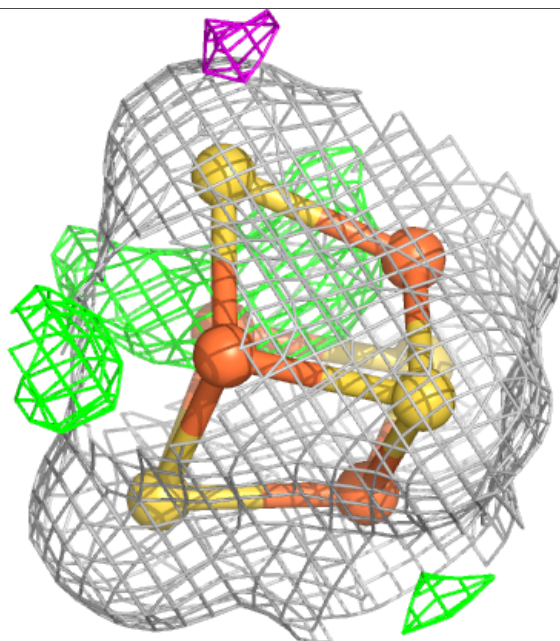
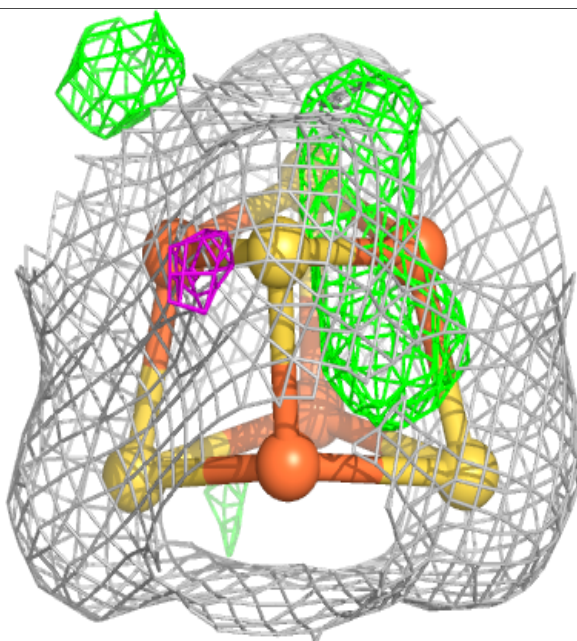
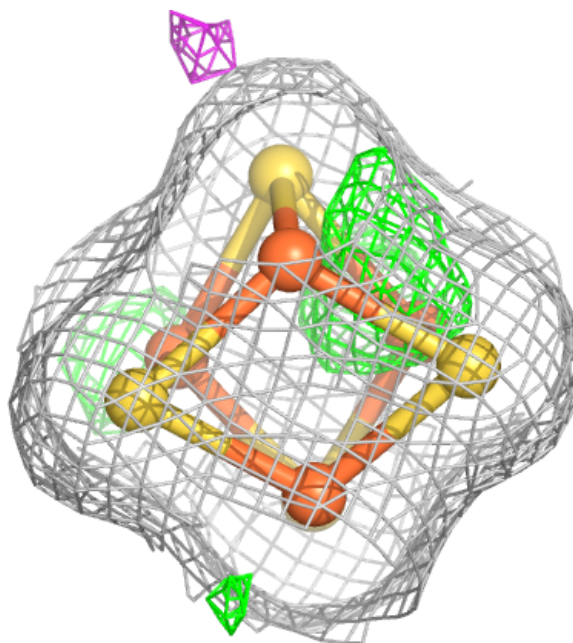
Electron density around SF4 B 402:

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



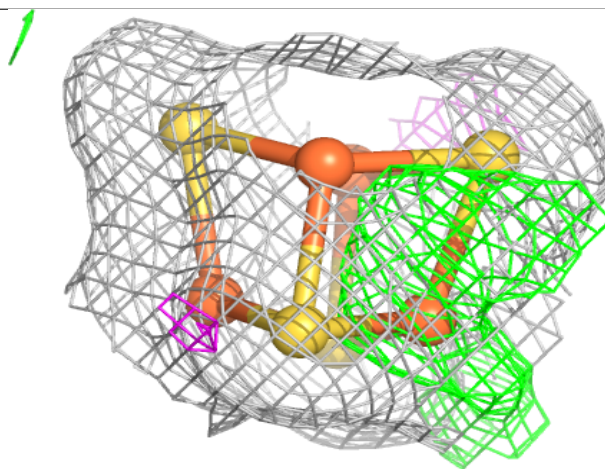
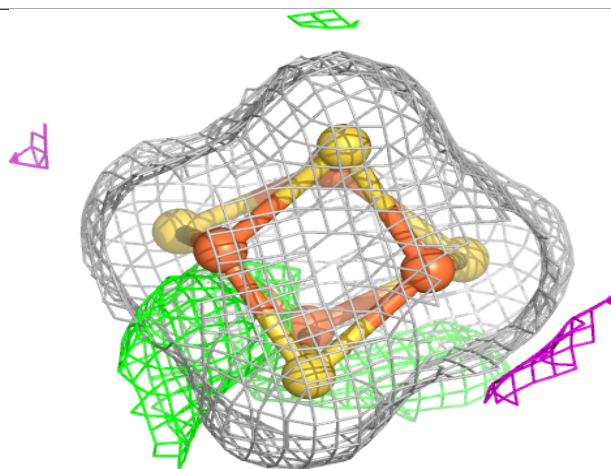
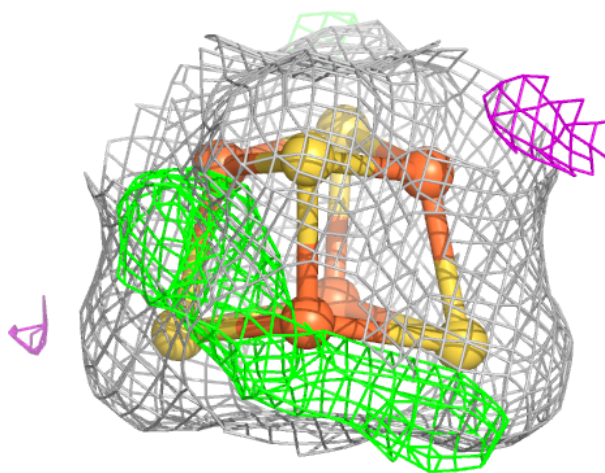
Electron density around SF4 B 403:

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



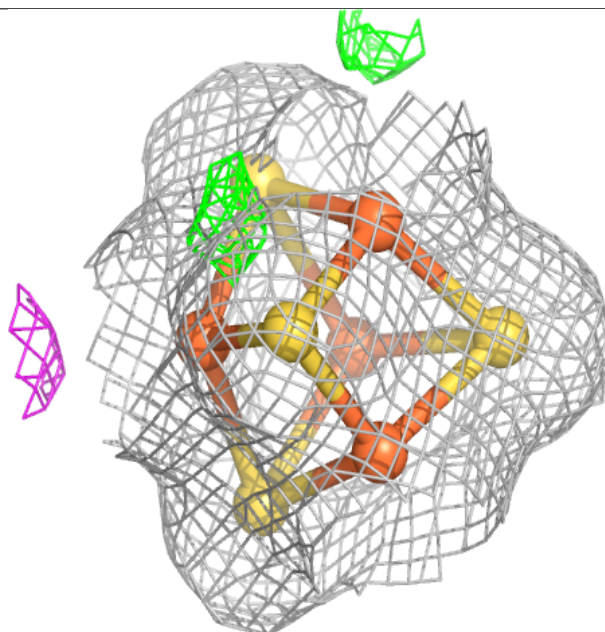
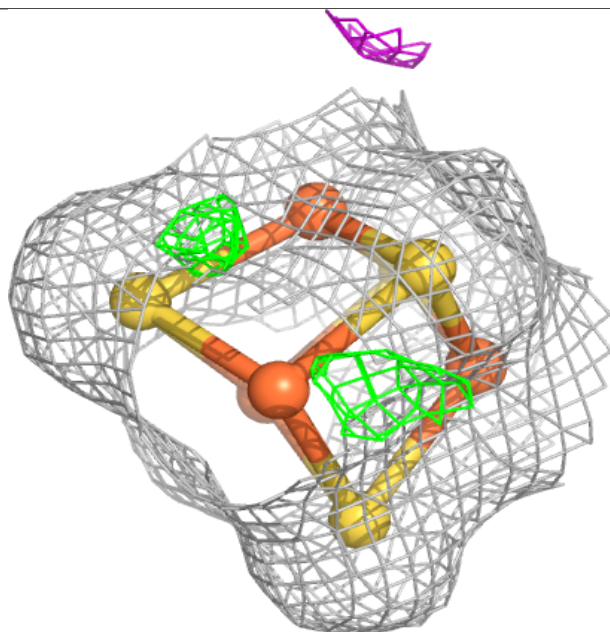
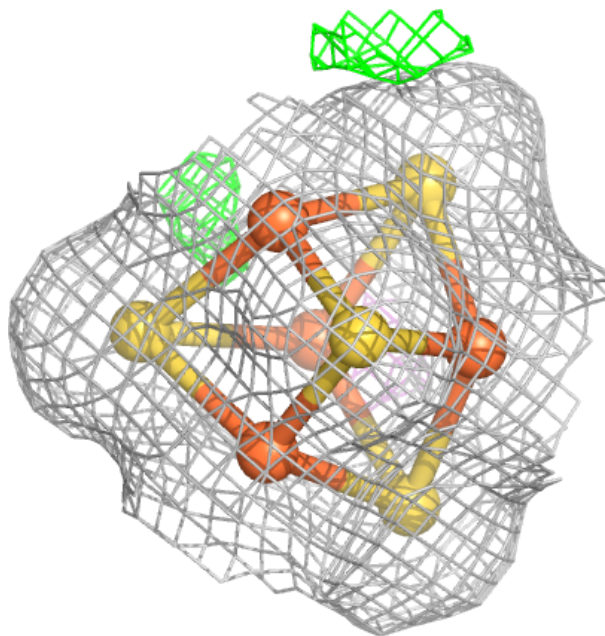
Electron density around SF4 A 809:

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



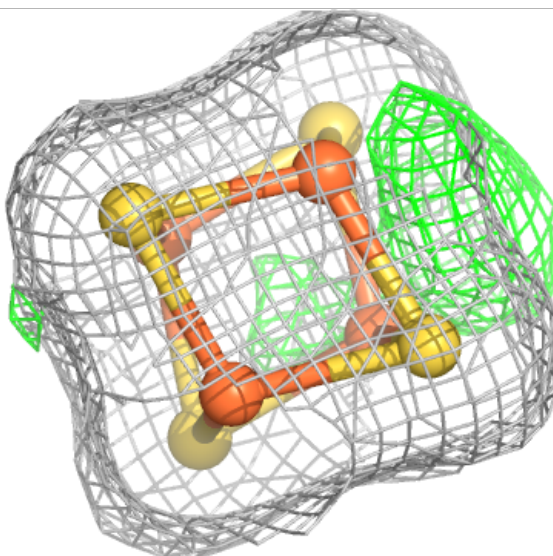
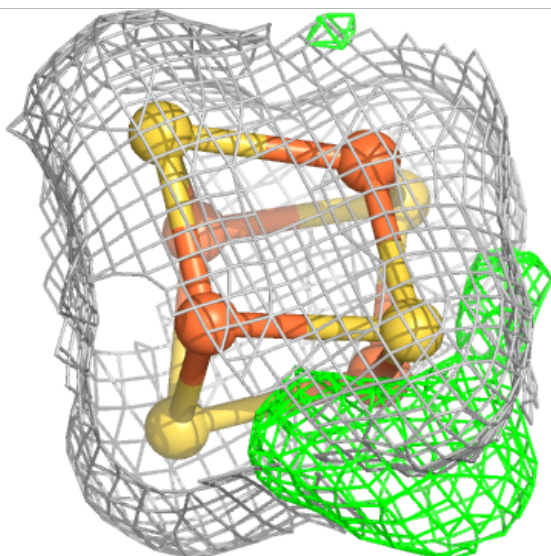
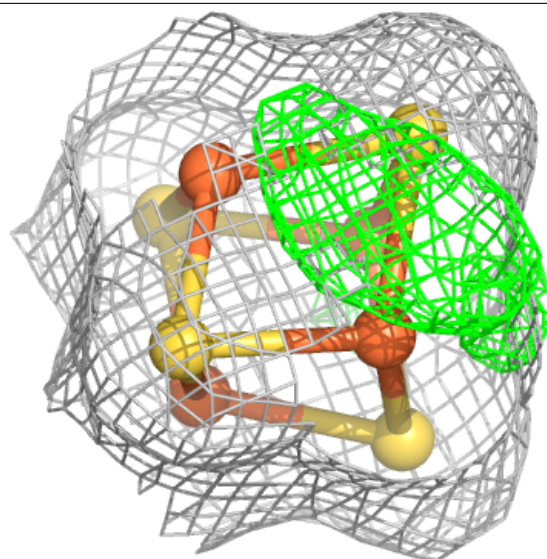
Electron density around SF4 D 803:

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



Electron density around SF4 D 804:

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



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.