



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:39 AM UTC

PDB ID : 9R51 / pdb_00009r51
Title : Dimeric state of the F420-reducing hydrogenase from *Methanothermococcus thermolithotrophicus* in crystalline form 1
Authors : Jespersen, M.; Lemaire, O.N.; Wagner, T.
Deposited on : 2025-05-08
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 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

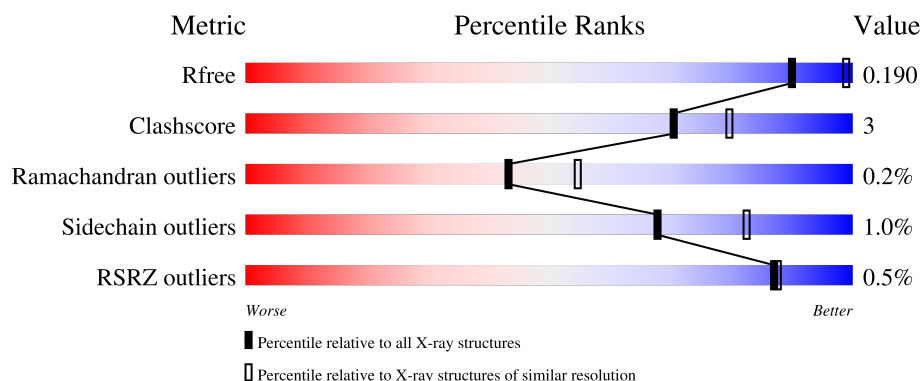
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	410	87% 8% .
1	D	410	88% 8% .
1	G	410	85% 10% ..
1	J	410	% 87% 9% .
2	B	282	94% 6%

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Mol	Chain	Length	Quality of chain
2	F	282	 92% 8%
2	I	282	 87% 13%
2	L	282	 89% 11%
3	C	241	 % 93% 7%
3	E	241	 93% 7%
3	H	241	 89% 10%
3	K	241	 % 92% 7%

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	NFU	G	501	-	-	X	-
9	SF4	B	401	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 30819 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 F420-reducing [NiFe]-hydrogenase from Methanothermococcus thermolithotrophicus subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3070	1954	525	576	15			
1	D	392	Total	C	N	O	S	0	0	0
			3070	1954	525	576	15			
1	G	392	Total	C	N	O	S	0	0	0
			3070	1954	525	576	15			
1	J	392	Total	C	N	O	S	0	0	0
			3070	1954	525	576	15			

- Molecule 2 is a protein called F420-reducing [NiFe]-hydrogenase from Methanothermococcus thermolithotrophicus subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	282	Total	C	N	O	S	0	0	0
			2177	1394	356	412	15			
2	F	282	Total	C	N	O	S	0	0	0
			2177	1394	356	412	15			
2	I	282	Total	C	N	O	S	0	0	0
			2177	1394	356	412	15			
2	L	282	Total	C	N	O	S	0	0	0
			2177	1394	356	412	15			

- Molecule 3 is a protein called F420-reducing [NiFe]-hydrogenase from Methanothermococcus thermolithotrophicus subunit gamma.

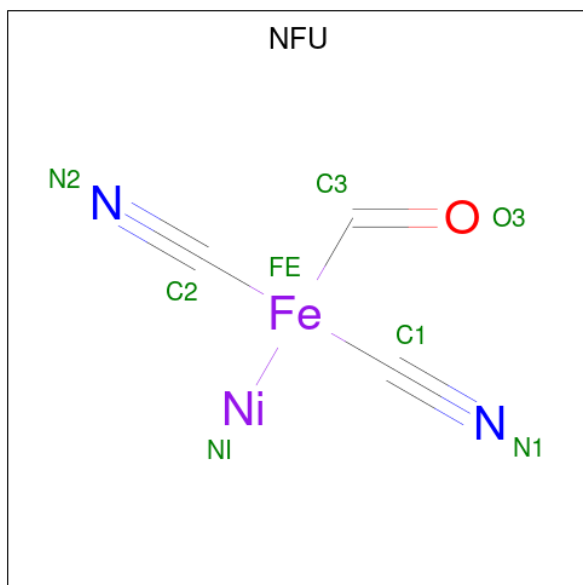
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1799	1130	299	349	21			
3	E	240	Total	C	N	O	S	0	1	0
			1805	1134	300	350	21			
3	H	240	Total	C	N	O	S	0	0	0
			1799	1130	299	349	21			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	240	Total	C	N	O	S	0	1	0
			1805	1134	300	350	21			

- Molecule 4 is formyl[bis(hydrocyanato-1kappaC)]ironnickel(Fe-Ni) (CCD ID: NFU) (formula: C_3HFeN_2NiO) (labeled as "Ligand of Interest" by depositor).

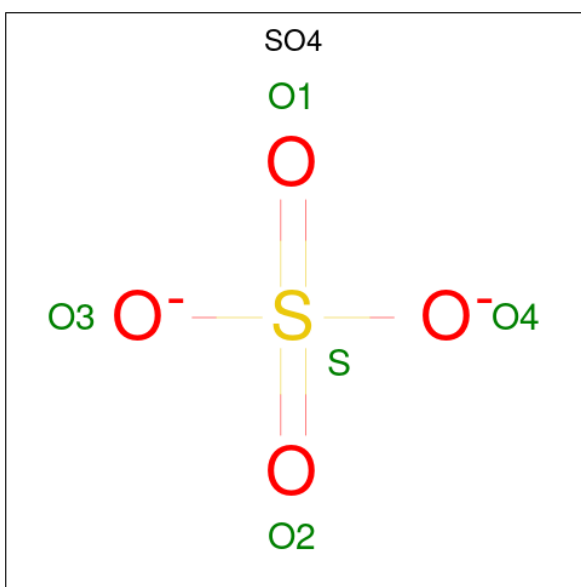


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 8	C 3	Fe 1	N 2	Ni 1	O 1	0	0
4	D	1	Total 8	C 3	Fe 1	N 2	Ni 1	O 1	0	0
4	G	1	Total 8	C 3	Fe 1	N 2	Ni 1	O 1	0	0
4	J	1	Total 8	C 3	Fe 1	N 2	Ni 1	O 1	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

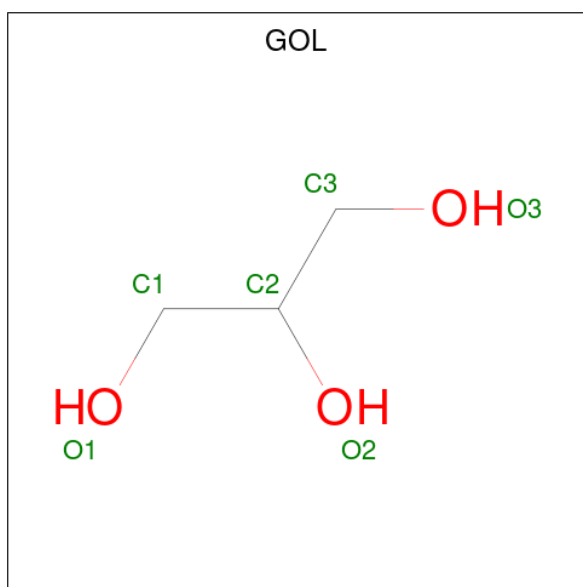
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total 6	C 3	O 3	0	0
7	D	1	Total 6	C 3	O 3	0	0
7	D	1	Total 6	C 3	O 3	0	0
7	D	1	Total 6	C 3	O 3	0	0
7	D	1	Total 6	C 3	O 3	0	0
7	E	1	Total 6	C 3	O 3	0	0
7	E	1	Total 6	C 3	O 3	0	0
7	E	1	Total 6	C 3	O 3	0	0
7	E	1	Total 6	C 3	O 3	0	0
7	F	1	Total 6	C 3	O 3	0	0
7	F	1	Total 6	C 3	O 3	0	0
7	G	1	Total 6	C 3	O 3	0	0
7	G	1	Total 6	C 3	O 3	0	0
7	G	1	Total 6	C 3	O 3	0	0
7	G	1	Total 6	C 3	O 3	0	0
7	H	1	Total 6	C 3	O 3	0	0
7	H	1	Total 6	C 3	O 3	0	0
7	H	1	Total 6	C 3	O 3	0	0
7	H	1	Total 6	C 3	O 3	0	0
7	I	1	Total 6	C 3	O 3	0	0
7	I	1	Total 6	C 3	O 3	0	0

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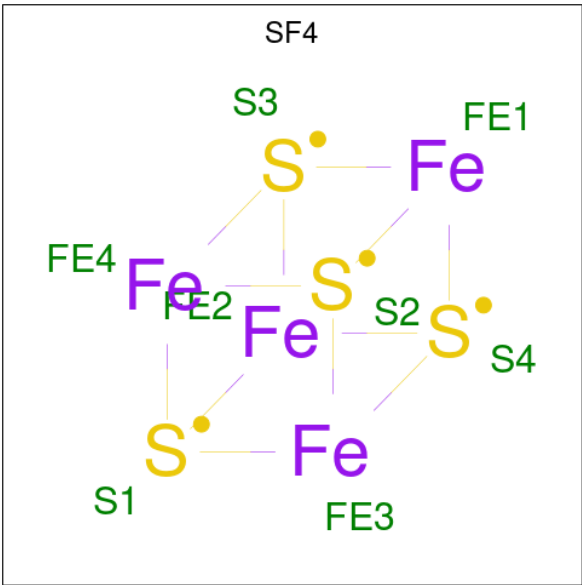
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	1	Total C O 6 3 3	0	0
7	J	1	Total C O 6 3 3	0	0
7	J	1	Total C O 6 3 3	0	0
7	J	1	Total C O 6 3 3	0	0
7	J	1	Total C O 6 3 3	0	0
7	J	1	Total C O 6 3 3	0	0
7	K	1	Total C O 6 3 3	0	0
7	K	1	Total C O 6 3 3	0	0
7	K	1	Total C O 6 3 3	0	0
7	L	1	Total C O 6 3 3	0	0
7	L	1	Total C O 6 3 3	0	0

- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Fe 1 1	0	0
8	D	1	Total Fe 1 1	0	0
8	G	1	Total Fe 1 1	0	0
8	J	1	Total Fe 1 1	0	0

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



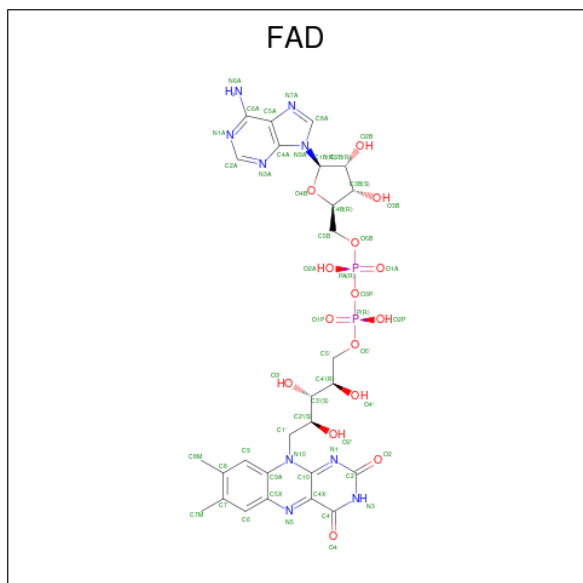
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		
9	C	1	Total	Fe	S	0	0
			8	4	4		
9	C	1	Total	Fe	S	0	0
			8	4	4		
9	C	1	Total	Fe	S	0	0
			8	4	4		
9	E	1	Total	Fe	S	0	0
			8	4	4		
9	E	1	Total	Fe	S	0	0
			8	4	4		
9	E	1	Total	Fe	S	0	0
			8	4	4		
9	F	1	Total	Fe	S	0	0
			8	4	4		
9	H	1	Total	Fe	S	0	0
			8	4	4		
9	H	1	Total	Fe	S	0	0
			8	4	4		
9	H	1	Total	Fe	S	0	0
			8	4	4		
9	I	1	Total	Fe	S	0	0
			8	4	4		
9	K	1	Total	Fe	S	0	0
			8	4	4		
9	K	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	K	1	Total 8	Fe 4	S 4	0	0
9	L	1	Total 8	Fe 4	S 4	0	0

- Molecule 10 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).

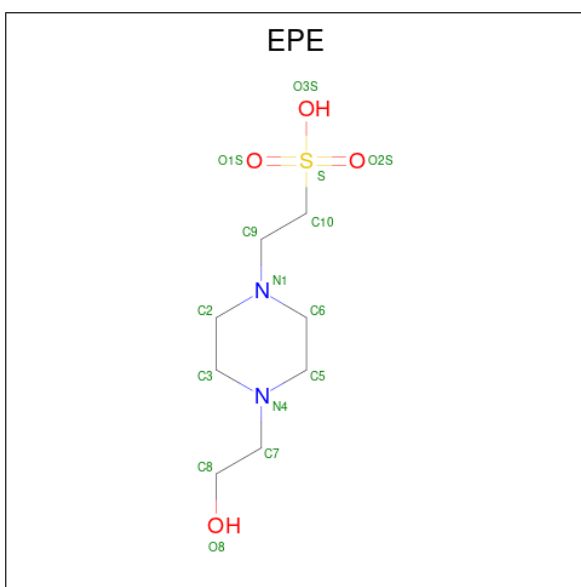


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
10	F	1	Total 53	C 27	N 9	O 15	P 2	0	0
10	I	1	Total 53	C 27	N 9	O 15	P 2	0	0
10	L	1	Total 53	C 27	N 9	O 15	P 2	0	0

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

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

- Molecule 12 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
12	J	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

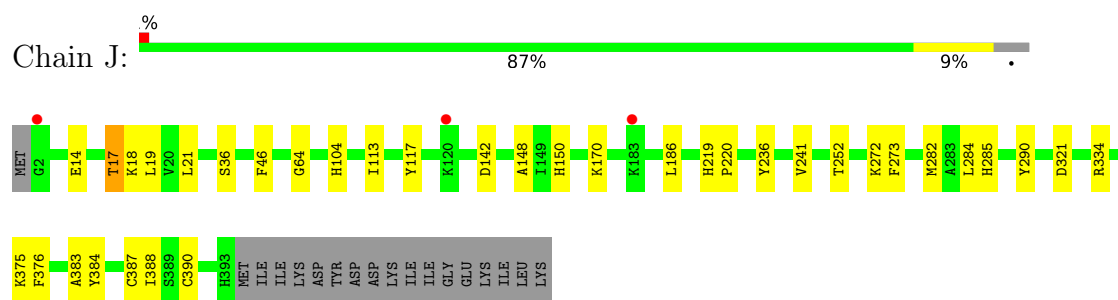
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	226	Total	O	0	0
			226	226		
13	B	136	Total	O	0	0
			136	136		
13	C	128	Total	O	0	0
			128	128		
13	D	258	Total	O	0	0
			258	258		
13	E	146	Total	O	0	0
			146	146		
13	F	131	Total	O	0	0
			131	131		
13	G	209	Total	O	0	0
			209	209		
13	H	112	Total	O	0	0
			112	112		
13	I	109	Total	O	0	0
			109	109		
13	J	198	Total	O	0	0
			198	198		

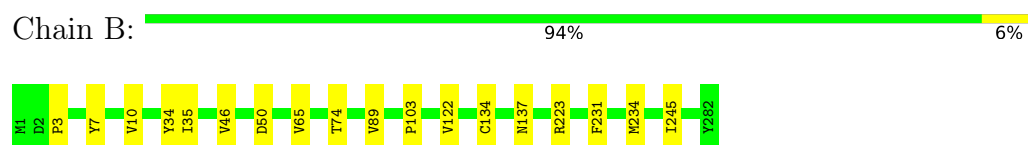
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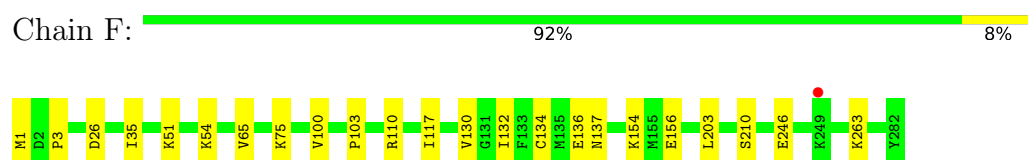
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	K	118	Total 118	O 118	0	0
13	L	117	Total 117	O 117	0	0



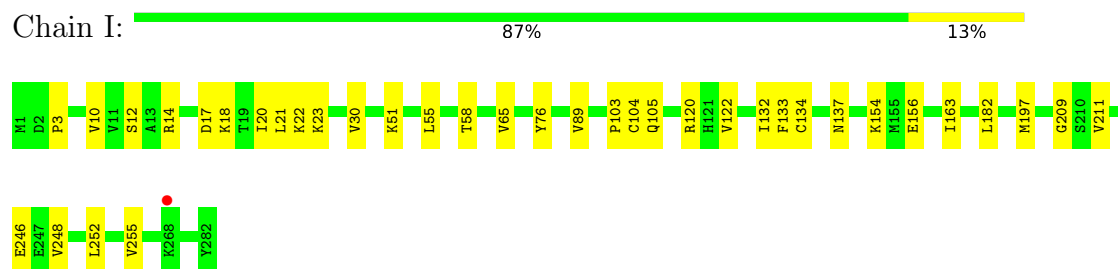
- Molecule 2: F420-reducing [NiFe]-hydrogenase from Methanothermococcus thermolithotrophicus subunit beta



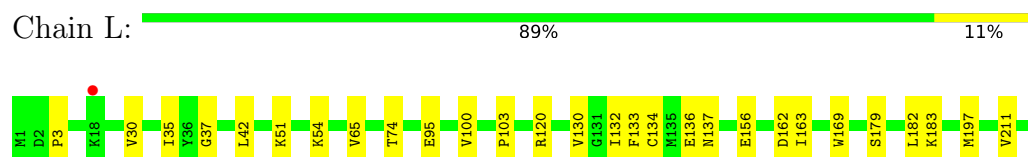
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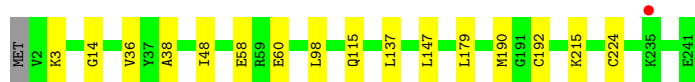


- Molecule 3: F420-reducing [NiFe]-hydrogenase from Methanothermococcus thermolithotrophicus subunit gamma

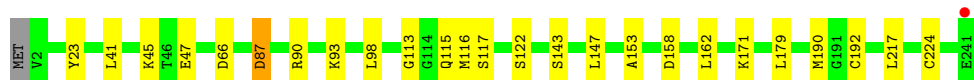
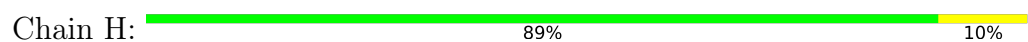




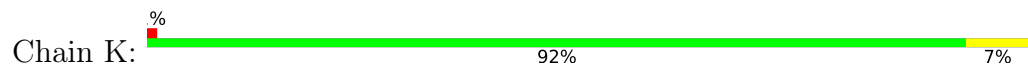
- Molecule 3: F420-reducing [NiFe]-hydrogenase from Methanothermococcus thermolithotrophicus subunit gamma



- Molecule 3: F420-reducing [NiFe]-hydrogenase from Methanothermococcus thermolithotrophicus subunit gamma



- Molecule 3: F420-reducing [NiFe]-hydrogenase from Methanothermococcus thermolithotrophicus subunit gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	192.71Å 192.71Å 386.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.55 – 2.30 31.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.55-2.30) 99.8 (31.55-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???), BUSTER	Depositor
R, R_{free}	0.180 , 0.207 (Not available) , 0.190	Depositor DCC
R_{free} test set	18436 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	30819	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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: SO4, GOL, CL, FAD, EPE, NA, SF4, NFU, FE

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	0.29	0/3140	0.53	1/4251 (0.0%)
1	D	0.31	0/3140	0.52	0/4251
1	G	0.34	0/3140	0.57	0/4251
1	J	0.33	0/3140	0.54	0/4251
2	B	0.29	0/2219	0.52	0/2994
2	F	0.35	0/2219	0.58	0/2994
2	I	0.31	0/2219	0.54	0/2994
2	L	0.32	0/2219	0.53	0/2994
3	C	0.34	0/1821	0.51	0/2465
3	E	0.31	0/1830	0.52	0/2477
3	H	0.33	0/1821	0.52	0/2465
3	K	0.33	0/1830	0.55	0/2477
All	All	0.32	0/28738	0.54	1/38864 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ARG	CA-CB-CG	-6.83	100.44	114.10

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	3070	0	3049	20	0
1	D	3070	0	3049	22	0
1	G	3070	0	3049	27	0
1	J	3070	0	3049	22	0
2	B	2177	0	2224	10	0
2	F	2177	0	2224	14	0
2	I	2177	0	2224	24	0
2	L	2177	0	2224	19	0
3	C	1799	0	1836	10	0
3	E	1805	0	1844	14	0
3	H	1799	0	1836	18	0
3	K	1805	0	1844	12	0
4	A	8	0	0	1	0
4	D	8	0	0	1	0
4	G	8	0	0	2	0
4	J	8	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	10	0	0	0	0
6	D	10	0	0	0	0
6	E	5	0	0	0	0
6	F	10	0	0	0	0
6	G	5	0	0	0	0
6	J	10	0	0	0	0
7	A	36	0	48	0	0
7	B	12	0	16	0	0
7	C	24	0	32	2	0
7	D	42	0	56	0	0
7	E	24	0	32	0	0
7	F	12	0	16	0	0
7	G	24	0	32	0	0
7	H	24	0	32	1	0
7	I	18	0	24	0	0
7	J	30	0	40	1	0
7	K	18	0	24	0	0
7	L	12	0	16	0	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
8	G	1	0	0	0	0
8	J	1	0	0	0	0
9	B	8	0	0	2	0
9	C	24	0	0	0	0
9	E	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	8	0	0	1	0
9	H	24	0	0	0	0
9	I	8	0	0	1	0
9	K	24	0	0	0	0
9	L	8	0	0	1	0
10	B	53	0	31	1	0
10	F	53	0	31	0	0
10	I	53	0	31	2	0
10	L	53	0	31	2	0
11	D	1	0	0	0	0
12	G	15	0	17	2	0
12	J	15	0	18	3	0
13	A	226	0	0	0	0
13	B	136	0	0	0	0
13	C	128	0	0	0	0
13	D	258	0	0	0	0
13	E	146	0	0	0	0
13	F	131	0	0	0	0
13	G	209	0	0	0	0
13	H	112	0	0	0	0
13	I	109	0	0	0	0
13	J	198	0	0	0	0
13	K	118	0	0	0	0
13	L	117	0	0	0	0
All	All	30819	0	28979	196	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 3.

All (196) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:THR:HG23	1:A:388:ILE:HG13	1.85	0.58
3:E:137:LEU:HD13	3:E:147:LEU:HD23	1.85	0.58
1:D:17:THR:HG23	1:D:388:ILE:HG13	1.86	0.58
1:J:17:THR:HG23	1:J:388:ILE:HG13	1.85	0.57
1:G:19:LEU:HD22	1:G:21:LEU:HD21	1.86	0.57
2:F:35:ILE:HG12	2:F:65:VAL:HG13	1.86	0.56
1:G:17:THR:HG23	1:G:388:ILE:HG13	1.87	0.56
1:G:36:SER:HB2	1:G:388:ILE:HG23	1.89	0.55
1:J:19:LEU:HD22	1:J:21:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:259:GLY:O	12:G:503:EPE:H22	2.08	0.54
2:F:137:ASN:HB2	9:F:401:SF4:S2	2.50	0.52
3:K:196:ALA:HA	3:K:204:ILE:HB	1.92	0.52
1:G:285:HIS:CE1	1:G:383:ALA:HA	2.46	0.51
1:J:36:SER:HB3	1:J:252:THR:HG23	1.92	0.51
1:J:334:ARG:HD2	4:J:501:NFU:C1	2.40	0.51
2:B:103:PRO:HD2	9:B:401:SF4:S3	2.50	0.51
3:H:190:MET:SD	3:H:192:CYS:HB3	2.51	0.51
1:D:17:THR:HG22	1:D:36:SER:HA	1.92	0.51
2:I:30:VAL:HG11	10:I:402:FAD:H4B	1.92	0.51
2:L:137:ASN:HB2	9:L:401:SF4:S2	2.50	0.51
1:A:155:LYS:HD2	1:A:160:ALA:HB2	1.91	0.51
1:A:241:VAL:HG11	1:A:254:VAL:HG11	1.93	0.51
2:F:103:PRO:HD2	2:F:134:CYS:HB3	1.92	0.51
1:A:334:ARG:HD2	4:A:501:NFU:C1	2.41	0.51
1:J:272:LYS:HG2	1:J:273:PHE:CE2	2.46	0.50
3:H:190:MET:HE1	3:H:192:CYS:HB3	1.94	0.50
1:G:15:GLY:HA3	1:G:388:ILE:HB	1.93	0.50
2:B:35:ILE:HG12	2:B:65:VAL:HG13	1.93	0.50
1:D:111:PHE:HB2	1:D:130:VAL:HG11	1.94	0.50
1:J:142:ASP:OD1	1:J:148:ALA:N	2.45	0.50
2:L:103:PRO:HD3	2:L:132:ILE:O	2.13	0.49
1:J:321:ASP:HB3	7:J:506:GOL:H31	1.94	0.49
2:I:103:PRO:HD2	2:I:134:CYS:HB3	1.95	0.49
1:D:36:SER:HB3	1:D:252:THR:HG23	1.95	0.49
2:I:17:ASP:HB3	2:I:20:ILE:HD12	1.94	0.49
1:D:2:GLY:N	1:D:25:ASP:OD1	2.46	0.48
3:H:87:ASP:OD1	3:H:90:ARG:NH2	2.45	0.48
2:B:7:TYR:HA	2:B:223:ARG:HA	1.94	0.48
3:K:190:MET:SD	3:K:192:CYS:HB3	2.53	0.48
1:G:267:ARG:HB2	1:G:284:LEU:HD23	1.95	0.48
2:I:163:ILE:HG23	2:I:182:LEU:HD21	1.94	0.48
2:L:54:LYS:HE2	2:L:156:GLU:CG	2.44	0.48
3:C:190:MET:HE1	3:C:192:CYS:HB3	1.97	0.47
7:C:304:GOL:H31	1:D:49:GLY:HA2	1.95	0.47
1:D:108:LEU:HB2	1:D:134:ARG:HD3	1.94	0.47
1:G:334:ARG:HD2	4:G:501:NFU:C1	2.44	0.47
2:B:89:VAL:HG21	2:B:122:VAL:HG22	1.95	0.47
3:H:98:LEU:HD11	3:H:147:LEU:HD21	1.96	0.47
1:J:186:LEU:HD11	1:J:290:TYR:CD1	2.48	0.47
2:I:18:LYS:HG2	2:I:22:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:103:PRO:HD3	2:I:132:ILE:O	2.15	0.47
3:H:153:ALA:HB3	3:H:162:LEU:HD21	1.96	0.47
3:E:179:LEU:HD11	3:E:224:CYS:HB2	1.96	0.47
2:I:154:LYS:HA	2:I:154:LYS:HD2	1.64	0.47
1:A:119:PRO:HD2	1:A:188:TYR:OH	2.15	0.47
1:D:334:ARG:HD2	4:D:501:NFU:C1	2.44	0.47
1:A:277:LYS:HA	1:A:277:LYS:HD3	1.76	0.47
3:C:190:MET:SD	3:C:192:CYS:HB3	2.55	0.47
1:D:241:VAL:HG11	1:D:254:VAL:HG11	1.97	0.47
1:J:334:ARG:HD3	1:J:387:CYS:HB2	1.97	0.47
2:F:103:PRO:HD3	2:F:132:ILE:O	2.16	0.46
3:C:113:GLY:HA3	3:C:122:SER:HB3	1.96	0.46
1:D:8:HIS:O	3:E:58:GLU:HA	2.16	0.46
1:J:14:GLU:O	1:J:388:ILE:HG12	2.15	0.46
2:I:51:LYS:HD2	2:I:55:LEU:HD23	1.98	0.46
3:E:190:MET:SD	3:E:192:CYS:HB3	2.56	0.46
1:J:241:VAL:HG12	12:J:504:EPE:H91	1.96	0.46
1:D:15:GLY:HA3	1:D:388:ILE:HB	1.96	0.46
1:D:46:PHE:C	1:D:46:PHE:CD1	2.94	0.46
2:L:163:ILE:HG23	2:L:182:LEU:HD21	1.98	0.46
2:L:197:MET:HB3	2:L:197:MET:HE3	1.66	0.46
3:C:98:LEU:HD11	3:C:147:LEU:HD21	1.98	0.46
2:F:100:VAL:HA	2:F:130:VAL:O	2.16	0.46
2:I:10:VAL:HG21	2:I:252:LEU:HD13	1.98	0.46
1:D:36:SER:HB2	1:D:388:ILE:HG23	1.98	0.45
1:G:358:THR:HB	1:G:391:ALA:HB2	1.98	0.45
1:A:142:ASP:OD1	1:A:148:ALA:N	2.49	0.45
2:B:74:THR:HG23	10:B:402:FAD:HM83	1.99	0.45
1:G:255:PRO:HB2	1:G:360:TRP:CE3	2.52	0.45
2:L:156:GLU:H	2:L:156:GLU:CD	2.25	0.45
1:A:111:PHE:CZ	7:C:305:GOL:H2	2.52	0.45
1:J:36:SER:HB2	1:J:388:ILE:HG23	1.97	0.45
2:L:103:PRO:HD2	2:L:134:CYS:HB3	1.98	0.45
1:G:311:LYS:NZ	1:G:315:ASP:OD2	2.50	0.45
3:C:116:MET:HE3	3:C:117:SER:HA	1.99	0.45
1:J:285:HIS:CE1	1:J:383:ALA:HA	2.52	0.45
1:G:42:GLY:HA2	3:H:115:GLN:CD	2.42	0.45
1:A:64:GLY:HA3	3:C:14:GLY:CA	2.47	0.45
1:G:8:HIS:HB2	1:G:18:LYS:HB2	1.98	0.45
1:G:337:ASN:OD1	1:G:356:VAL:HA	2.17	0.45
1:J:113:ILE:HD13	1:J:285:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:HIS:CE1	1:D:383:ALA:HA	2.52	0.44
2:L:169:TRP:CE3	2:L:179:SER:HB3	2.53	0.44
2:F:154:LYS:HD3	2:F:154:LYS:HA	1.84	0.44
2:L:162:ASP:OD1	2:L:163:ILE:N	2.49	0.44
1:G:108:LEU:HB2	1:G:134:ARG:HD3	1.98	0.44
1:A:217:ALA:HB3	1:A:272:LYS:HG3	1.99	0.44
1:G:135:ARG:HG3	3:H:23:TYR:CD2	2.52	0.44
3:H:98:LEU:CD1	3:H:147:LEU:HD21	2.48	0.44
1:J:219:HIS:CG	1:J:220:PRO:HD2	2.52	0.44
3:C:216:GLU:OE2	3:E:215:LYS:N	2.44	0.44
1:D:219:HIS:CG	1:D:220:PRO:HD2	2.53	0.44
2:F:51:LYS:HD3	2:F:75:LYS:HD2	2.00	0.44
1:J:117:TYR:OH	1:J:282:MET:HE1	2.17	0.44
1:A:229:ASP:HB3	1:A:232:LYS:HD2	1.99	0.44
2:F:1:MET:HE3	2:F:263:LYS:HB3	2.00	0.44
3:H:113:GLY:HA3	3:H:122:SER:HB3	1.99	0.43
3:E:137:LEU:HD22	2:F:117:ILE:HD11	1.99	0.43
3:K:137:LEU:HD21	3:K:150:LEU:HD13	2.00	0.43
3:C:137:LEU:HD21	3:C:150:LEU:HD13	1.99	0.43
1:D:64:GLY:HA3	3:E:14:GLY:CA	2.47	0.43
3:H:153:ALA:HB1	3:H:158:ASP:HB3	2.00	0.43
2:I:14:ARG:HG3	2:I:21:LEU:HD21	2.00	0.43
2:L:37:GLY:HA2	2:L:42:LEU:HB2	2.00	0.43
3:E:137:LEU:CD1	3:E:147:LEU:HD23	2.49	0.43
1:J:46:PHE:CD1	1:J:46:PHE:C	2.96	0.43
1:G:284:LEU:HD11	1:G:384:TYR:CZ	2.54	0.43
2:B:137:ASN:HB2	9:B:401:SF4:S2	2.58	0.43
1:G:334:ARG:HD2	4:G:501:NFU:N1	2.34	0.43
3:K:153:ALA:HB1	3:K:158:ASP:HB3	2.01	0.43
1:A:12:ARG:HB2	1:A:382:ARG:HE	1.84	0.43
1:A:136:ILE:HG23	1:A:174:LYS:HB3	2.00	0.43
12:J:504:EPE:H102	12:J:504:EPE:H61	1.47	0.43
3:K:49:ARG:NH1	3:K:58:GLU:OE1	2.52	0.43
3:E:98:LEU:HD11	3:E:147:LEU:HD21	2.00	0.43
2:L:100:VAL:HA	2:L:130:VAL:O	2.19	0.43
3:H:192:CYS:HA	2:I:105:GLN:HG2	2.01	0.42
3:K:241:GLU:HB2	2:L:224:THR:HB	2.00	0.42
2:I:76:TYR:CZ	2:I:163:ILE:HG13	2.54	0.42
1:D:42:GLY:HA2	3:E:115:GLN:CD	2.44	0.42
3:K:190:MET:HE1	3:K:192:CYS:HB3	2.00	0.42
1:G:155:LYS:HD2	1:G:160:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:45:LYS:HE3	3:H:47:GLU:OE2	2.19	0.42
1:J:236:TYR:CZ	12:J:504:EPE:H71	2.54	0.42
3:H:41:LEU:HB3	7:H:306:GOL:H12	2.01	0.42
2:I:154:LYS:HB3	2:I:156:GLU:HG2	2.01	0.42
2:F:26:ASP:CG	2:F:210:SER:HB2	2.45	0.42
2:F:246:GLU:H	2:F:246:GLU:CD	2.26	0.42
1:J:170:LYS:NZ	2:L:95:GLU:OE2	2.39	0.42
1:A:8:HIS:O	3:C:58:GLU:HA	2.19	0.42
1:D:334:ARG:HD3	1:D:387:CYS:HB2	2.02	0.42
1:G:261:LEU:HG	12:G:503:EPE:H101	2.01	0.42
1:A:42:GLY:HA2	3:C:115:GLN:CD	2.45	0.42
1:D:215:TYR:HB3	1:D:268:ALA:HB1	2.01	0.42
2:F:54:LYS:HD3	2:F:156:GLU:HG3	2.02	0.42
2:I:12:SER:HB3	2:I:248:VAL:HG11	2.00	0.42
2:L:74:THR:HG23	10:L:402:FAD:HM83	2.02	0.42
1:A:129:ARG:NH1	1:A:185:GLN:OE1	2.47	0.42
2:F:26:ASP:OD1	2:F:210:SER:HB2	2.20	0.42
1:J:64:GLY:HA3	3:K:14:GLY:CA	2.49	0.42
3:K:4:ILE:HG12	3:K:33:VAL:HG21	2.02	0.42
2:L:30:VAL:HG11	10:L:402:FAD:H4B	2.02	0.42
1:A:219:HIS:CG	1:A:220:PRO:HD2	2.55	0.41
2:B:10:VAL:HG13	2:B:245:ILE:HG21	2.03	0.41
1:G:103:MET:HG2	1:G:178:TYR:CZ	2.55	0.41
3:H:179:LEU:HD11	3:H:224:CYS:HB2	2.03	0.41
2:L:35:ILE:HG12	2:L:65:VAL:HG13	2.01	0.41
2:I:51:LYS:HD2	2:I:55:LEU:CD2	2.50	0.41
2:L:211:VAL:HG23	2:L:255:VAL:HG22	2.01	0.41
3:E:215:LYS:HE3	3:E:215:LYS:HB2	1.93	0.41
2:I:89:VAL:HG21	2:I:122:VAL:HG22	2.01	0.41
2:I:137:ASN:HB2	9:I:401:SF4:S2	2.60	0.41
2:I:211:VAL:HG23	2:I:255:VAL:HG22	2.01	0.41
3:K:204:ILE:HG12	3:K:213:VAL:HG22	2.02	0.41
3:E:48:ILE:O	3:K:49:ARG:HA	2.21	0.41
3:H:143:SER:HB2	2:I:120:ARG:HA	2.02	0.41
1:D:59:VAL:HG21	1:D:74:ALA:HB2	2.01	0.41
3:H:66:ASP:OD1	3:H:93:LYS:NZ	2.43	0.41
2:I:12:SER:CB	2:I:248:VAL:HG11	2.51	0.41
1:J:375:LYS:HE3	1:J:376:PHE:CZ	2.55	0.41
3:K:143:SER:HB2	2:L:120:ARG:HA	2.03	0.41
1:A:111:PHE:HB2	1:A:130:VAL:HG11	2.03	0.41
3:E:190:MET:HE1	3:E:192:CYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:10:VAL:HG21	2:I:252:LEU:CD1	2.51	0.41
1:D:219:HIS:O	1:D:331:GLU:HG3	2.21	0.41
3:E:3:LYS:HD3	3:E:36:VAL:HG11	2.03	0.41
2:F:110:ARG:HG3	2:F:203:LEU:HB3	2.03	0.41
2:I:197:MET:HE3	2:I:197:MET:HB3	1.75	0.41
2:B:34:TYR:CE2	2:B:46:VAL:HB	2.56	0.41
1:G:14:GLU:O	1:G:388:ILE:HG12	2.20	0.41
1:G:60:SER:OG	1:G:67:PRO:HB2	2.21	0.41
3:H:116:MET:HA	3:H:117:SER:HA	1.82	0.40
10:I:402:FAD:H9	10:I:402:FAD:H1'1	1.86	0.40
1:A:45:LYS:HD3	1:A:45:LYS:HA	1.71	0.40
2:B:231:PHE:HA	2:B:234:MET:CE	2.51	0.40
1:D:111:PHE:HD1	1:D:127:ILE:HG12	1.86	0.40
1:G:13:HIS:CE1	1:G:17:THR:OG1	2.74	0.40
1:G:63:CYS:SG	1:G:65:ILE:HB	2.62	0.40
1:J:284:LEU:HD11	1:J:384:TYR:CZ	2.56	0.40
2:B:103:PRO:HD2	2:B:134:CYS:HB3	2.04	0.40
1:G:43:PHE:HA	1:G:46:PHE:CE2	2.56	0.40
1:G:269:ARG:HH12	1:G:335:GLY:HA2	1.86	0.40
2:I:133:PHE:CD2	2:I:209:GLY:HA3	2.56	0.40
2:L:133:PHE:N	2:L:133:PHE:CD1	2.89	0.40
1:A:145:GLY:HA3	1:A:151:SER:HB3	2.03	0.40
3:H:190:MET:HE2	2:I:104:CYS:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	390/410 (95%)	380 (97%)	10 (3%)	0	100	100
1	D	390/410 (95%)	379 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	390/410 (95%)	380 (97%)	10 (3%)	0	100	100
1	J	390/410 (95%)	379 (97%)	10 (3%)	1 (0%)	36	46
2	B	280/282 (99%)	271 (97%)	8 (3%)	1 (0%)	30	38
2	F	280/282 (99%)	271 (97%)	8 (3%)	1 (0%)	30	38
2	I	280/282 (99%)	270 (96%)	9 (3%)	1 (0%)	30	38
2	L	280/282 (99%)	271 (97%)	8 (3%)	1 (0%)	30	38
3	C	238/241 (99%)	226 (95%)	11 (5%)	1 (0%)	30	38
3	E	239/241 (99%)	228 (95%)	10 (4%)	1 (0%)	30	38
3	H	238/241 (99%)	223 (94%)	15 (6%)	0	100	100
3	K	239/241 (99%)	226 (95%)	12 (5%)	1 (0%)	30	38
All	All	3634/3732 (97%)	3504 (96%)	122 (3%)	8 (0%)	43	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	38	ALA
1	J	150	HIS
3	K	38	ALA
2	B	3	PRO
3	E	38	ALA
2	I	3	PRO
2	F	3	PRO
2	L	3	PRO

5.3.2 Protein sidechains ⓘ

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	330/347 (95%)	326 (99%)	4 (1%)	63	79
1	D	330/347 (95%)	327 (99%)	3 (1%)	70	84
1	G	330/347 (95%)	325 (98%)	5 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	330/347 (95%)	326 (99%)	4 (1%)	63	79
2	B	238/238 (100%)	237 (100%)	1 (0%)	84	92
2	F	238/238 (100%)	237 (100%)	1 (0%)	84	92
2	I	238/238 (100%)	234 (98%)	4 (2%)	53	72
2	L	238/238 (100%)	235 (99%)	3 (1%)	61	77
3	C	204/205 (100%)	203 (100%)	1 (0%)	81	90
3	E	205/205 (100%)	204 (100%)	1 (0%)	81	90
3	H	204/205 (100%)	201 (98%)	3 (2%)	57	75
3	K	205/205 (100%)	203 (99%)	2 (1%)	68	82
All	All	3090/3160 (98%)	3058 (99%)	32 (1%)	68	82

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	18	LYS
1	A	104	HIS
1	A	390	CYS
2	B	50	ASP
3	C	87	ASP
1	D	46	PHE
1	D	104	HIS
1	D	390	CYS
3	E	60	GLU
2	F	136	GLU
1	G	17	THR
1	G	21	LEU
1	G	104	HIS
1	G	267	ARG
1	G	390	CYS
3	H	87	ASP
3	H	171	LYS
3	H	217	LEU
2	I	23	LYS
2	I	58	THR
2	I	65	VAL
2	I	246	GLU
1	J	17	THR
1	J	18	LYS

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Mol	Chain	Res	Type
1	J	104	HIS
1	J	390	CYS
3	K	150	LEU
3	K	217	LEU
2	L	51	LYS
2	L	136	GLU
2	L	183	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	A	340	GLN
1	A	353	ASN
2	B	56	GLN
2	B	190	GLN
2	B	272	HIS
3	C	8	HIS
3	C	25	GLN
3	C	182	ASN
1	D	336	HIS
3	E	80	HIS
3	E	182	ASN
2	F	272	HIS
1	G	162	GLN
1	G	285	HIS
1	G	340	GLN
1	G	353	ASN
3	H	8	HIS
3	H	25	GLN
2	I	194	HIS
2	I	272	HIS
1	J	124	ASN
1	J	162	GLN
1	J	285	HIS
1	J	330	HIS
2	L	186	HIS
2	L	272	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 89 ligands modelled in this entry, 7 are monoatomic - leaving 82 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	$\# Z > 2$
7	GOL	G	505	-	5,5,5	0.92	0	5,5,5	1.04	0
7	GOL	G	506	-	5,5,5	0.09	0	5,5,5	0.32	0
7	GOL	B	404	-	5,5,5	0.92	0	5,5,5	1.06	0
6	SO4	D	503	-	4,4,4	0.25	0	6,6,6	0.16	0
7	GOL	K	306	-	5,5,5	0.09	0	5,5,5	0.31	0
7	GOL	J	506	-	5,5,5	0.09	0	5,5,5	0.35	0
9	SF4	K	302	3	0,12,12	-	-	-	-	-
7	GOL	F	405	-	5,5,5	0.09	0	5,5,5	0.31	0
7	GOL	H	306	-	5,5,5	0.09	0	5,5,5	0.33	0
7	GOL	B	405	-	5,5,5	0.08	0	5,5,5	0.32	0
4	NFU	A	501	1	2,7,7	0.98	0	-	-	-
7	GOL	K	304	-	5,5,5	1.01	0	5,5,5	0.94	0
10	FAD	F	402	-	58,58,58	1.46	9 (15%)	85,89,89	1.56	12 (14%)
7	GOL	A	505	-	5,5,5	0.87	0	5,5,5	1.09	0
7	GOL	H	304	-	5,5,5	0.08	0	5,5,5	0.31	0
7	GOL	D	507	-	5,5,5	0.08	0	5,5,5	0.30	0
6	SO4	J	502	-	4,4,4	0.25	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	G	502	-	4,4,4	0.27	0	6,6,6	0.16	0
7	GOL	J	509	-	5,5,5	0.08	0	5,5,5	0.29	0
7	GOL	J	508	-	5,5,5	0.08	0	5,5,5	0.33	0
9	SF4	H	301	3	0,12,12	-	-	-		
7	GOL	C	306	-	5,5,5	0.08	0	5,5,5	0.31	0
9	SF4	C	302	3	0,12,12	-	-	-		
9	SF4	C	301	3	0,12,12	-	-	-		
7	GOL	E	305	-	5,5,5	0.93	0	5,5,5	1.01	0
9	SF4	H	303	3	0,12,12	-	-	-		
4	NFU	G	501	1	2,7,7	0.89	0	-		
6	SO4	F	403	-	4,4,4	0.26	0	6,6,6	0.15	0
7	GOL	A	507	-	5,5,5	0.74	0	5,5,5	1.01	0
7	GOL	D	510	-	5,5,5	0.09	0	5,5,5	0.30	0
7	GOL	I	404	-	5,5,5	0.07	0	5,5,5	0.30	0
7	GOL	H	305	-	5,5,5	0.08	0	5,5,5	0.33	0
4	NFU	J	501	1	2,7,7	1.18	0	-		
9	SF4	L	401	2	0,12,12	-	-	-		
7	GOL	A	508	-	5,5,5	0.91	0	5,5,5	1.09	0
7	GOL	D	505	-	5,5,5	0.09	0	5,5,5	0.33	0
7	GOL	D	504	-	5,5,5	0.99	0	5,5,5	0.99	0
7	GOL	A	509	-	5,5,5	0.08	0	5,5,5	0.32	0
7	GOL	D	508	-	5,5,5	0.08	0	5,5,5	0.30	0
7	GOL	G	507	-	5,5,5	0.07	0	5,5,5	0.30	0
7	GOL	E	307	-	5,5,5	0.08	0	5,5,5	0.33	0
9	SF4	E	302	3	0,12,12	-	-	-		
9	SF4	F	401	2	0,12,12	-	-	-		
7	GOL	H	307	-	5,5,5	0.09	0	5,5,5	0.32	0
6	SO4	D	502	-	4,4,4	0.26	0	6,6,6	0.12	0
9	SF4	H	302	3	0,12,12	-	-	-		
9	SF4	C	303	3	0,12,12	-	-	-		
9	SF4	K	301	3	0,12,12	-	-	-		
7	GOL	C	305	-	5,5,5	1.03	0	5,5,5	0.89	0
7	GOL	F	406	-	5,5,5	0.09	0	5,5,5	0.32	0
7	GOL	J	505	-	5,5,5	0.97	0	5,5,5	1.06	0
7	GOL	E	308	-	5,5,5	0.09	0	5,5,5	0.32	0
10	FAD	B	402	-	58,58,58	1.43	8 (13%)	85,89,89	1.57	17 (20%)
6	SO4	E	304	-	4,4,4	0.36	0	6,6,6	0.08	0
4	NFU	D	501	1	2,7,7	0.96	0	-		
7	GOL	J	507	-	5,5,5	0.93	0	5,5,5	0.99	0
7	GOL	D	506	-	5,5,5	0.98	0	5,5,5	1.03	0
6	SO4	A	504	-	4,4,4	0.28	0	6,6,6	0.22	0
7	GOL	A	510	-	5,5,5	0.09	0	5,5,5	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	EPE	G	503	-	15,15,15	0.86	1 (6%)	19,20,20	1.78	5 (26%)
6	SO4	J	503	-	4,4,4	0.35	0	6,6,6	0.07	0
7	GOL	K	305	-	5,5,5	0.08	0	5,5,5	0.32	0
7	GOL	I	405	-	5,5,5	0.09	0	5,5,5	0.30	0
7	GOL	L	404	-	5,5,5	0.08	0	5,5,5	0.33	0
7	GOL	L	403	-	5,5,5	0.09	0	5,5,5	0.33	0
9	SF4	E	303	3	0,12,12	-	-	-	-	-
9	SF4	B	401	2	0,12,12	-	-	-	-	-
6	SO4	A	503	-	4,4,4	0.25	0	6,6,6	0.13	0
6	SO4	F	404	-	4,4,4	0.35	0	6,6,6	0.07	0
9	SF4	E	301	3	0,12,12	-	-	-	-	-
7	GOL	C	304	-	5,5,5	1.09	0	5,5,5	0.91	0
7	GOL	C	307	-	5,5,5	0.09	0	5,5,5	0.32	0
10	FAD	I	402	-	58,58,58	1.42	9 (15%)	85,89,89	1.54	16 (18%)
7	GOL	E	306	-	5,5,5	0.09	0	5,5,5	0.34	0
7	GOL	G	504	-	5,5,5	1.25	0	5,5,5	0.83	0
9	SF4	I	401	2	0,12,12	-	-	-	-	-
7	GOL	A	506	-	5,5,5	0.93	0	5,5,5	1.03	0
7	GOL	D	509	-	5,5,5	0.10	0	5,5,5	0.32	0
9	SF4	K	303	3	0,12,12	-	-	-	-	-
12	EPE	J	504	-	15,15,15	0.58	1 (6%)	19,20,20	0.69	1 (5%)
10	FAD	L	402	-	58,58,58	1.48	11 (18%)	85,89,89	1.54	17 (20%)
7	GOL	I	403	-	5,5,5	0.09	0	5,5,5	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	I	405	-	-	2/4/4/4	-
7	GOL	J	509	-	-	1/4/4/4	-
7	GOL	E	307	-	-	4/4/4/4	-
7	GOL	G	505	-	-	0/4/4/4	-
7	GOL	L	404	-	-	3/4/4/4	-
7	GOL	L	403	-	-	2/4/4/4	-
7	GOL	J	508	-	-	4/4/4/4	-
9	SF4	H	301	3	-	-	0/6/5/5
7	GOL	C	306	-	-	1/4/4/4	-
9	SF4	E	303	3	-	-	0/6/5/5
9	SF4	B	401	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	C	302	3	-	-	0/6/5/5
9	SF4	E	302	3	-	-	0/6/5/5
9	SF4	C	301	3	-	-	0/6/5/5
7	GOL	E	305	-	-	4/4/4/4	-
7	GOL	G	506	-	-	0/4/4/4	-
9	SF4	H	303	3	-	-	0/6/5/5
9	SF4	F	401	2	-	-	0/6/5/5
7	GOL	H	307	-	-	2/4/4/4	-
9	SF4	E	301	3	-	-	0/6/5/5
7	GOL	A	507	-	-	3/4/4/4	-
7	GOL	C	304	-	-	0/4/4/4	-
7	GOL	C	307	-	-	4/4/4/4	-
9	SF4	H	302	3	-	-	0/6/5/5
7	GOL	D	510	-	-	2/4/4/4	-
7	GOL	I	404	-	-	4/4/4/4	-
7	GOL	H	305	-	-	0/4/4/4	-
7	GOL	K	306	-	-	2/4/4/4	-
7	GOL	J	506	-	-	4/4/4/4	-
9	SF4	L	401	2	-	-	0/6/5/5
10	FAD	I	402	-	-	2/34/50/50	0/6/6/6
7	GOL	E	306	-	-	2/4/4/4	-
7	GOL	F	405	-	-	1/4/4/4	-
9	SF4	C	303	3	-	-	0/6/5/5
7	GOL	G	504	-	-	4/4/4/4	-
9	SF4	K	301	3	-	-	0/6/5/5
7	GOL	C	305	-	-	2/4/4/4	-
7	GOL	H	306	-	-	2/4/4/4	-
9	SF4	I	401	2	-	-	0/6/5/5
9	SF4	K	302	3	-	-	0/6/5/5
7	GOL	F	406	-	-	4/4/4/4	-
7	GOL	A	508	-	-	0/4/4/4	-
7	GOL	J	505	-	-	1/4/4/4	-
7	GOL	B	405	-	-	3/4/4/4	-
7	GOL	E	308	-	-	2/4/4/4	-
10	FAD	B	402	-	-	0/34/50/50	0/6/6/6
7	GOL	A	506	-	-	4/4/4/4	-
7	GOL	K	304	-	-	0/4/4/4	-
10	FAD	F	402	-	-	3/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	J	507	-	-	0/4/4/4	-
7	GOL	D	506	-	-	0/4/4/4	-
7	GOL	A	505	-	-	0/4/4/4	-
7	GOL	D	505	-	-	2/4/4/4	-
7	GOL	D	504	-	-	0/4/4/4	-
7	GOL	H	304	-	-	4/4/4/4	-
7	GOL	A	509	-	-	2/4/4/4	-
7	GOL	D	507	-	-	4/4/4/4	-
7	GOL	I	403	-	-	4/4/4/4	-
7	GOL	D	509	-	-	4/4/4/4	-
7	GOL	D	508	-	-	1/4/4/4	-
9	SF4	K	303	3	-	-	0/6/5/5
7	GOL	A	510	-	-	0/4/4/4	-
12	EPE	G	503	-	-	3/9/19/19	0/1/1/1
12	EPE	J	504	-	-	5/9/19/19	0/1/1/1
7	GOL	K	305	-	-	1/4/4/4	-
7	GOL	G	507	-	-	2/4/4/4	-
10	FAD	L	402	-	-	2/34/50/50	0/6/6/6
7	GOL	B	404	-	-	2/4/4/4	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	402	FAD	C9A-C5X	5.38	1.49	1.41
10	F	402	FAD	C9A-C5X	5.34	1.49	1.41
10	L	402	FAD	C9A-C5X	5.07	1.49	1.41
10	I	402	FAD	C9A-C5X	5.02	1.49	1.41
10	I	402	FAD	C5A-C4A	4.88	1.47	1.39
10	L	402	FAD	C5A-C4A	4.64	1.47	1.39
10	F	402	FAD	C5A-C4A	4.57	1.47	1.39
10	B	402	FAD	C5A-C4A	4.51	1.47	1.39
10	L	402	FAD	C8-C7	3.24	1.48	1.40
10	B	402	FAD	C8-C7	3.23	1.48	1.40
10	I	402	FAD	C8-C7	3.10	1.48	1.40
10	F	402	FAD	C8-C7	2.88	1.47	1.40
10	F	402	FAD	C5A-C6A	2.81	1.48	1.41
10	I	402	FAD	C5A-C6A	2.79	1.48	1.41
10	L	402	FAD	C5A-C6A	2.77	1.48	1.41
12	G	503	EPE	C10-S	2.71	1.81	1.77
10	F	402	FAD	C4-N3	-2.70	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	402	FAD	C5A-C6A	2.68	1.48	1.41
10	L	402	FAD	PA-O3P	2.67	1.62	1.59
10	F	402	FAD	C8A-N7A	2.54	1.36	1.31
10	L	402	FAD	C4-N3	-2.45	1.34	1.38
10	L	402	FAD	C8A-N7A	2.43	1.36	1.31
10	B	402	FAD	C4-N3	-2.41	1.34	1.38
10	I	402	FAD	C4X-N5	2.41	1.36	1.30
10	B	402	FAD	C8A-N7A	2.36	1.36	1.31
10	I	402	FAD	C8A-N7A	2.33	1.36	1.31
10	L	402	FAD	C4X-N5	2.30	1.35	1.30
10	I	402	FAD	C4-N3	-2.20	1.34	1.38
10	F	402	FAD	C4X-N5	2.19	1.35	1.30
10	B	402	FAD	C5A-N7A	-2.18	1.35	1.39
10	L	402	FAD	C5A-N7A	-2.16	1.35	1.39
10	F	402	FAD	C4A-N9A	-2.15	1.33	1.37
10	I	402	FAD	C4A-N9A	-2.13	1.33	1.37
10	L	402	FAD	P-O3P	2.09	1.61	1.59
12	J	504	EPE	O3S-S	2.07	1.55	1.47
10	B	402	FAD	C4X-N5	2.04	1.35	1.30
10	L	402	FAD	C4A-N9A	-2.04	1.33	1.37
10	F	402	FAD	C2-N3	-2.03	1.34	1.39
10	I	402	FAD	C5A-N7A	-2.02	1.35	1.39

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	402	FAD	C5A-C4A-N3A	-5.73	118.83	126.72
10	L	402	FAD	C5A-C4A-N3A	-5.66	118.92	126.72
10	F	402	FAD	C5A-C4A-N3A	-5.35	119.35	126.72
10	I	402	FAD	C5A-C4A-N3A	-5.04	119.77	126.72
10	B	402	FAD	N3A-C4A-N9A	4.59	134.97	127.17
10	L	402	FAD	N3A-C4A-N9A	4.33	134.53	127.17
10	F	402	FAD	N3A-C4A-N9A	4.27	134.43	127.17
10	I	402	FAD	N3A-C4A-N9A	4.07	134.08	127.17
12	G	503	EPE	C5-N4-C3	3.80	117.03	108.84
10	F	402	FAD	C4A-C5A-N7A	-3.79	106.24	110.58
10	B	402	FAD	C2A-N3A-C4A	3.71	120.89	111.83
10	L	402	FAD	C4A-C5A-N7A	-3.69	106.36	110.58
10	F	402	FAD	C2A-N3A-C4A	3.67	120.79	111.83
10	F	402	FAD	C4A-N9A-C8A	3.64	109.56	105.74
10	L	402	FAD	C2A-N3A-C4A	3.63	120.69	111.83
10	I	402	FAD	C2A-N3A-C4A	3.52	120.44	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	402	FAD	C4A-C5A-N7A	-3.38	106.72	110.58
10	F	402	FAD	N3A-C2A-N1A	-3.35	123.51	128.58
10	B	402	FAD	C4A-C5A-N7A	-3.33	106.77	110.58
10	I	402	FAD	N3A-C2A-N1A	-3.33	123.55	128.58
10	B	402	FAD	N3A-C2A-N1A	-3.30	123.59	128.58
10	L	402	FAD	N3A-C2A-N1A	-3.03	124.00	128.58
10	I	402	FAD	C4A-N9A-C8A	3.02	108.91	105.74
10	I	402	FAD	C4-C4X-N5	3.01	122.36	118.21
12	G	503	EPE	C7-N4-C3	2.92	119.03	111.24
10	B	402	FAD	C4A-N9A-C8A	2.88	108.76	105.74
12	G	503	EPE	C7-N4-C5	2.84	118.80	111.24
10	B	402	FAD	O2A-PA-O3P	2.81	114.86	107.27
10	L	402	FAD	C4-C4X-N5	2.76	122.02	118.21
12	G	503	EPE	C6-N1-C2	2.76	114.78	108.84
10	L	402	FAD	C4A-N9A-C8A	2.75	108.62	105.74
12	G	503	EPE	O1S-S-C10	2.74	110.87	106.73
10	F	402	FAD	C5A-N7A-C8A	2.71	107.70	103.45
10	L	402	FAD	C5'-C4'-C3'	-2.69	107.14	112.22
10	B	402	FAD	C4-C4X-N5	2.67	121.90	118.21
10	F	402	FAD	C6A-C5A-N7A	2.60	137.11	132.09
10	F	402	FAD	N9A-C8A-N7A	-2.59	110.27	113.94
10	I	402	FAD	O2-C2-N1	-2.57	117.53	121.80
10	F	402	FAD	C4-C4X-N5	2.55	121.73	118.21
10	B	402	FAD	C5A-N7A-C8A	2.54	107.44	103.45
10	L	402	FAD	C5A-N7A-C8A	2.53	107.43	103.45
10	B	402	FAD	O4-C4-C4X	-2.52	119.87	126.53
10	I	402	FAD	O4-C4-C4X	-2.51	119.90	126.53
10	I	402	FAD	C6A-C5A-N7A	2.48	136.88	132.09
10	I	402	FAD	C5A-N7A-C8A	2.45	107.30	103.45
10	I	402	FAD	O2A-PA-O3P	2.42	113.82	107.27
10	L	402	FAD	C6A-C5A-N7A	2.34	136.60	132.09
10	B	402	FAD	C4X-C10-N1	-2.26	119.06	124.59
10	F	402	FAD	C4X-C10-N1	-2.25	119.06	124.59
10	I	402	FAD	C5'-C4'-C3'	-2.25	107.97	112.22
10	I	402	FAD	C4X-C10-N10	2.21	119.65	116.48
10	B	402	FAD	N9A-C8A-N7A	-2.19	110.83	113.94
10	L	402	FAD	O4-C4-C4X	-2.18	120.78	126.53
10	B	402	FAD	C4X-C10-N10	2.17	119.59	116.48
10	B	402	FAD	O2-C2-N1	-2.14	118.24	121.80
10	L	402	FAD	O2-C2-N1	-2.12	118.28	121.80
10	I	402	FAD	N9A-C8A-N7A	-2.12	110.93	113.94
10	L	402	FAD	O2A-PA-O3P	2.11	112.98	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	402	FAD	C2A-N1A-C6A	2.11	122.19	118.73
10	F	402	FAD	O4-C4-C4X	-2.11	120.98	126.53
10	L	402	FAD	C4X-C10-N10	2.10	119.49	116.48
10	B	402	FAD	C6A-C5A-N7A	2.07	136.08	132.09
10	L	402	FAD	C9A-C5X-N5	-2.07	120.26	122.45
12	J	504	EPE	O3S-S-C10	-2.06	101.97	106.00
10	L	402	FAD	C4X-C10-N1	-2.04	119.58	124.59
10	B	402	FAD	C10-N1-C2	2.04	121.26	116.85
10	L	402	FAD	N9A-C8A-N7A	-2.04	111.05	113.94
10	B	402	FAD	C3B-C2B-C1B	2.00	105.25	101.46

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	506	GOL	O1-C1-C2-C3
7	A	506	GOL	C1-C2-C3-O3
7	A	507	GOL	O1-C1-C2-C3
7	B	404	GOL	C1-C2-C3-O3
7	C	305	GOL	O1-C1-C2-C3
7	D	505	GOL	C1-C2-C3-O3
7	D	507	GOL	O1-C1-C2-O2
7	D	507	GOL	O1-C1-C2-C3
7	D	509	GOL	C1-C2-C3-O3
7	D	510	GOL	C1-C2-C3-O3
7	E	305	GOL	O1-C1-C2-O2
7	E	305	GOL	O1-C1-C2-C3
7	E	305	GOL	C1-C2-C3-O3
7	E	307	GOL	C1-C2-C3-O3
7	E	307	GOL	O2-C2-C3-O3
7	F	406	GOL	O1-C1-C2-C3
7	H	304	GOL	O1-C1-C2-C3
7	H	307	GOL	C1-C2-C3-O3
7	I	403	GOL	O1-C1-C2-C3
7	I	404	GOL	O1-C1-C2-C3
7	I	404	GOL	C1-C2-C3-O3
7	I	404	GOL	O2-C2-C3-O3
7	I	405	GOL	O1-C1-C2-C3
7	J	506	GOL	O1-C1-C2-C3
7	J	506	GOL	C1-C2-C3-O3
7	J	508	GOL	O1-C1-C2-C3
7	K	306	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	L	404	GOL	O1-C1-C2-C3
12	J	504	EPE	C10-C9-N1-C6
12	J	504	EPE	S-C10-C9-N1
12	J	504	EPE	C8-C7-N4-C5
7	H	306	GOL	O2-C2-C3-O3
7	I	403	GOL	O2-C2-C3-O3
7	A	509	GOL	C1-C2-C3-O3
7	B	405	GOL	C1-C2-C3-O3
7	C	307	GOL	O1-C1-C2-C3
7	D	507	GOL	C1-C2-C3-O3
7	E	307	GOL	O1-C1-C2-C3
7	E	308	GOL	O1-C1-C2-C3
7	F	406	GOL	C1-C2-C3-O3
7	G	504	GOL	C1-C2-C3-O3
7	G	507	GOL	C1-C2-C3-O3
7	H	304	GOL	C1-C2-C3-O3
7	H	306	GOL	C1-C2-C3-O3
7	I	403	GOL	C1-C2-C3-O3
7	J	508	GOL	C1-C2-C3-O3
7	L	403	GOL	O1-C1-C2-C3
7	A	506	GOL	O1-C1-C2-O2
7	B	404	GOL	O2-C2-C3-O3
7	C	305	GOL	O1-C1-C2-O2
7	D	509	GOL	O2-C2-C3-O3
7	E	305	GOL	O2-C2-C3-O3
7	F	406	GOL	O2-C2-C3-O3
7	G	507	GOL	O2-C2-C3-O3
7	H	304	GOL	O2-C2-C3-O3
7	H	307	GOL	O2-C2-C3-O3
7	I	403	GOL	O1-C1-C2-O2
7	I	404	GOL	O1-C1-C2-O2
7	J	506	GOL	O1-C1-C2-O2
7	J	506	GOL	O2-C2-C3-O3
7	J	508	GOL	O1-C1-C2-O2
7	K	306	GOL	O1-C1-C2-O2
7	L	404	GOL	O1-C1-C2-O2
7	A	507	GOL	O1-C1-C2-O2
7	A	509	GOL	O2-C2-C3-O3
7	B	405	GOL	O2-C2-C3-O3
7	C	307	GOL	O2-C2-C3-O3
7	D	505	GOL	O2-C2-C3-O3
7	D	507	GOL	O2-C2-C3-O3

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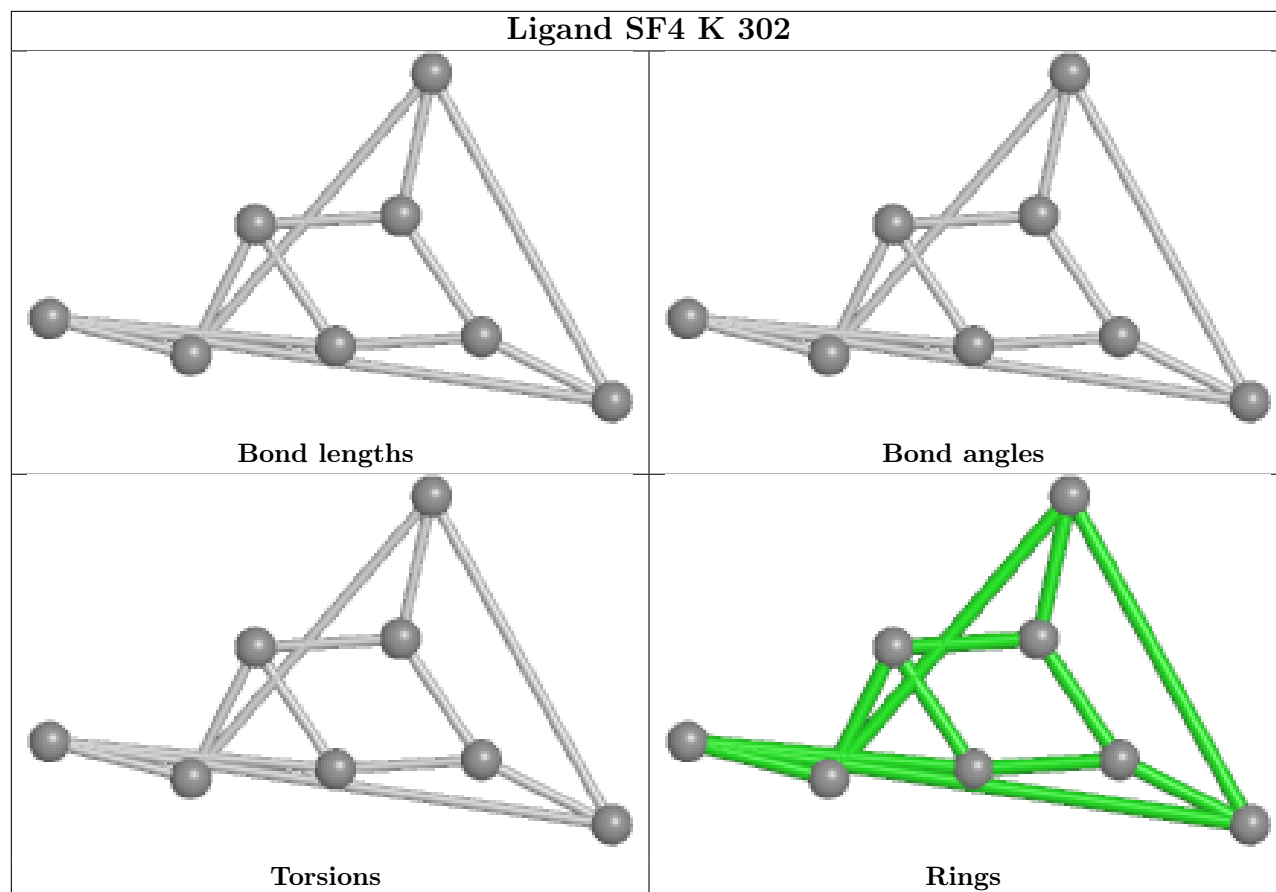
Mol	Chain	Res	Type	Atoms
7	F	406	GOL	O1-C1-C2-O2
7	H	304	GOL	O1-C1-C2-O2
7	C	307	GOL	O1-C1-C2-O2
7	D	508	GOL	O2-C2-C3-O3
7	D	510	GOL	O2-C2-C3-O3
7	E	306	GOL	O1-C1-C2-O2
7	E	307	GOL	O1-C1-C2-O2
7	G	504	GOL	O1-C1-C2-O2
7	J	505	GOL	O2-C2-C3-O3
7	A	506	GOL	O2-C2-C3-O3
7	F	405	GOL	O1-C1-C2-O2
7	G	504	GOL	O2-C2-C3-O3
7	J	508	GOL	O2-C2-C3-O3
7	L	403	GOL	O1-C1-C2-O2
7	L	404	GOL	O2-C2-C3-O3
12	G	503	EPE	C9-C10-S-O1S
12	G	503	EPE	C9-C10-S-O2S
7	C	307	GOL	C1-C2-C3-O3
7	D	509	GOL	O1-C1-C2-C3
7	K	305	GOL	C1-C2-C3-O3
10	L	402	FAD	P-O3P-PA-O2A
12	G	503	EPE	C9-C10-S-O3S
7	B	405	GOL	O1-C1-C2-O2
12	J	504	EPE	C10-C9-N1-C2
7	G	504	GOL	O1-C1-C2-C3
7	J	509	GOL	O1-C1-C2-C3
12	J	504	EPE	N4-C7-C8-O8
7	E	308	GOL	O1-C1-C2-O2
7	I	405	GOL	O1-C1-C2-O2
10	F	402	FAD	P-O3P-PA-O2A
7	C	306	GOL	O2-C2-C3-O3
7	E	306	GOL	O1-C1-C2-C3
7	A	507	GOL	O2-C2-C3-O3
10	F	402	FAD	P-O3P-PA-O1A
10	I	402	FAD	PA-O3P-P-O2P
10	L	402	FAD	P-O3P-PA-O1A
7	D	509	GOL	O1-C1-C2-O2
10	F	402	FAD	O4B-C4B-C5B-O5B
10	I	402	FAD	O4B-C4B-C5B-O5B

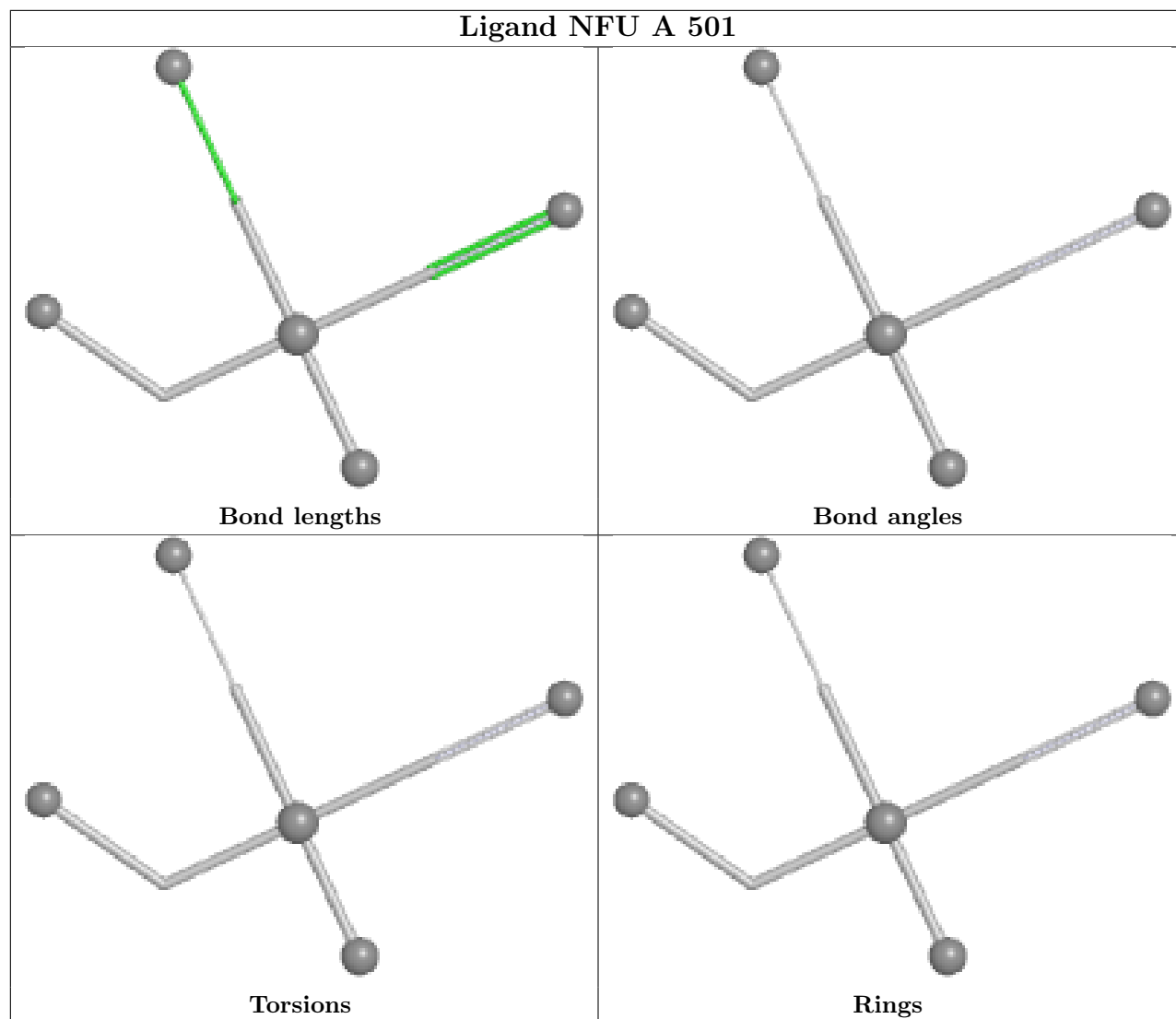
There are no ring outliers.

17 monomers are involved in 24 short contacts:

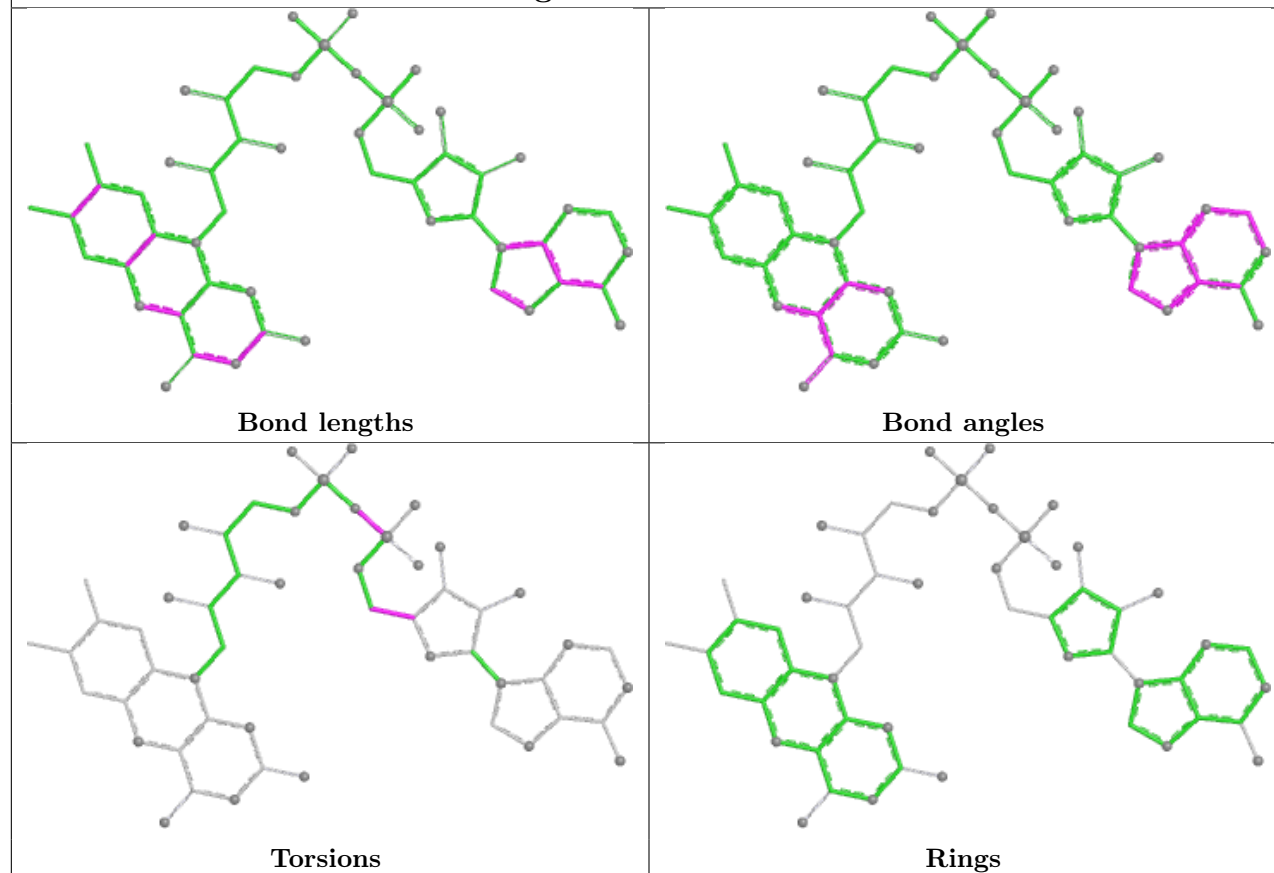
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	506	GOL	1	0
7	H	306	GOL	1	0
4	A	501	NFU	1	0
4	G	501	NFU	2	0
4	J	501	NFU	1	0
9	L	401	SF4	1	0
9	F	401	SF4	1	0
7	C	305	GOL	1	0
10	B	402	FAD	1	0
4	D	501	NFU	1	0
12	G	503	EPE	2	0
9	B	401	SF4	2	0
7	C	304	GOL	1	0
10	I	402	FAD	2	0
9	I	401	SF4	1	0
12	J	504	EPE	3	0
10	L	402	FAD	2	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.

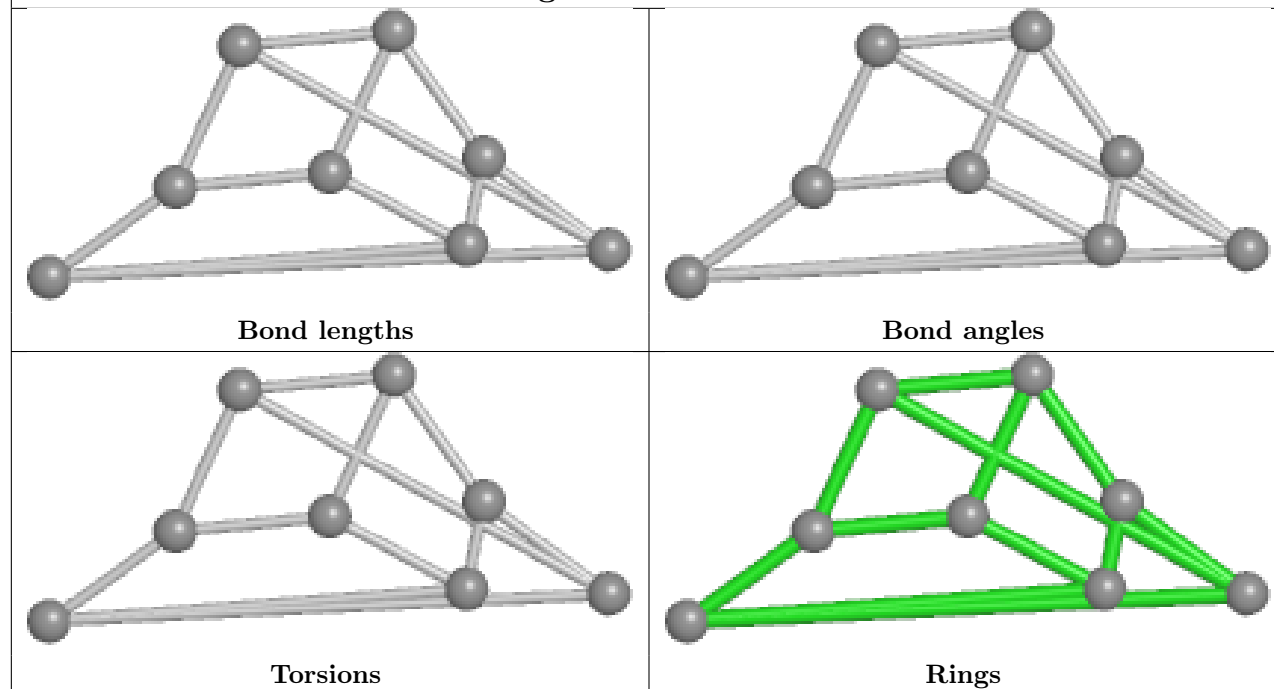


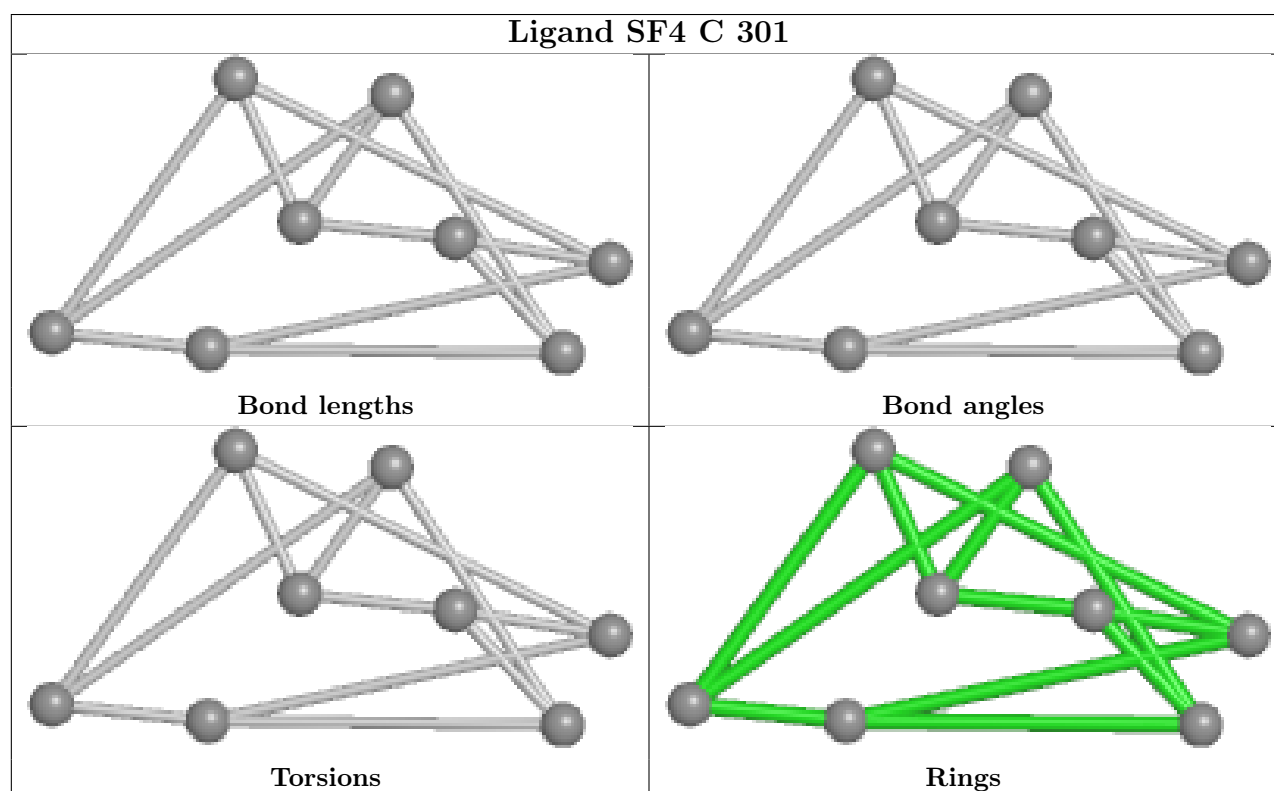
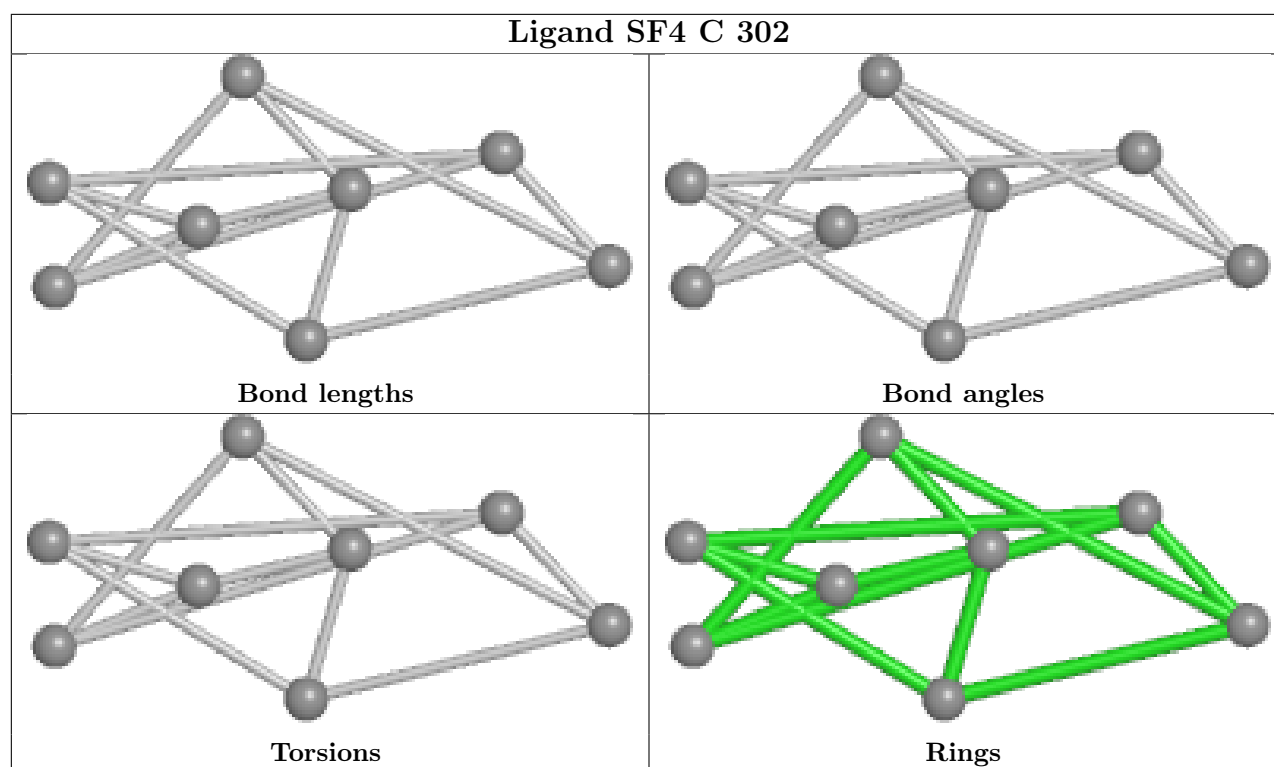


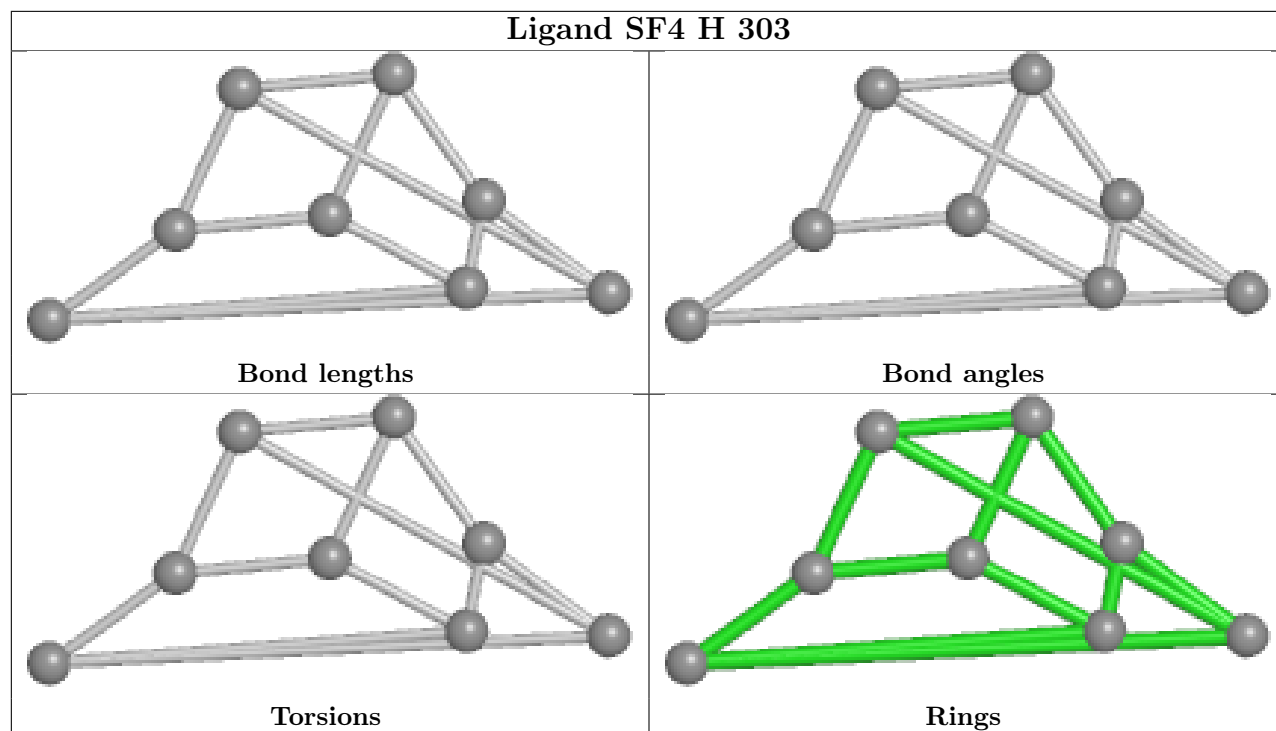
Ligand FAD F 402

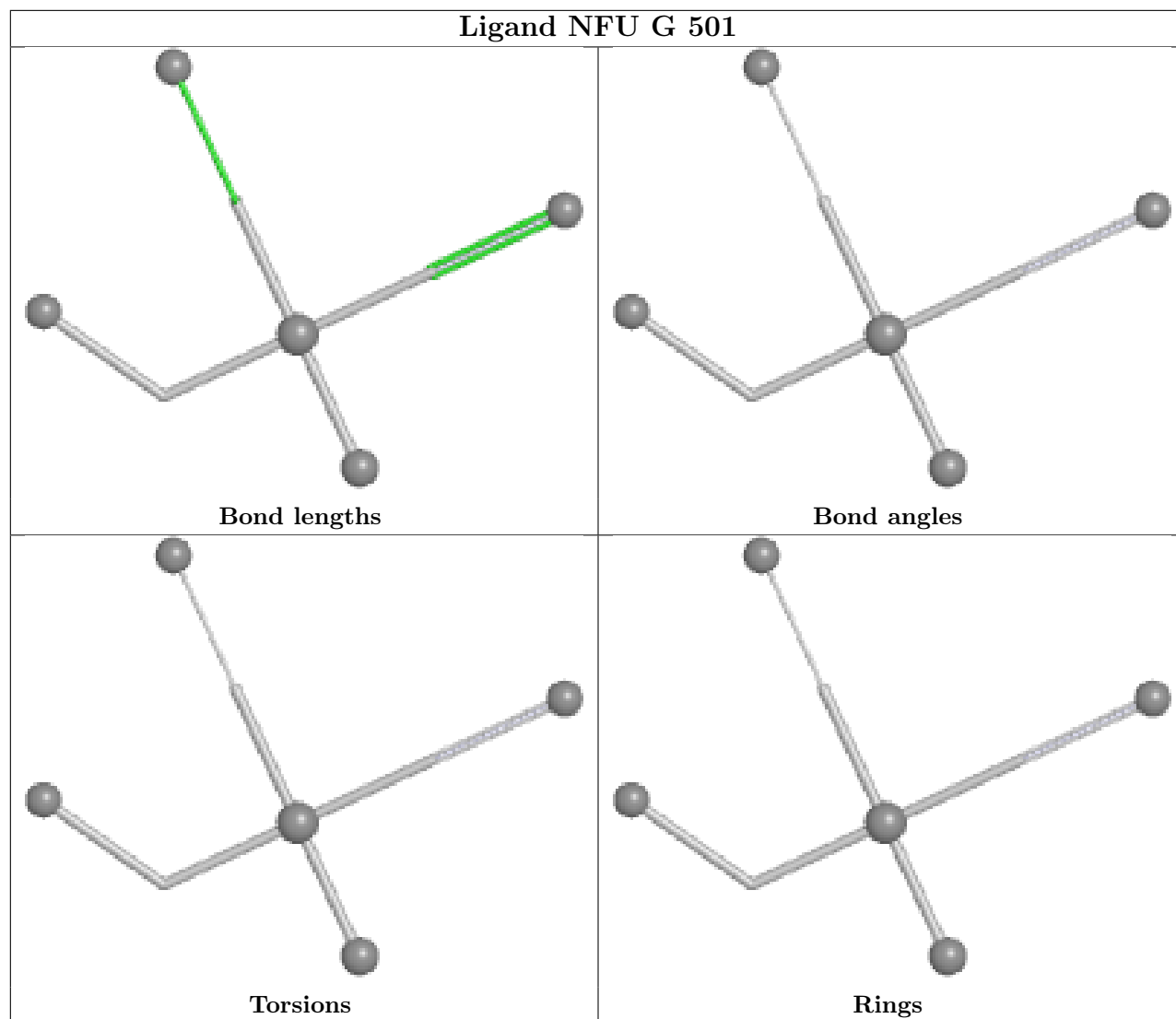


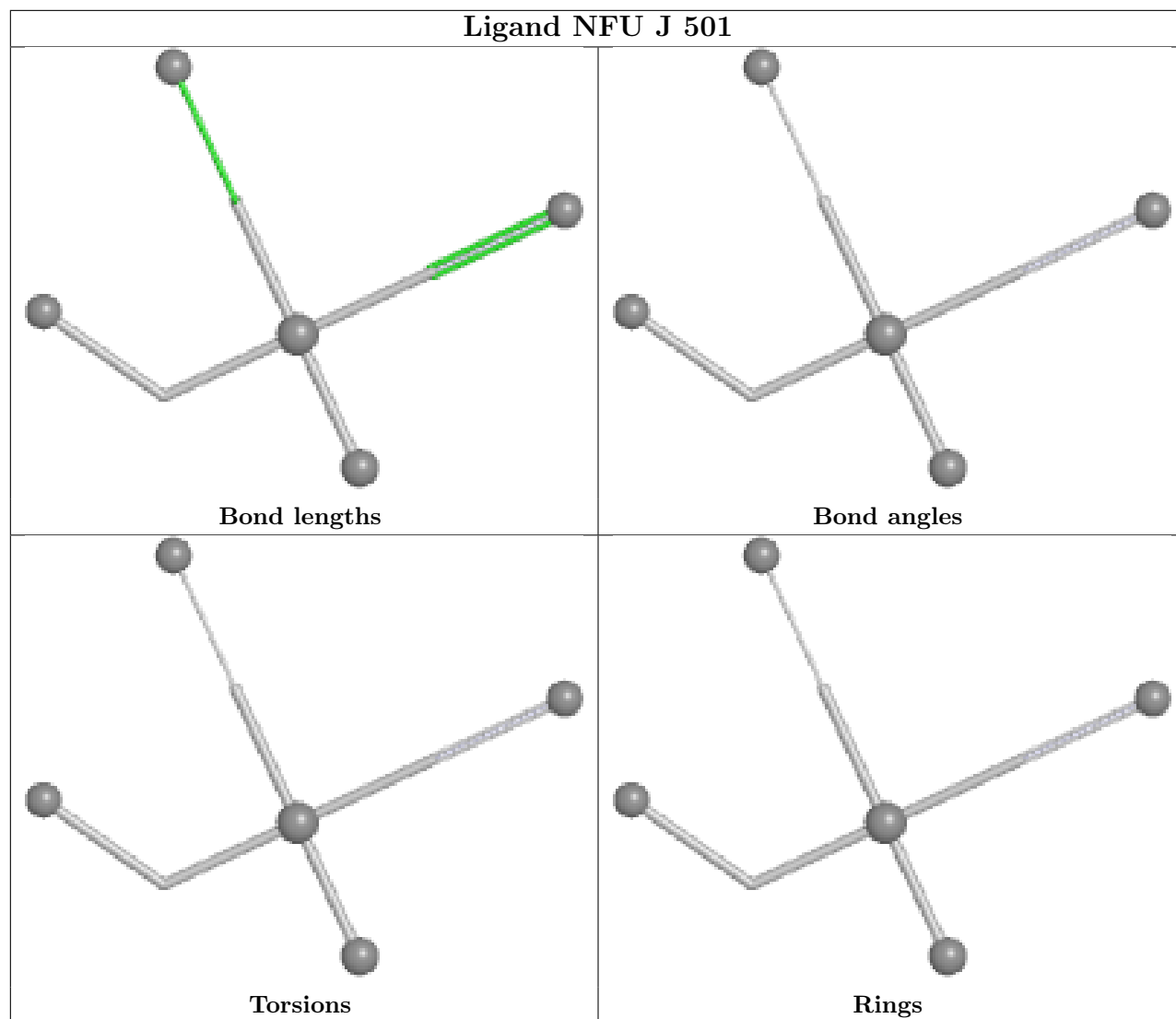
Ligand SF4 H 301



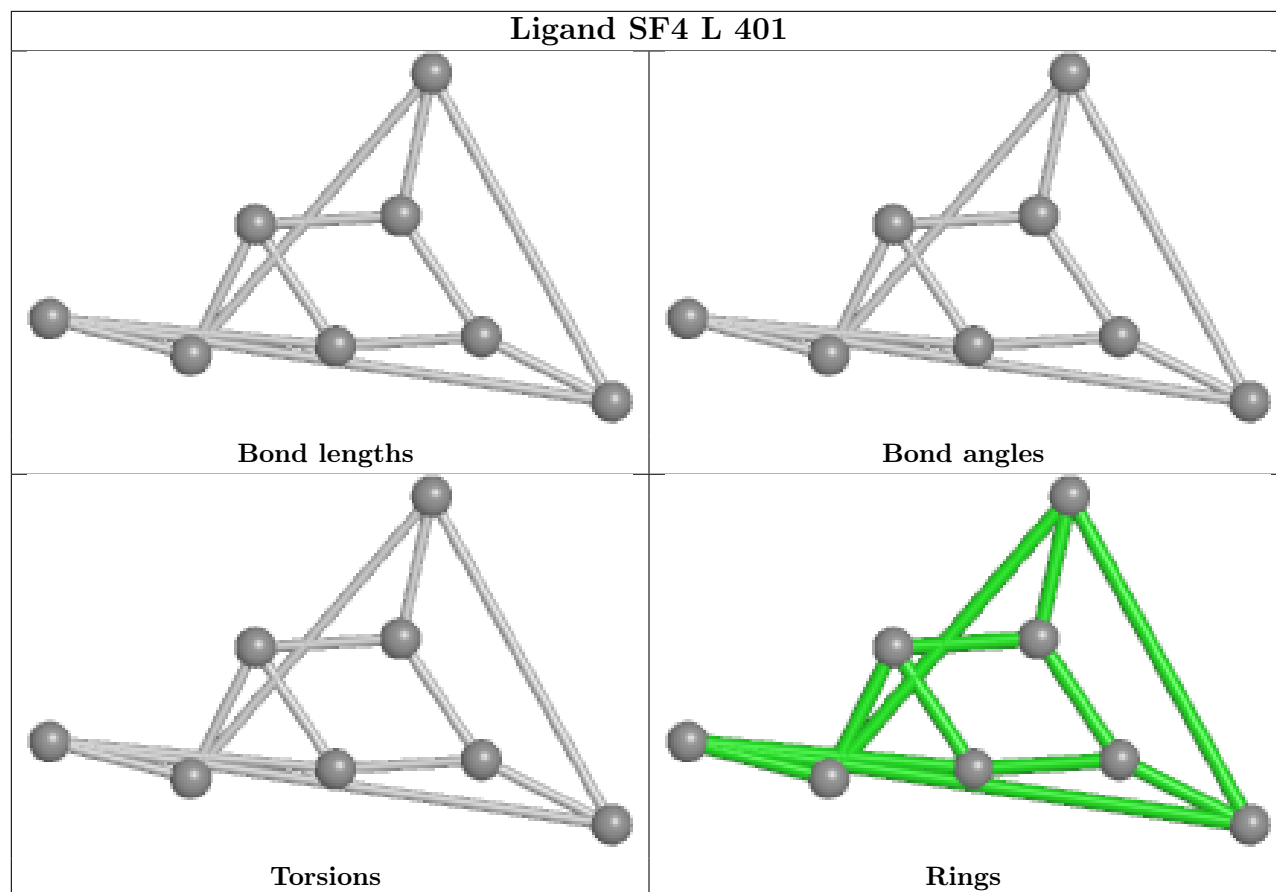




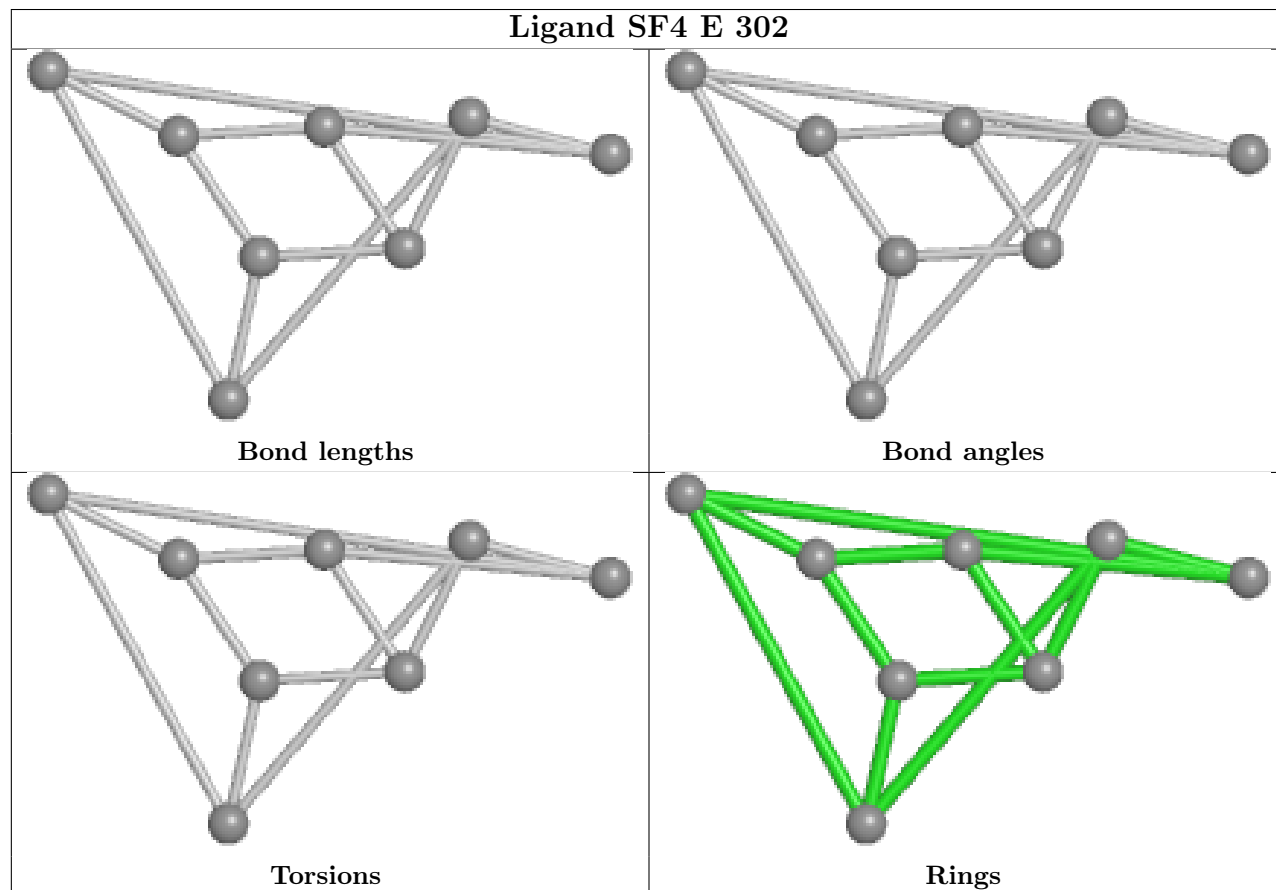




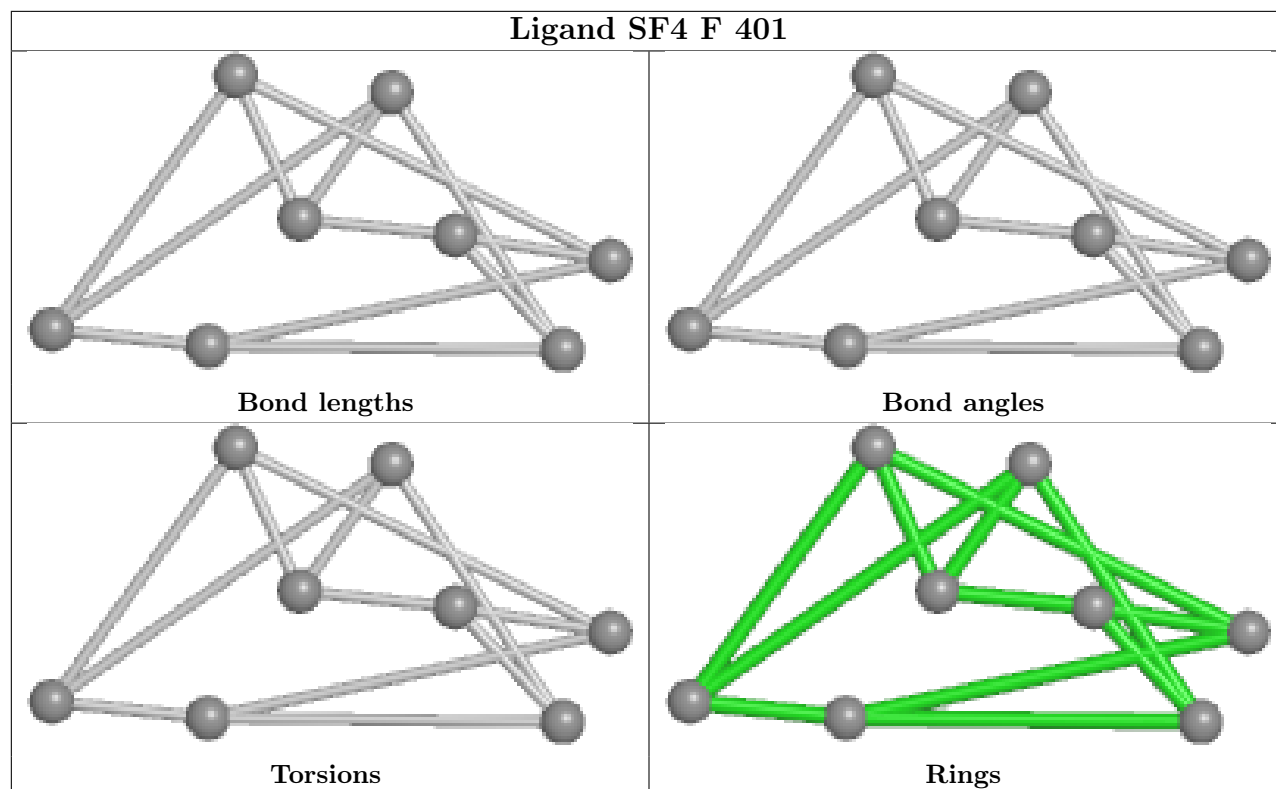
Ligand SF4 L 401



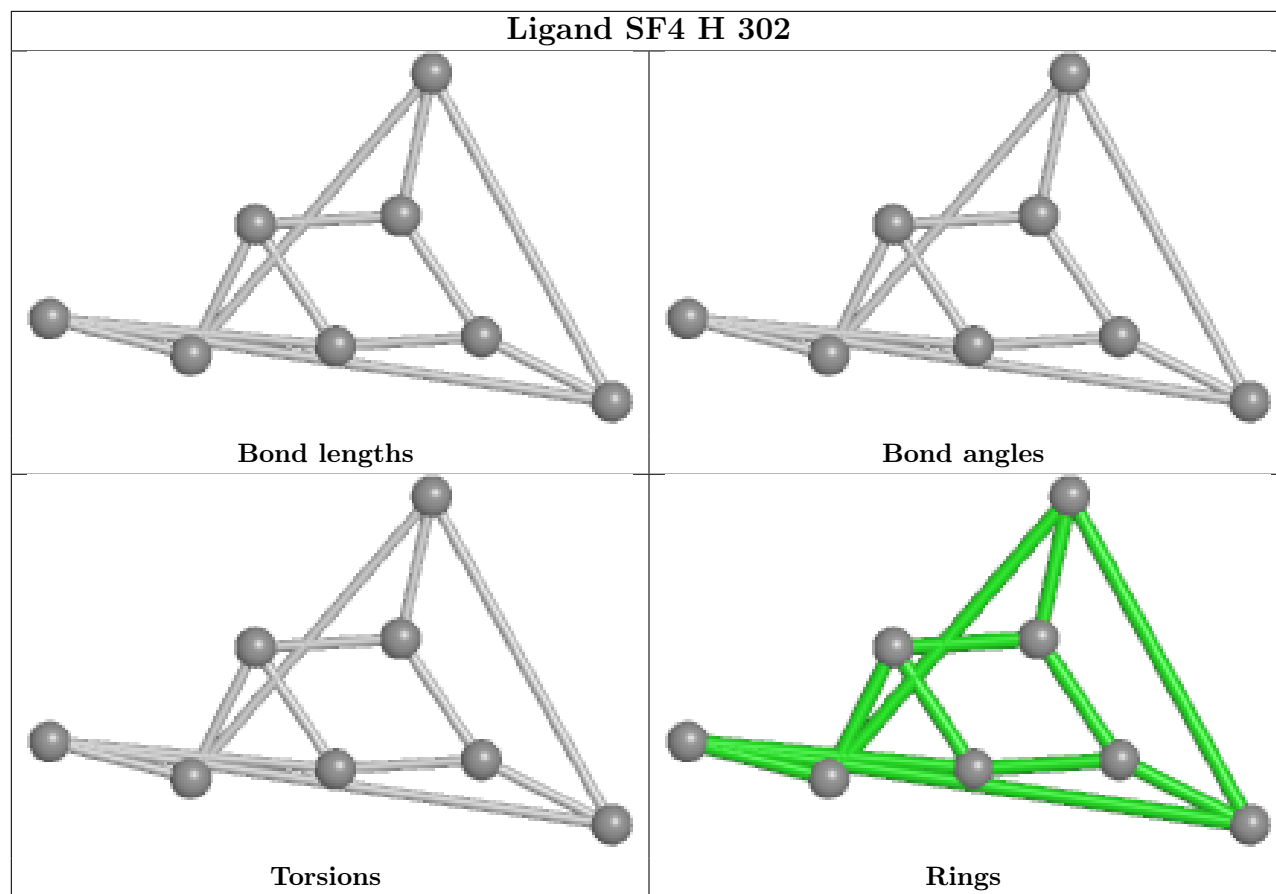
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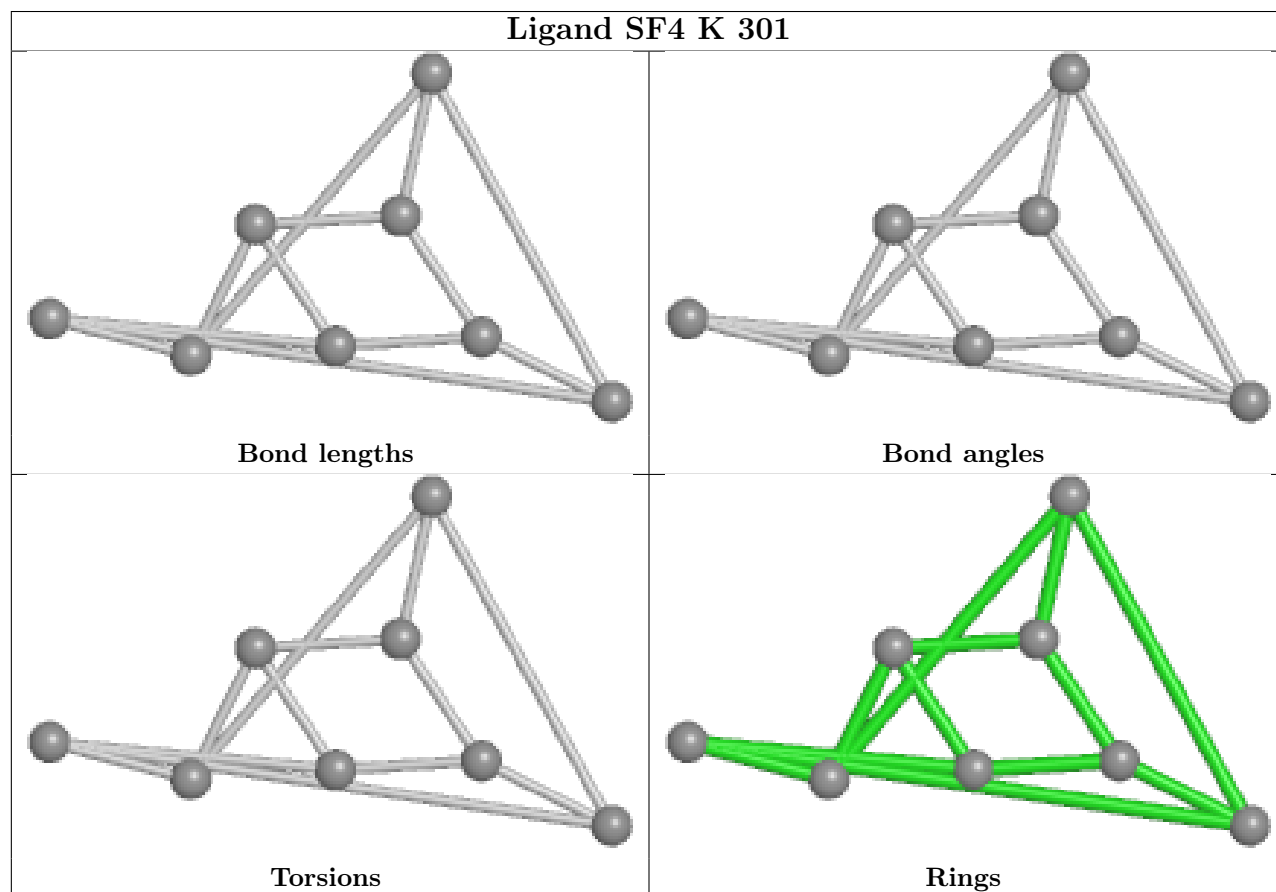
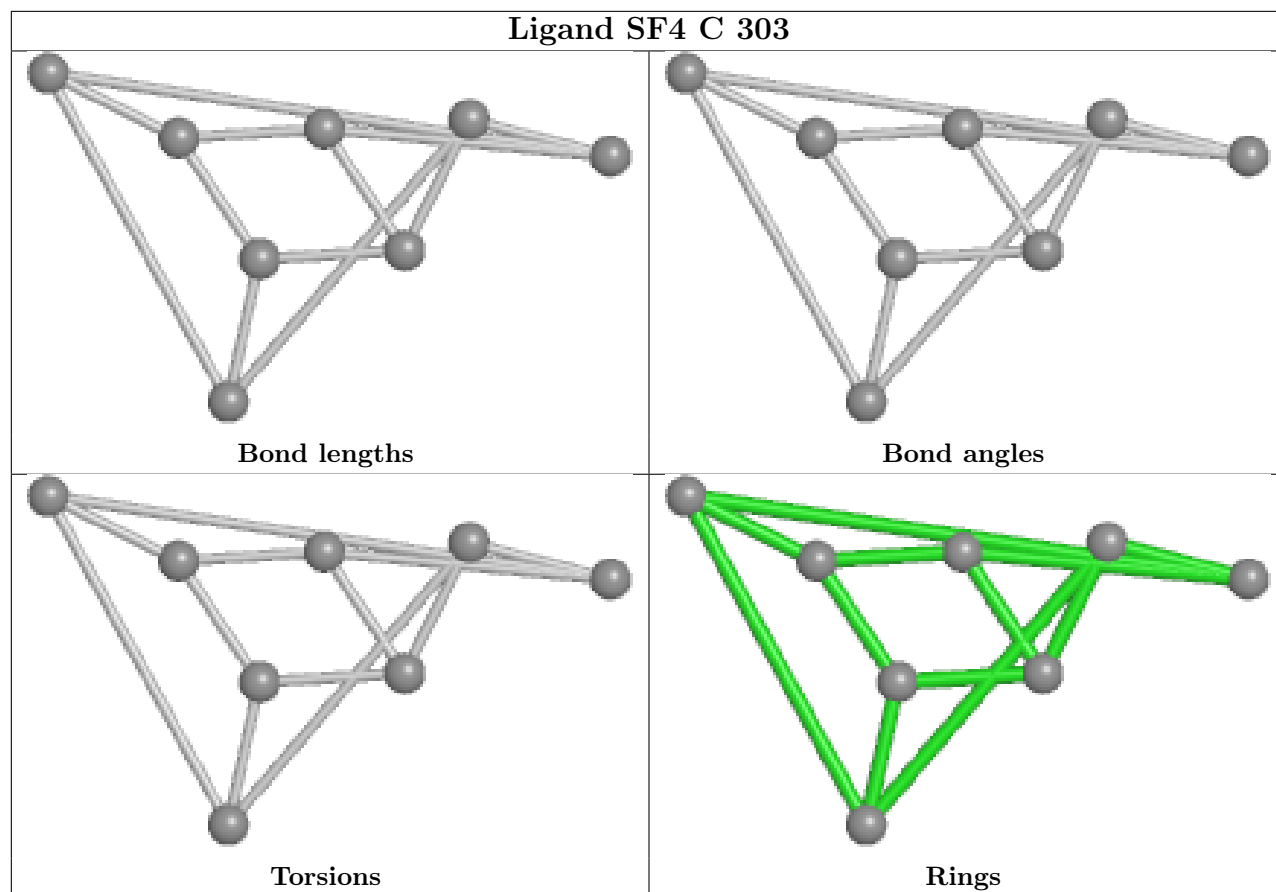


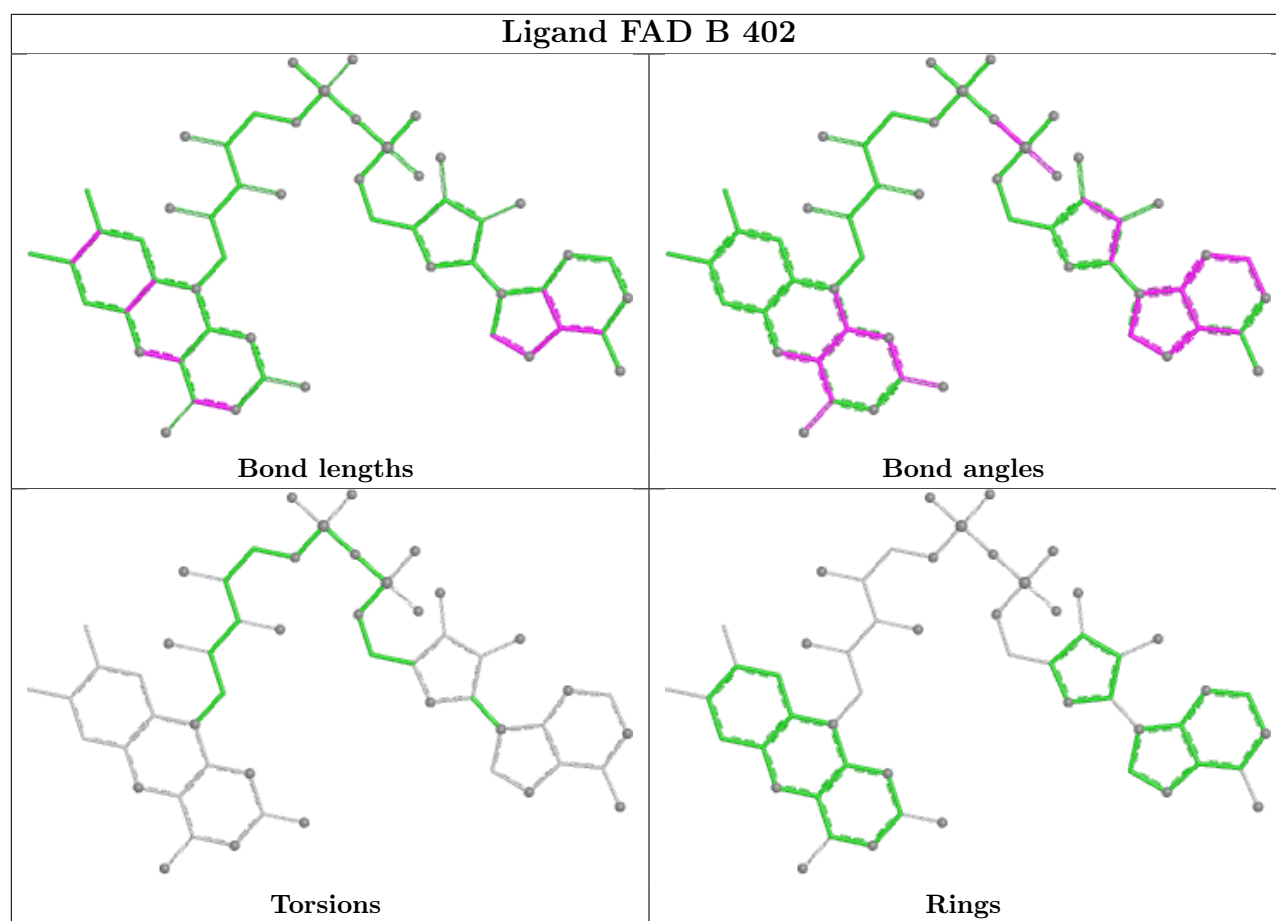
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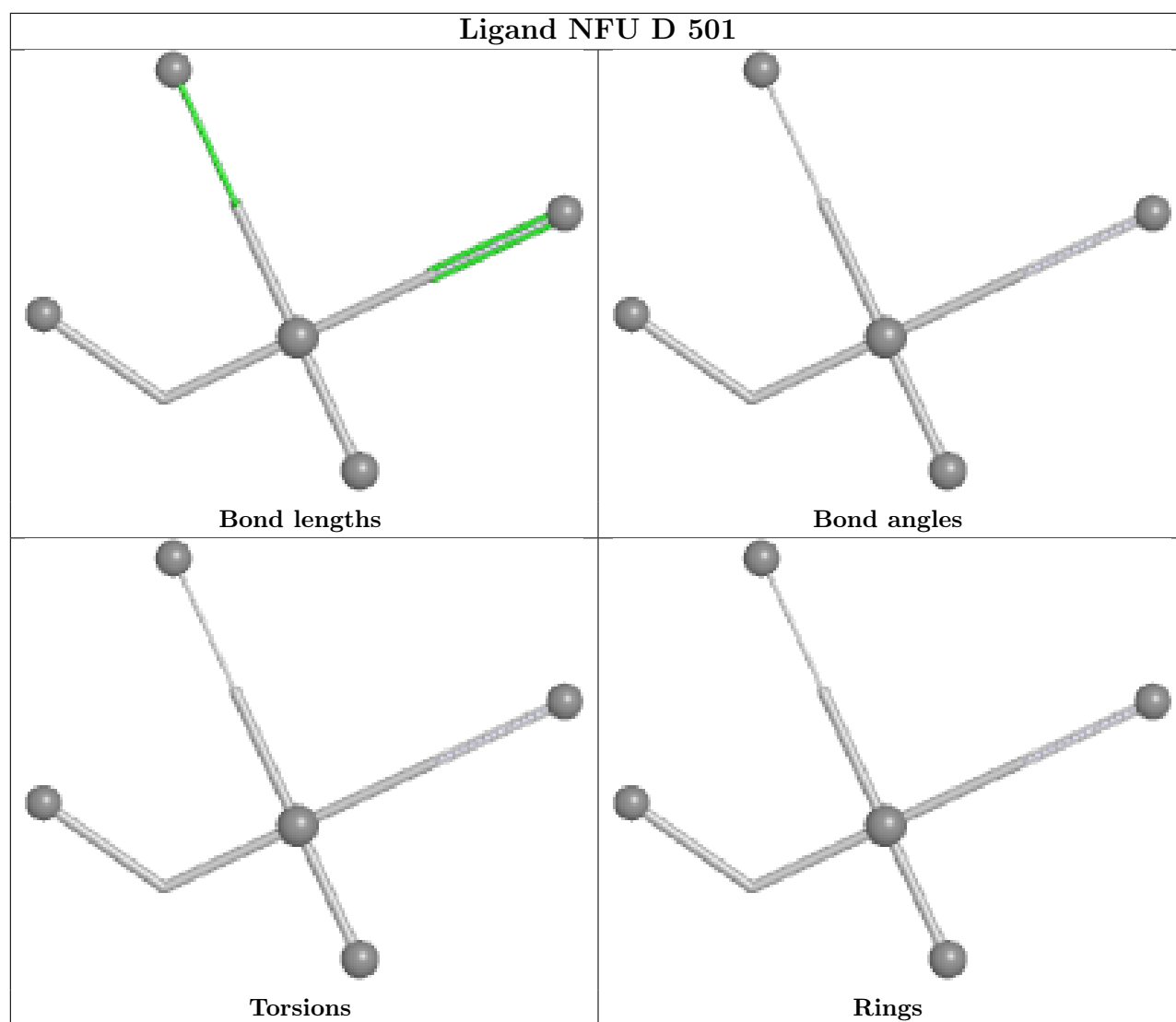


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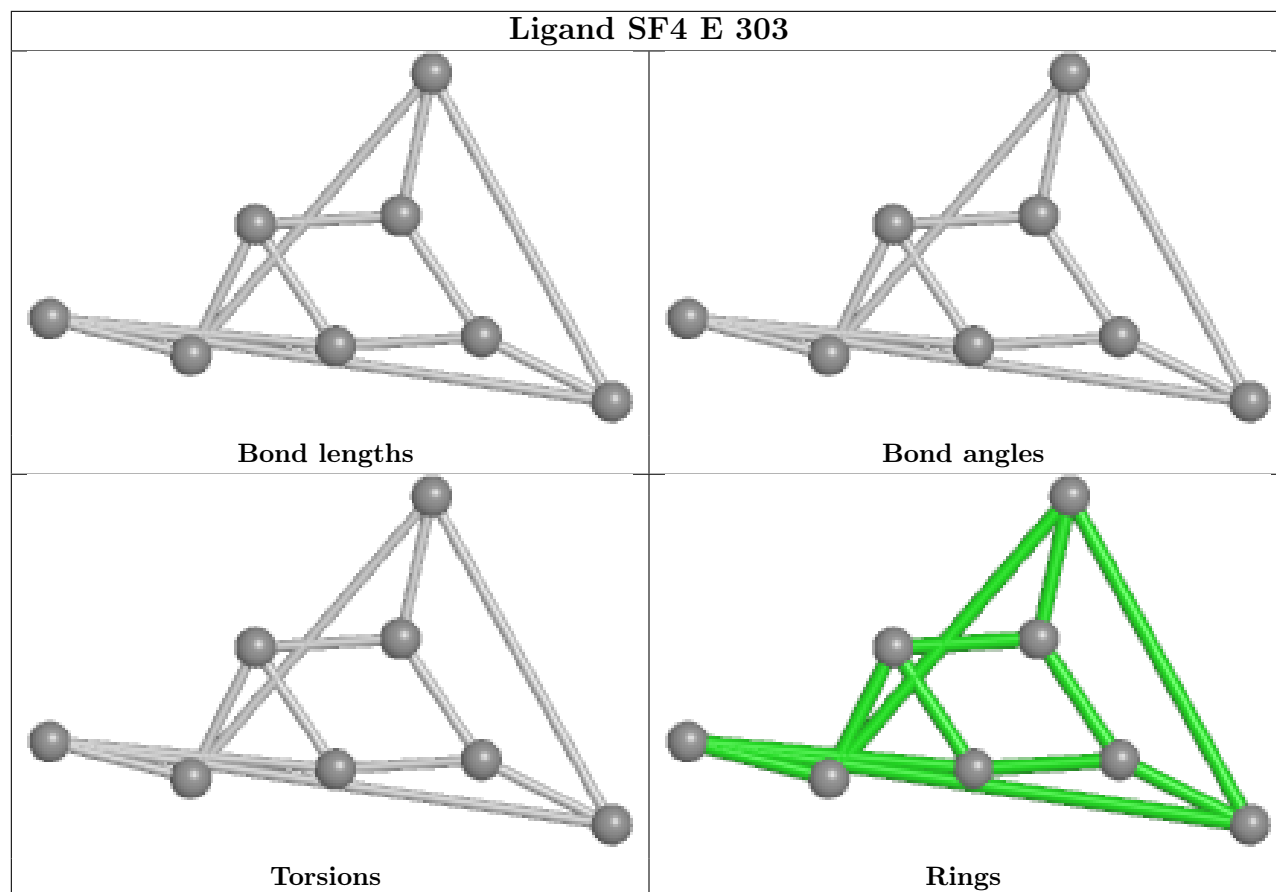




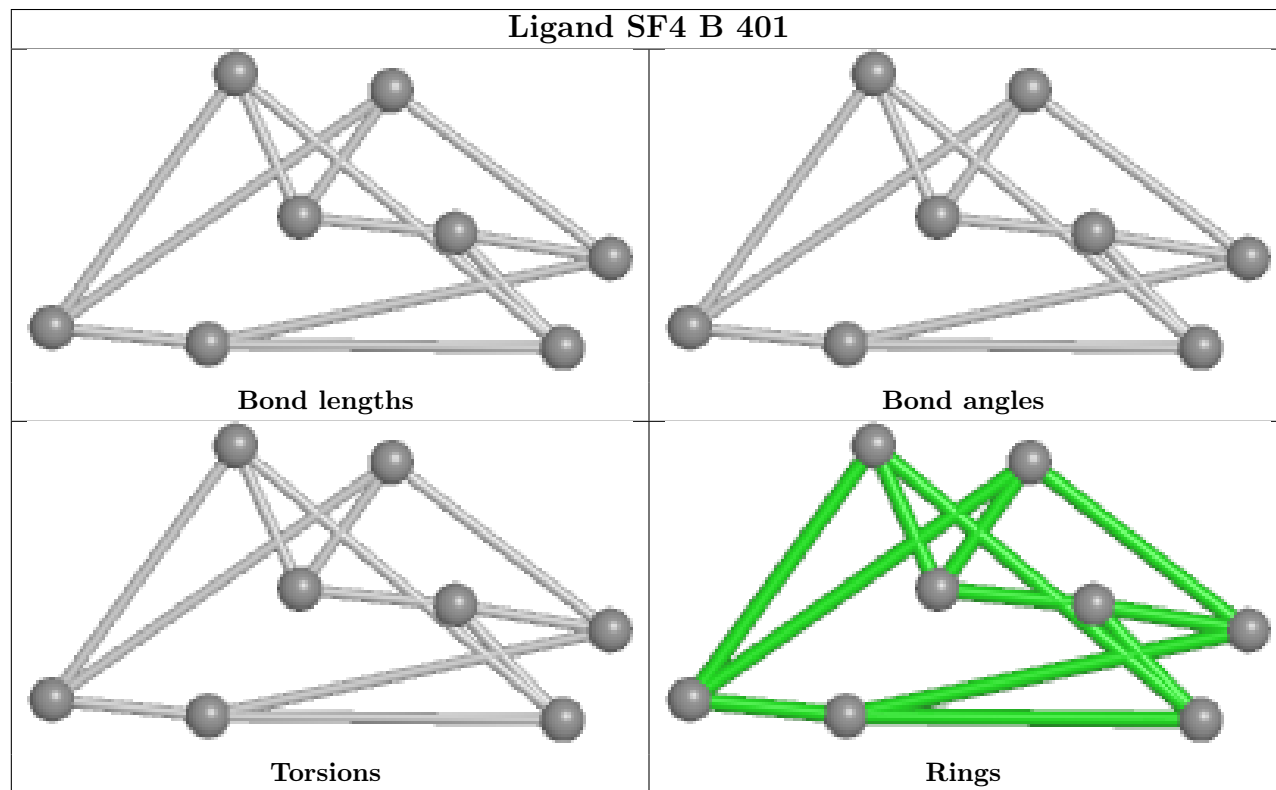


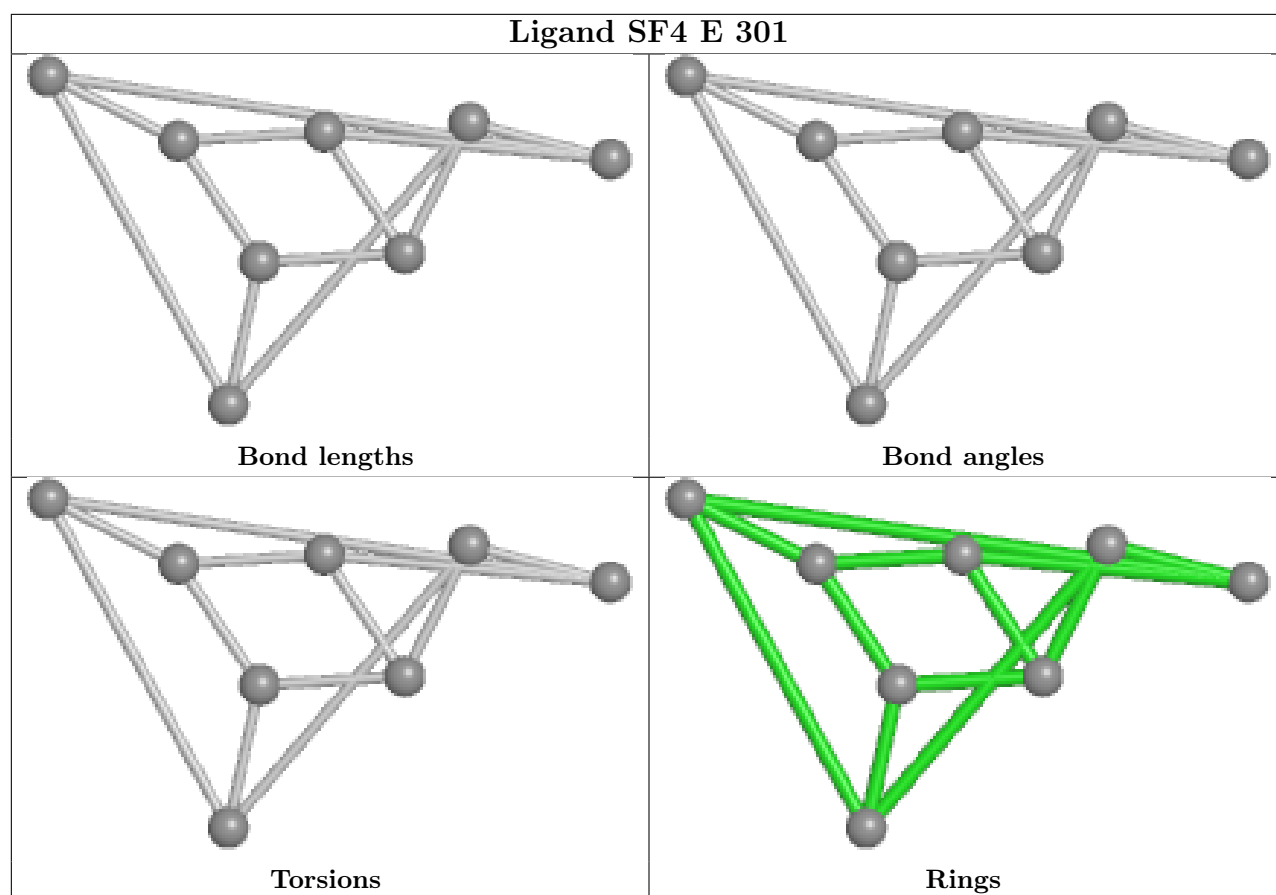


Ligand SF4 E 303

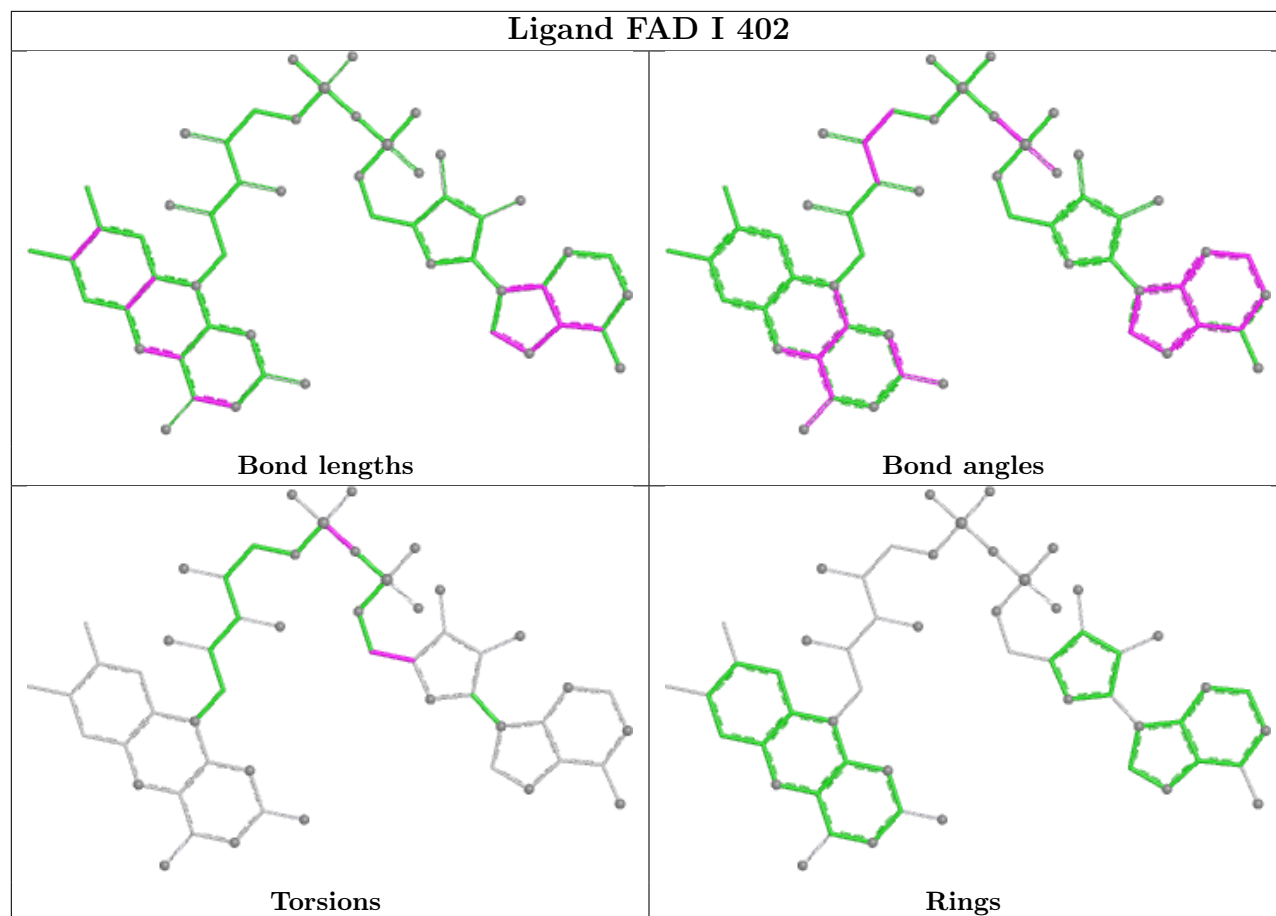


Ligand SF4 B 401

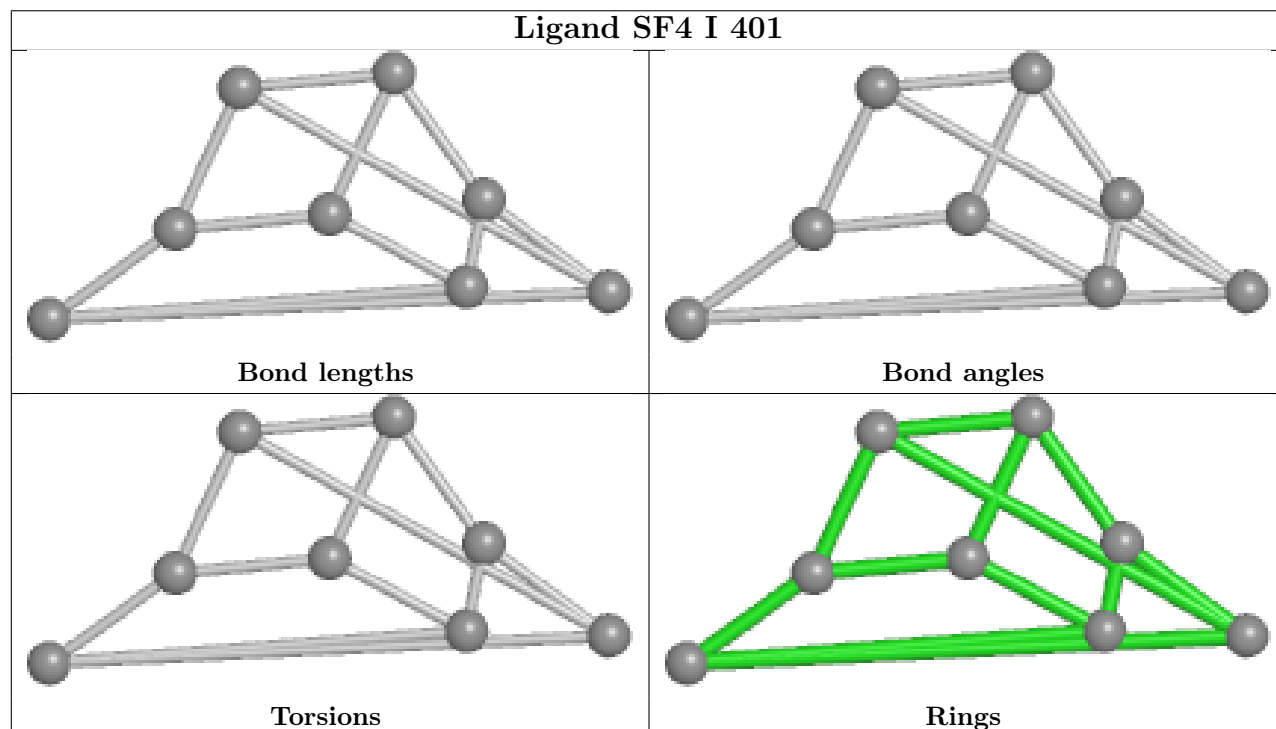




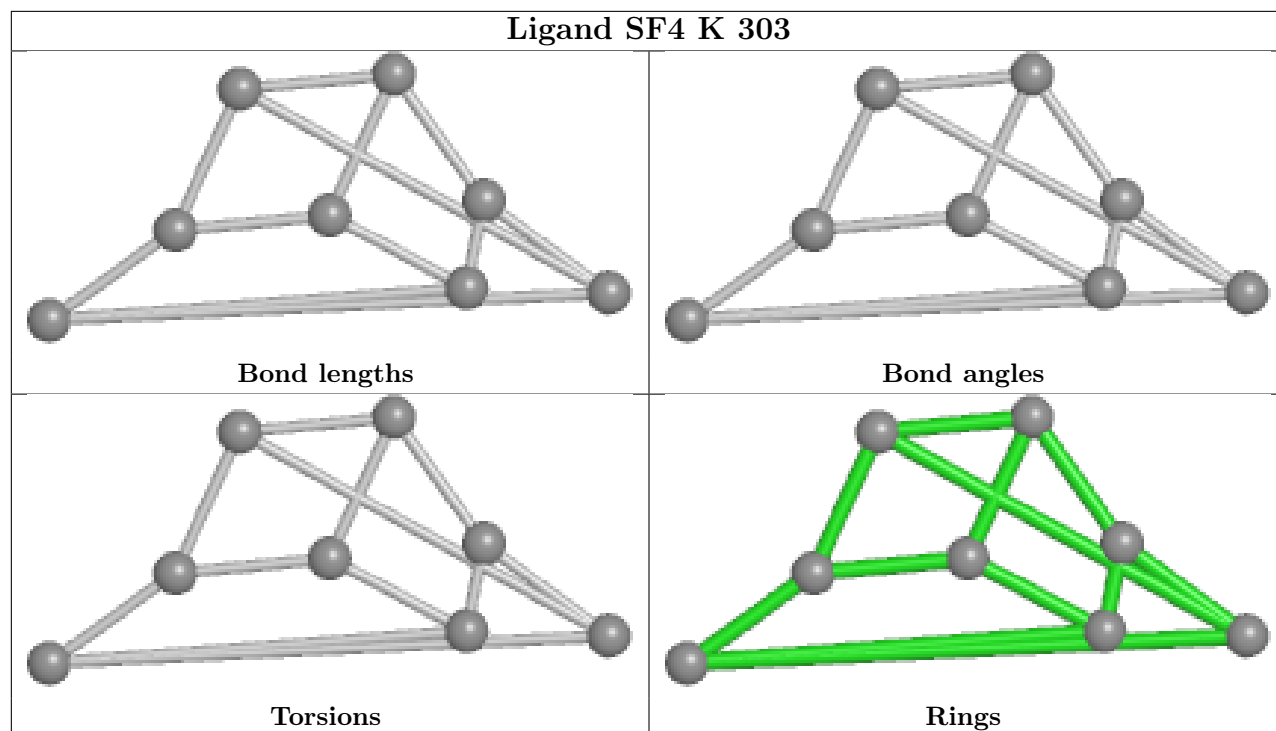
Ligand FAD I 402



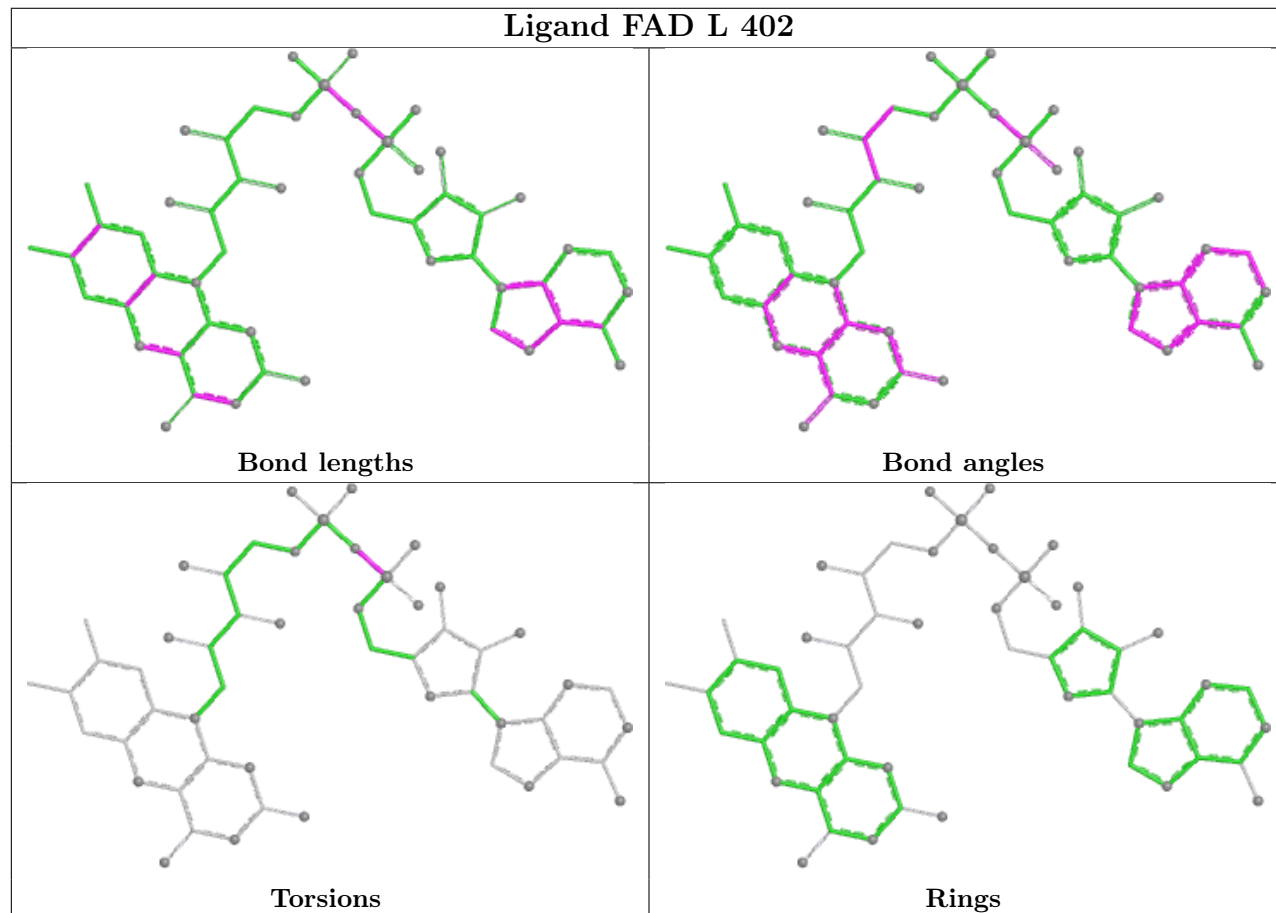
Ligand SF4 I 401



Ligand SF4 K 303



Ligand FAD L 402



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	392/410 (95%)	-0.39	2 (0%) 87 87	36, 47, 70, 84	0
1	D	392/410 (95%)	-0.47	1 (0%) 90 90	33, 44, 67, 83	0
1	G	392/410 (95%)	-0.35	1 (0%) 90 90	39, 51, 76, 93	0
1	J	392/410 (95%)	-0.31	3 (0%) 82 83	38, 51, 77, 93	0
2	B	282/282 (100%)	-0.19	0 100 100	38, 56, 75, 98	0
2	F	282/282 (100%)	-0.26	1 (0%) 88 89	35, 53, 76, 96	0
2	I	282/282 (100%)	-0.14	1 (0%) 88 89	42, 59, 82, 104	0
2	L	282/282 (100%)	-0.10	1 (0%) 88 89	40, 60, 82, 112	0
3	C	240/241 (99%)	-0.28	2 (0%) 82 83	36, 48, 76, 101	0
3	E	240/241 (99%)	-0.31	1 (0%) 88 89	35, 45, 69, 95	1 (0%)
3	H	240/241 (99%)	-0.20	1 (0%) 88 89	38, 54, 80, 117	0
3	K	240/241 (99%)	-0.13	3 (1%) 75 76	40, 51, 78, 115	1 (0%)
All	All	3656/3732 (97%)	-0.28	17 (0%) 87 87	33, 51, 77, 117	2 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	241	GLU	3.9
3	H	241	GLU	3.9
1	J	2	GLY	3.5
3	K	241	GLU	3.5
1	A	2	GLY	2.8
1	D	2	GLY	2.7
1	G	2	GLY	2.6
3	K	25[A]	GLN	2.5
3	C	53	ASP	2.5
2	I	268	LYS	2.4
3	E	235	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	120	LYS	2.2
1	J	183	LYS	2.2
2	F	249	LYS	2.2
2	L	18	LYS	2.2
1	A	22	LYS	2.1
3	K	235	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
7	GOL	L	403	6/6	0.57	0.24	90,94,98,100	0
7	GOL	H	307	6/6	0.64	0.28	74,86,90,92	0
7	GOL	K	305	6/6	0.70	0.32	76,79,81,85	0
7	GOL	E	308	6/6	0.70	0.23	79,83,91,98	0
7	GOL	L	404	6/6	0.72	0.27	78,83,90,90	0
7	GOL	D	510	6/6	0.73	0.23	44,59,69,74	0
7	GOL	B	405	6/6	0.73	0.23	78,87,90,90	0
7	GOL	C	304	6/6	0.73	0.23	72,81,91,101	0
6	SO4	F	404	5/5	0.74	0.11	116,123,140,143	0
7	GOL	A	510	6/6	0.74	0.22	77,92,97,98	0
7	GOL	C	306	6/6	0.75	0.23	77,80,91,92	0
7	GOL	I	404	6/6	0.76	0.26	63,73,84,99	0
7	GOL	I	403	6/6	0.78	0.20	79,87,97,98	0
7	GOL	E	306	6/6	0.79	0.21	51,61,70,80	0
12	EPE	J	504	15/15	0.79	0.20	41,73,88,114	0
6	SO4	F	403	5/5	0.80	0.11	93,100,115,124	0
7	GOL	K	306	6/6	0.82	0.17	80,85,98,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	G	506	6/6	0.82	0.18	65,70,82,84	0
7	GOL	H	304	6/6	0.82	0.17	72,76,79,86	0
7	GOL	A	506	6/6	0.82	0.20	72,76,82,99	0
7	GOL	I	405	6/6	0.83	0.20	66,68,78,79	0
6	SO4	D	503	5/5	0.83	0.13	84,99,120,128	0
7	GOL	C	307	6/6	0.83	0.20	62,64,82,93	0
7	GOL	F	406	6/6	0.84	0.17	78,86,95,100	0
7	GOL	D	505	6/6	0.84	0.20	57,70,74,76	0
7	GOL	E	307	6/6	0.84	0.18	62,69,75,77	0
6	SO4	E	304	5/5	0.84	0.12	110,110,118,133	0
6	SO4	J	502	5/5	0.85	0.12	81,82,101,110	0
7	GOL	G	504	6/6	0.85	0.21	62,68,72,76	0
7	GOL	J	506	6/6	0.85	0.20	69,75,83,102	0
12	EPE	G	503	15/15	0.85	0.17	47,69,121,138	0
6	SO4	G	502	5/5	0.85	0.11	76,84,105,106	0
7	GOL	G	505	6/6	0.86	0.18	48,76,84,91	0
7	GOL	J	507	6/6	0.86	0.18	64,77,84,90	0
7	GOL	H	305	6/6	0.86	0.18	65,76,79,85	0
7	GOL	D	508	6/6	0.86	0.19	75,81,92,94	0
7	GOL	A	508	6/6	0.87	0.16	73,78,81,83	0
6	SO4	A	504	5/5	0.87	0.12	87,92,109,130	0
7	GOL	K	304	6/6	0.87	0.15	62,68,77,85	0
7	GOL	G	507	6/6	0.88	0.18	73,82,84,86	0
7	GOL	D	504	6/6	0.88	0.15	63,71,72,72	0
6	SO4	A	503	5/5	0.88	0.09	72,77,106,106	0
7	GOL	F	405	6/6	0.88	0.18	66,74,79,81	0
7	GOL	C	305	6/6	0.88	0.16	60,66,78,82	0
7	GOL	D	509	6/6	0.88	0.18	41,55,78,81	0
7	GOL	B	404	6/6	0.88	0.14	67,72,80,83	0
6	SO4	D	502	5/5	0.88	0.10	62,81,94,106	0
7	GOL	E	305	6/6	0.89	0.15	59,69,73,88	0
7	GOL	D	506	6/6	0.90	0.15	55,83,86,91	0
7	GOL	D	507	6/6	0.90	0.18	65,68,78,80	0
7	GOL	J	508	6/6	0.90	0.14	64,74,82,83	0
5	NA	B	403	1/1	0.90	0.41	64,64,64,64	0
7	GOL	J	505	6/6	0.90	0.13	62,65,68,72	0
7	GOL	A	509	6/6	0.91	0.13	64,71,73,95	0
11	CL	D	512	1/1	0.91	0.14	70,70,70,70	0
7	GOL	J	509	6/6	0.92	0.19	53,67,72,94	0
6	SO4	J	503	5/5	0.92	0.12	99,109,115,170	0
7	GOL	H	306	6/6	0.92	0.12	64,65,75,78	0
7	GOL	A	505	6/6	0.93	0.15	44,65,73,75	0

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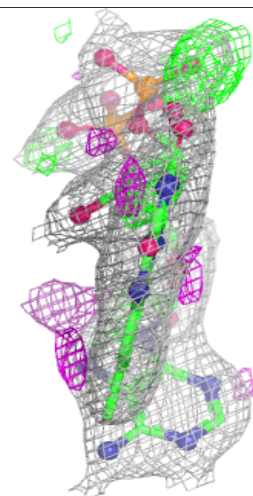
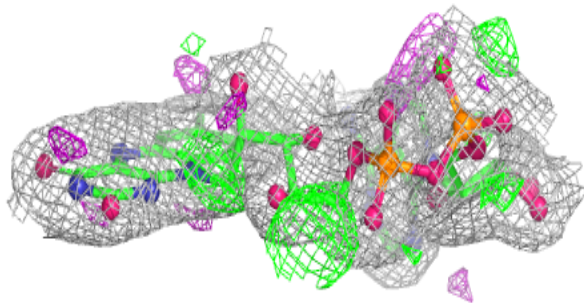
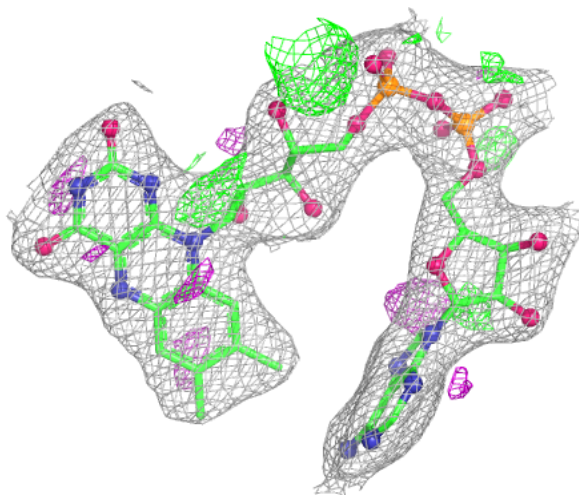
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	A	507	6/6	0.94	0.10	47,51,58,77	0
10	FAD	L	402	53/53	0.96	0.09	39,48,61,69	0
5	NA	A	502	1/1	0.97	0.15	46,46,46,46	0
10	FAD	I	402	53/53	0.97	0.08	33,47,56,66	0
4	NFU	G	501	8/8	0.98	0.11	28,43,54,62	0
4	NFU	J	501	8/8	0.98	0.12	31,40,60,73	0
4	NFU	A	501	8/8	0.98	0.09	28,40,56,57	0
10	FAD	B	402	53/53	0.98	0.07	36,46,55,62	0
10	FAD	F	402	53/53	0.98	0.07	36,45,52,56	0
9	SF4	E	302	8/8	0.99	0.03	29,35,37,40	0
9	SF4	E	303	8/8	0.99	0.03	32,34,37,37	0
9	SF4	F	401	8/8	0.99	0.04	42,44,46,47	0
9	SF4	H	301	8/8	0.99	0.03	33,38,42,43	0
9	SF4	H	302	8/8	0.99	0.03	33,38,41,43	0
9	SF4	H	303	8/8	0.99	0.03	30,36,37,39	0
9	SF4	I	401	8/8	0.99	0.03	38,41,44,44	0
9	SF4	K	301	8/8	0.99	0.03	35,38,41,41	0
9	SF4	K	302	8/8	0.99	0.03	32,37,39,42	0
9	SF4	K	303	8/8	0.99	0.03	32,36,38,39	0
9	SF4	L	401	8/8	0.99	0.04	45,47,48,49	0
4	NFU	D	501	8/8	0.99	0.08	30,38,44,58	0
8	FE	A	511	1/1	0.99	0.04	37,37,37,37	0
9	SF4	B	401	8/8	0.99	0.02	34,39,41,41	0
9	SF4	C	301	8/8	0.99	0.03	32,37,41,42	0
9	SF4	C	302	8/8	0.99	0.02	35,37,40,42	0
9	SF4	C	303	8/8	0.99	0.03	30,35,38,38	0
9	SF4	E	301	8/8	0.99	0.03	35,38,40,41	0
8	FE	J	510	1/1	1.00	0.03	40,40,40,40	0
8	FE	D	511	1/1	1.00	0.03	40,40,40,40	0
8	FE	G	508	1/1	1.00	0.03	43,43,43,43	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.

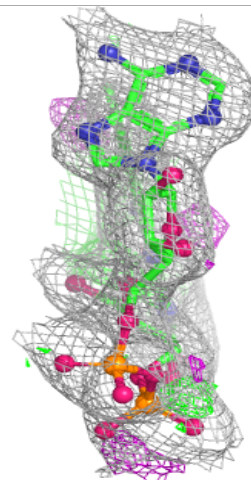
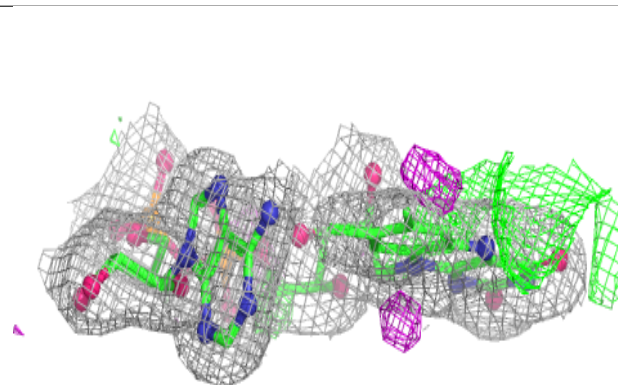
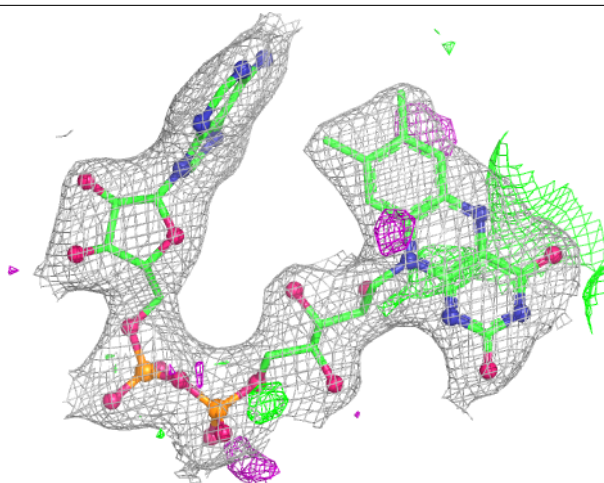
Electron density around FAD L 402:

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



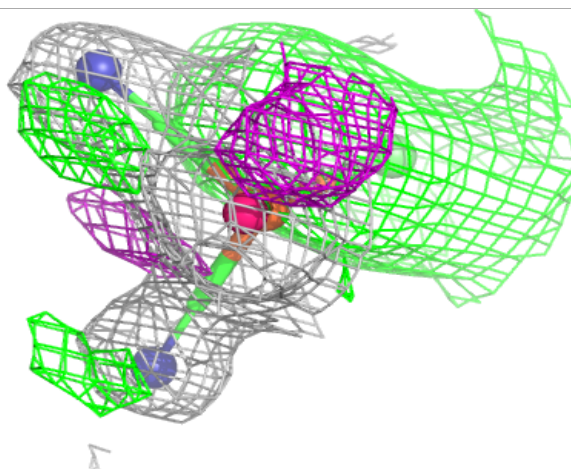
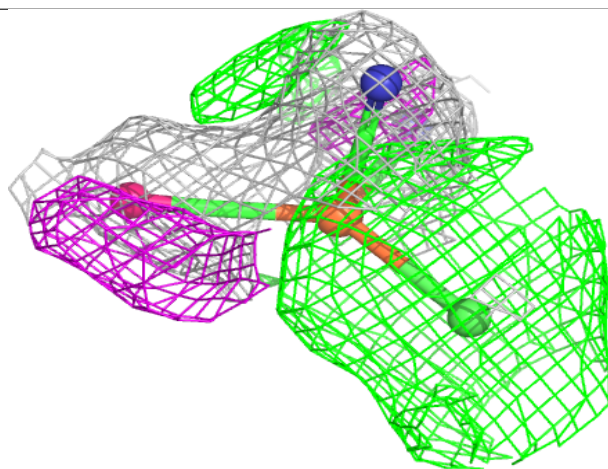
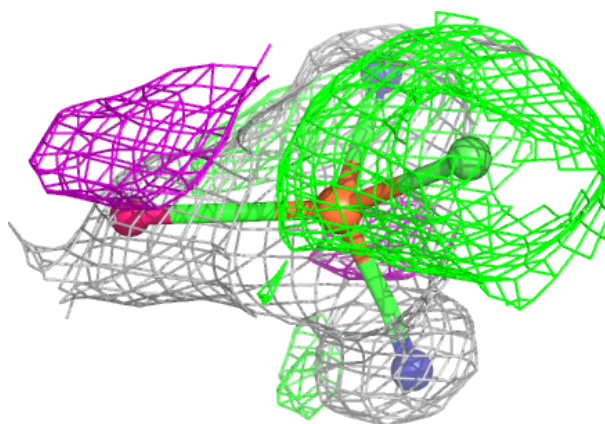
Electron density around FAD I 402:

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



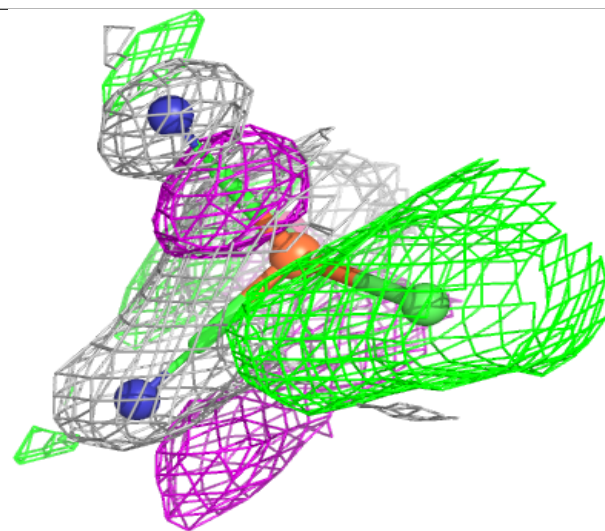
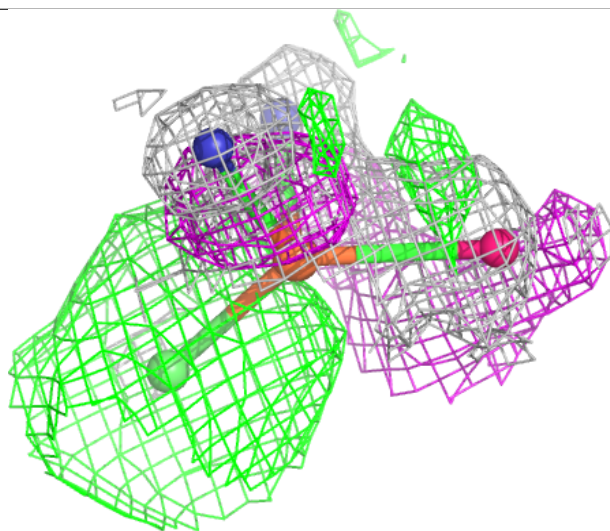
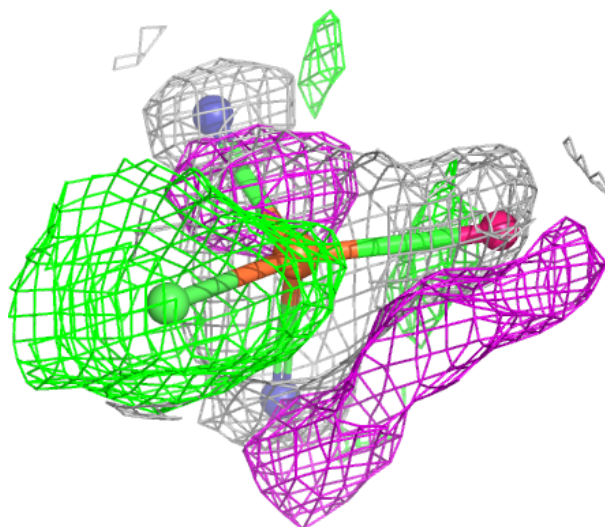
Electron density around NFU G 501:

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



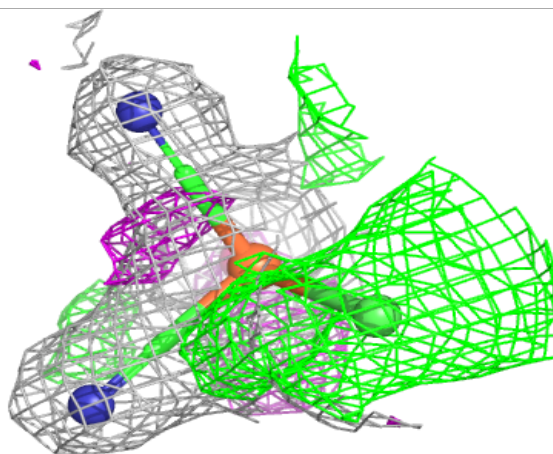
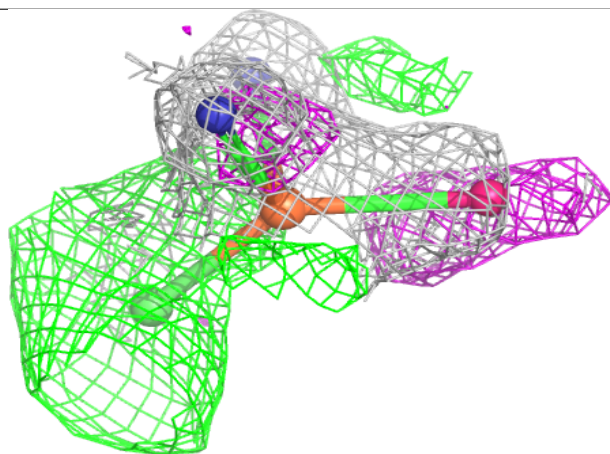
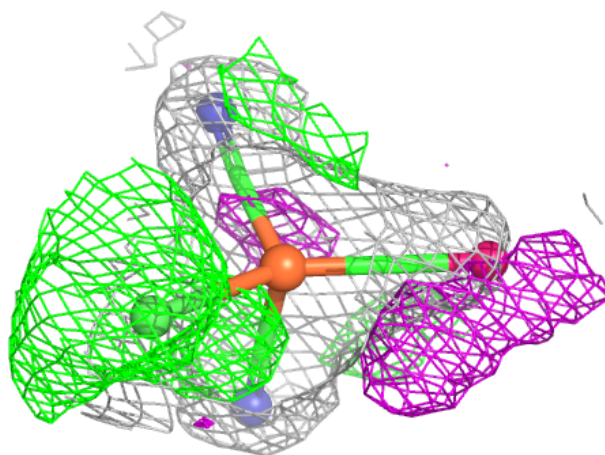
Electron density around NFU J 501:

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



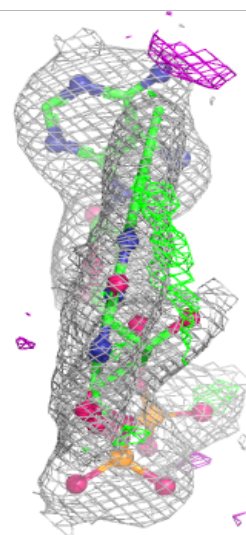
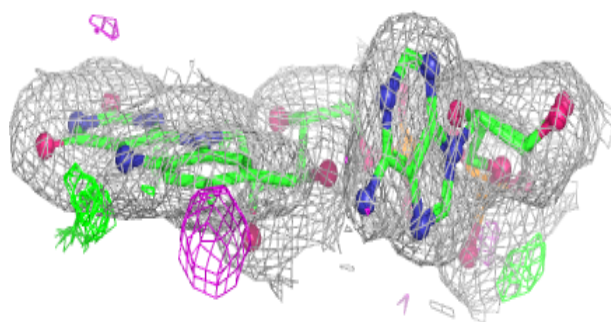
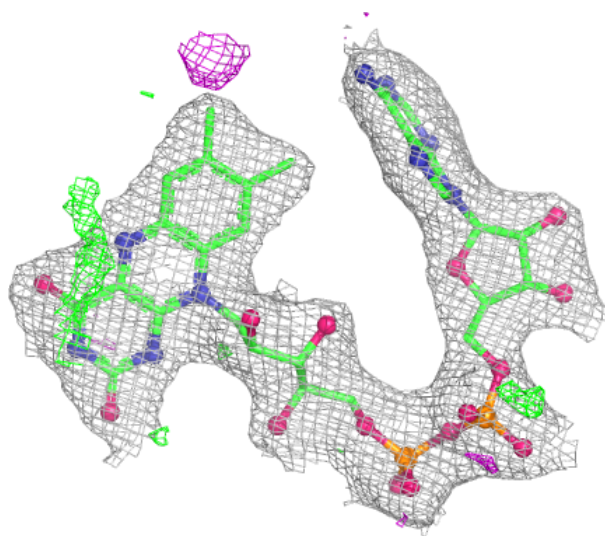
Electron density around NFU A 501:

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



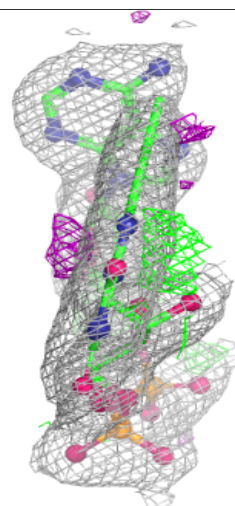
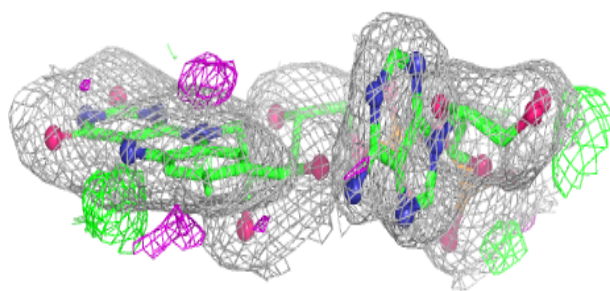
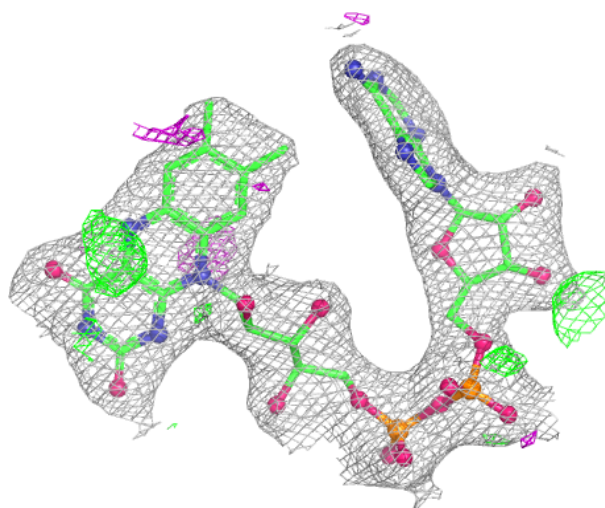
Electron density around FAD B 402:

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



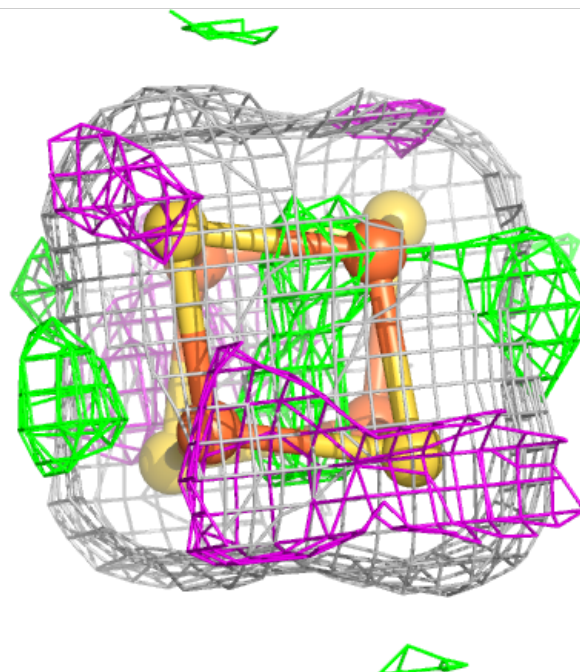
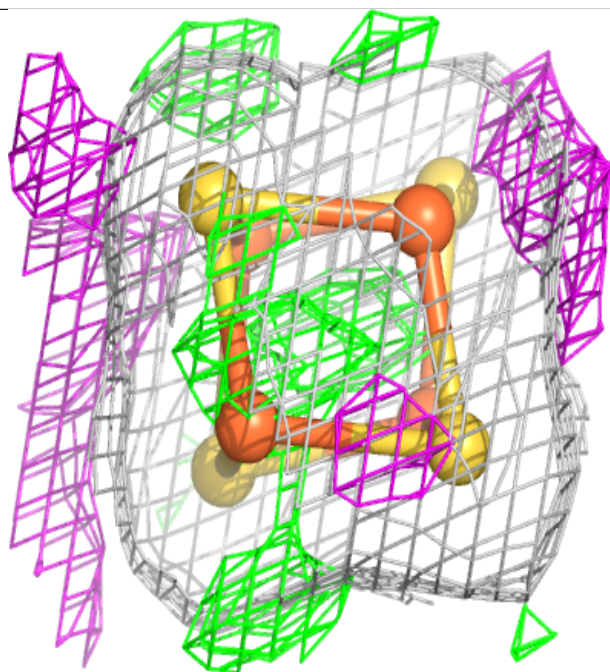
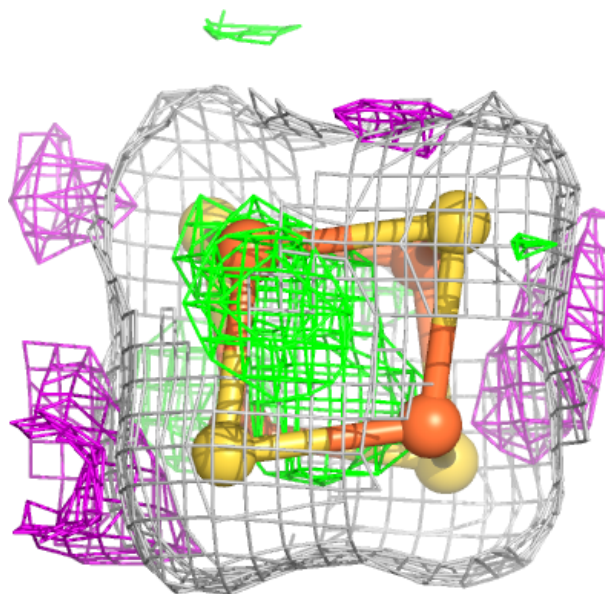
Electron density around FAD F 402:

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



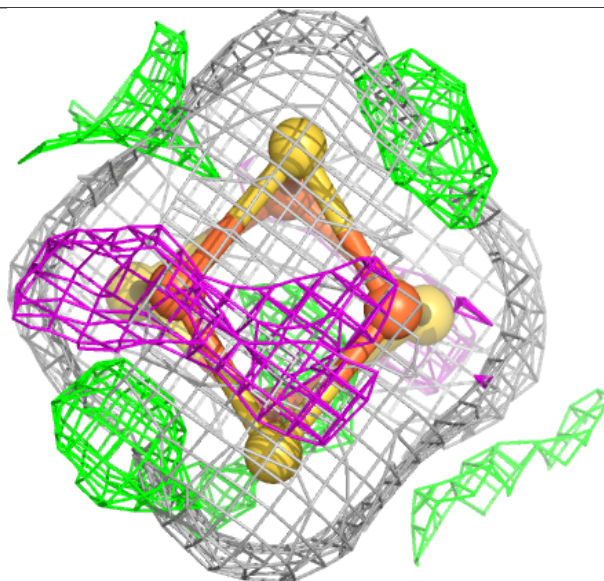
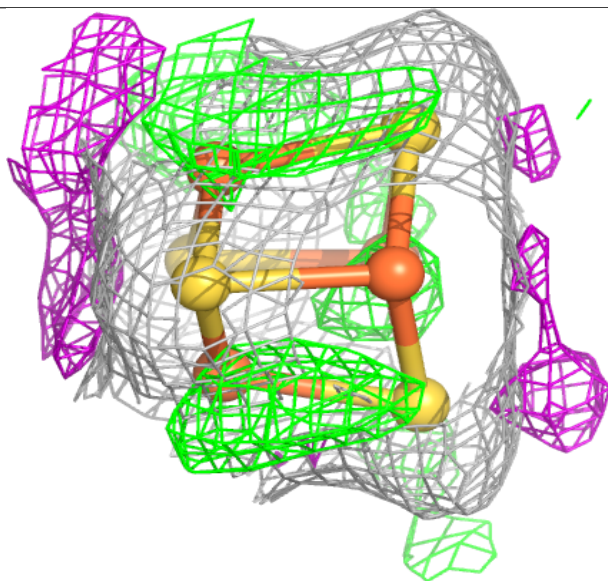
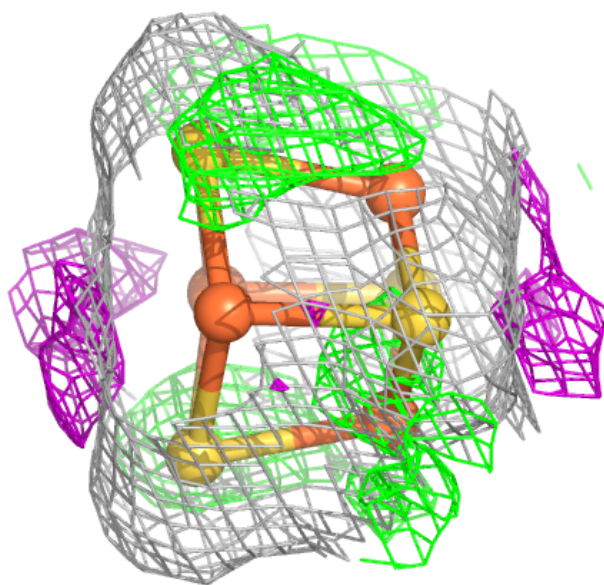
Electron density around SF4 E 302:

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and green (positive)



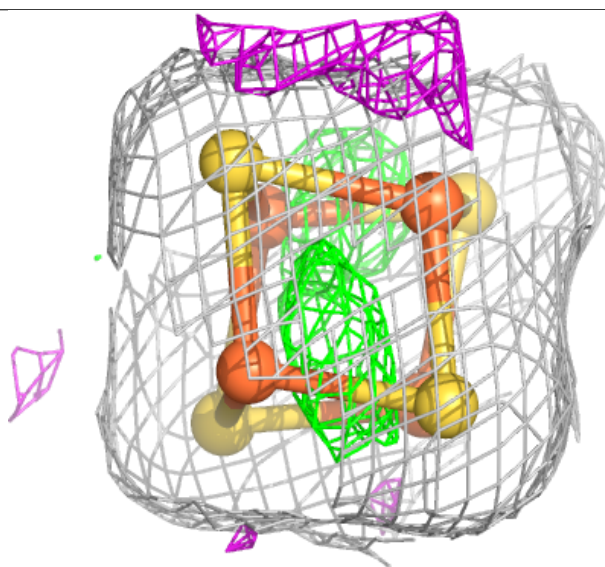
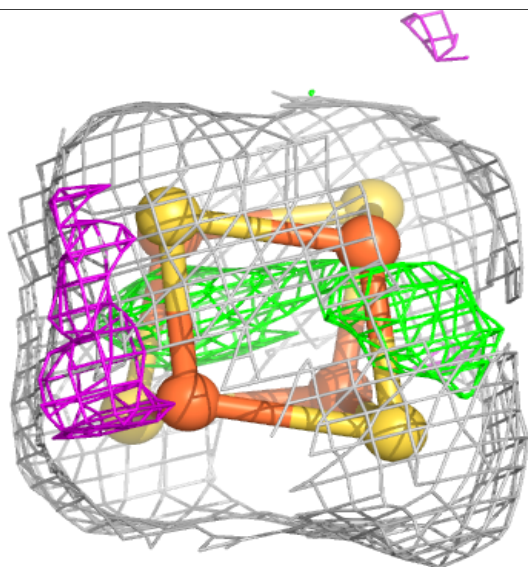
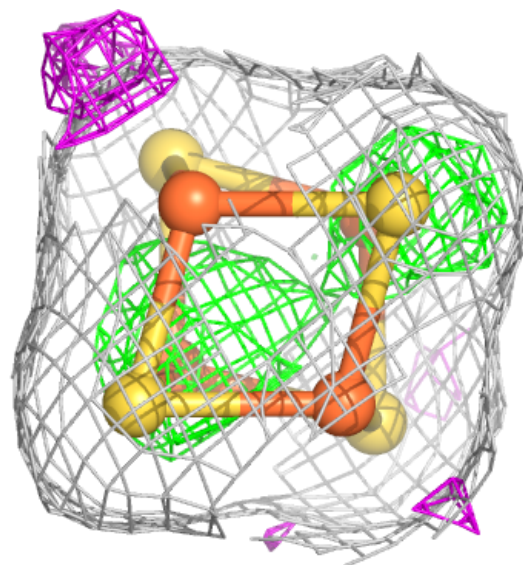
Electron density around SF4 E 303:

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and green (positive)



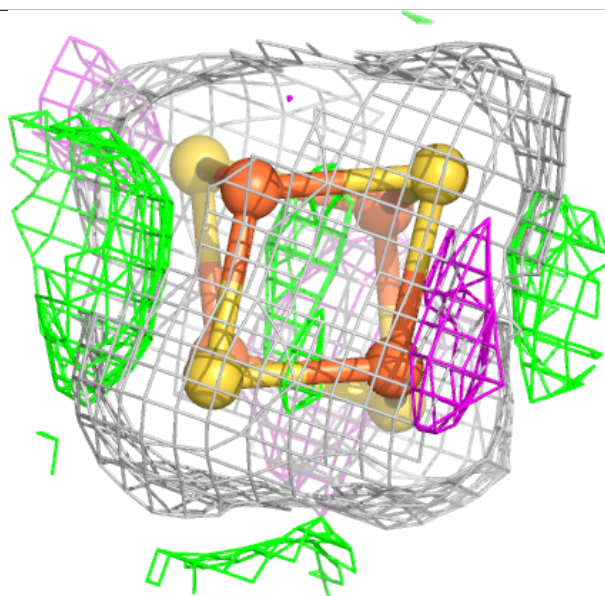
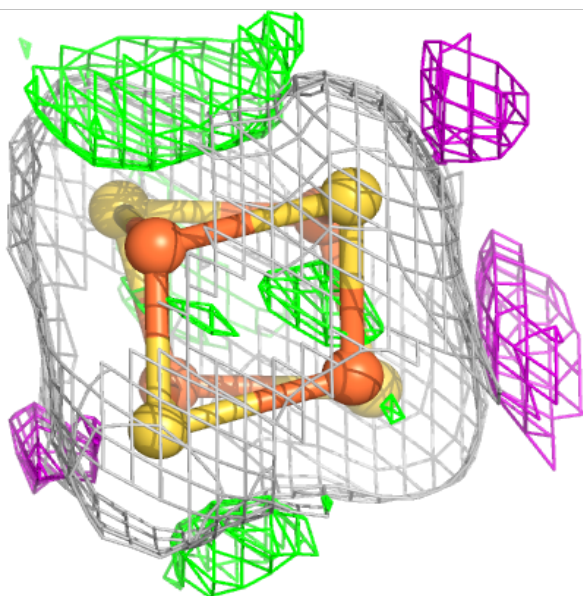
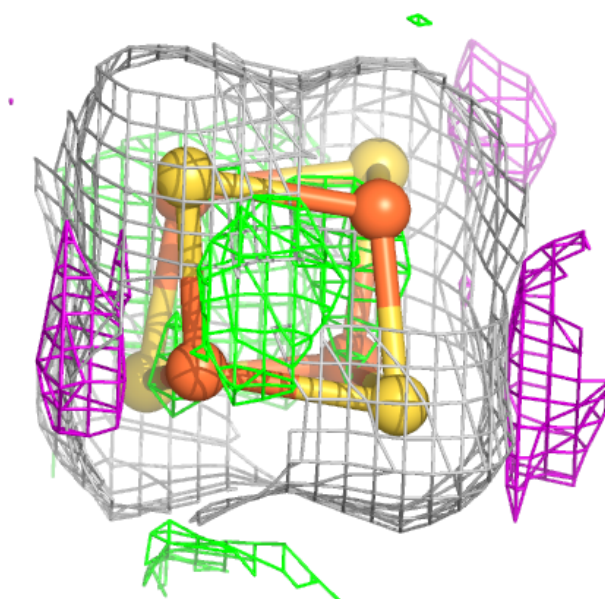
Electron density around SF4 F 401:

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



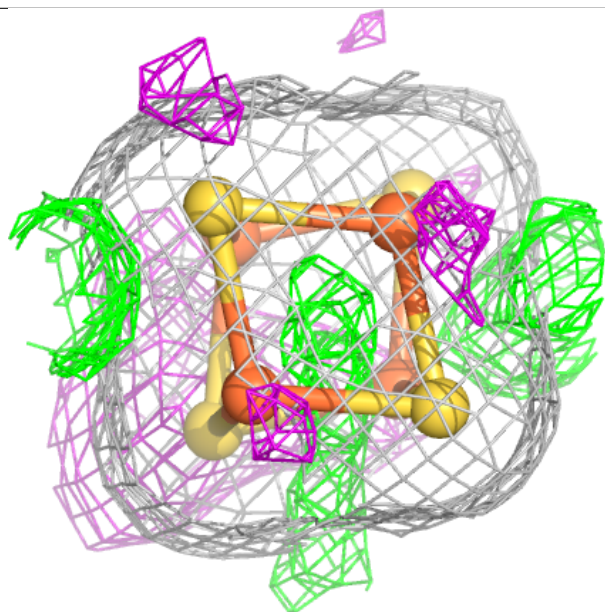
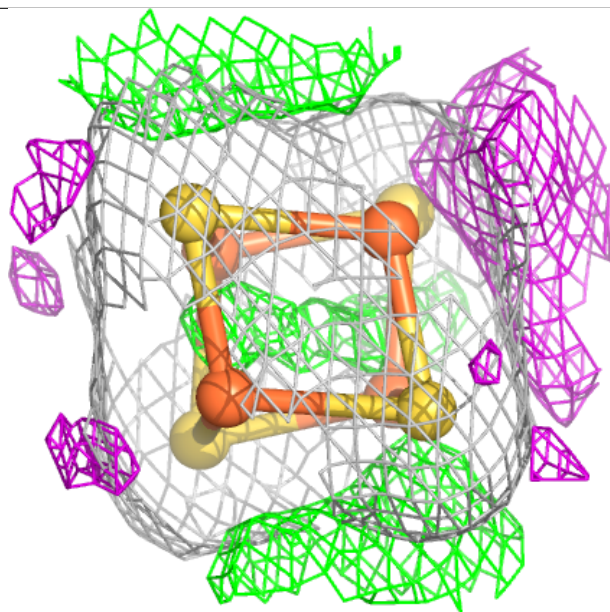
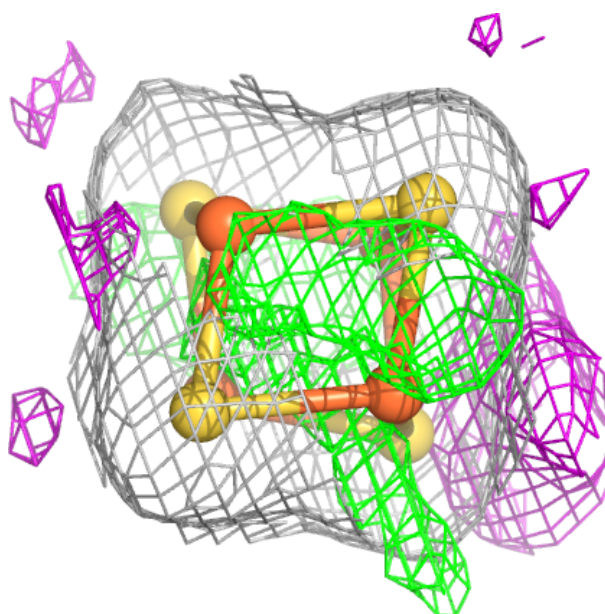
Electron density around SF4 H 301:

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and green (positive)



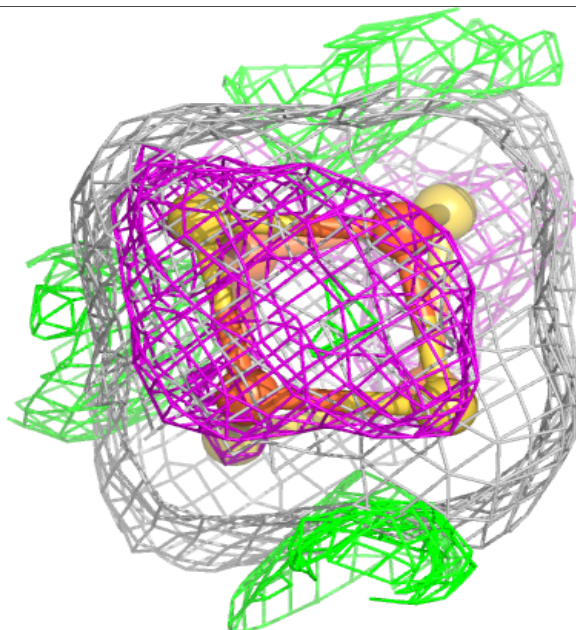
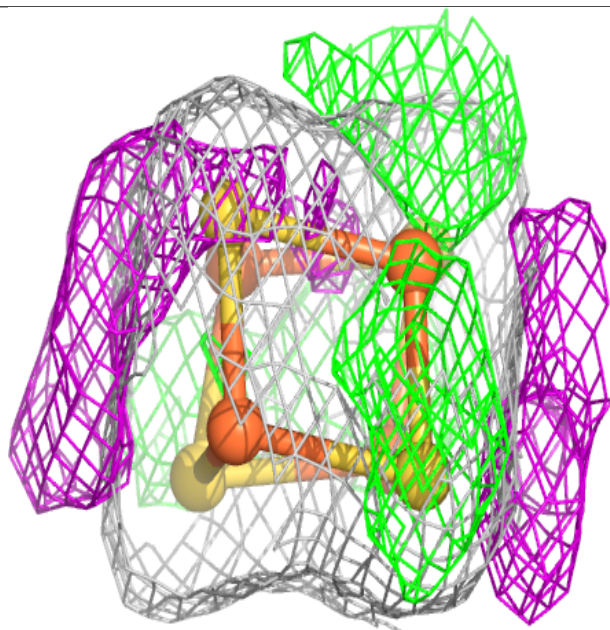
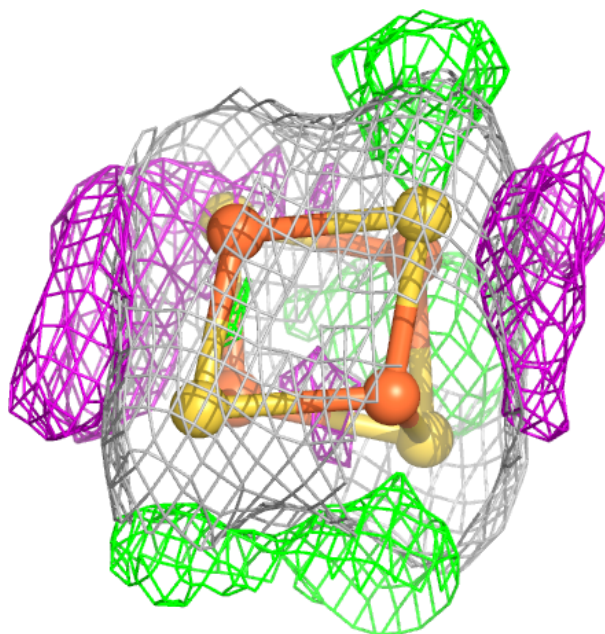
Electron density around SF4 H 302:

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and green (positive)



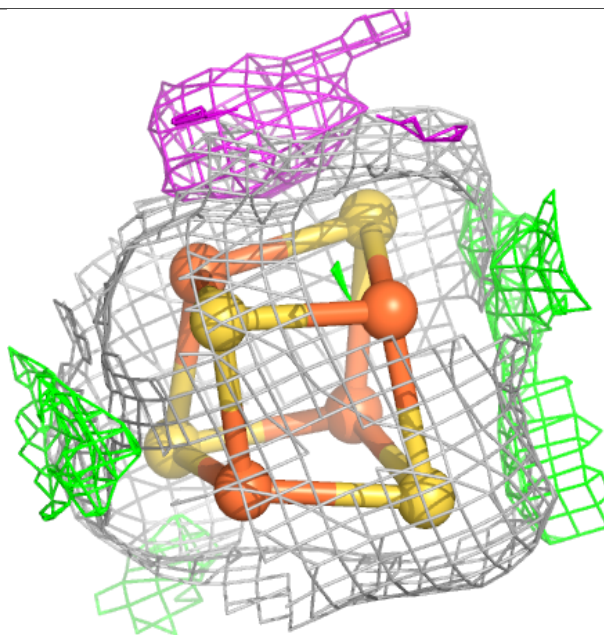
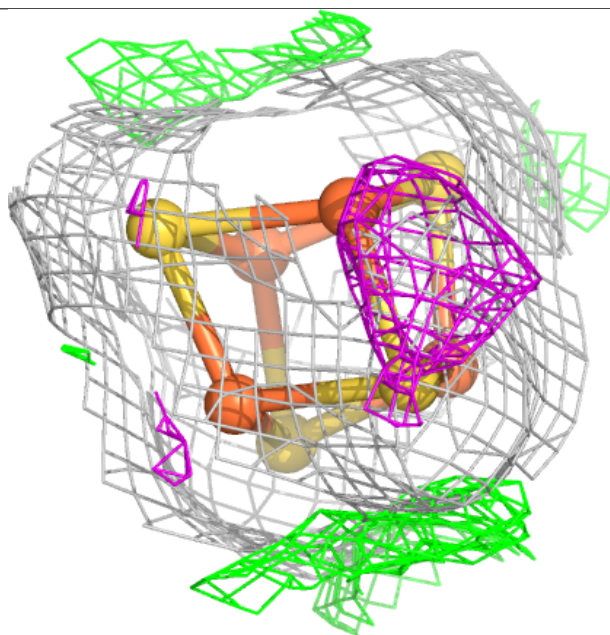
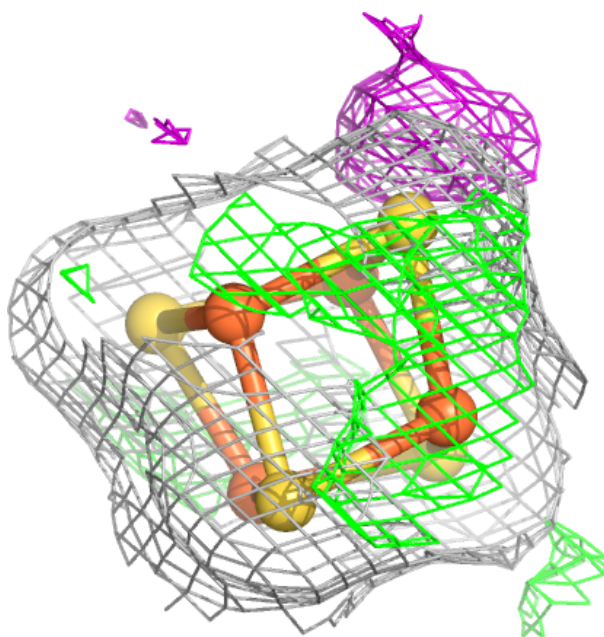
Electron density around SF4 H 303:

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and green (positive)



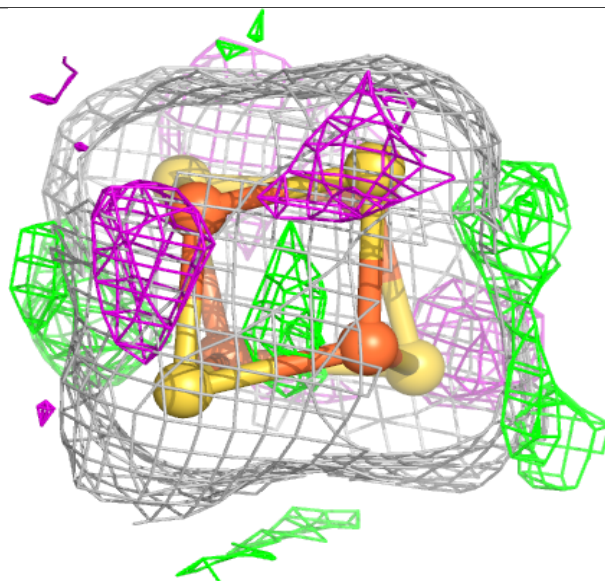
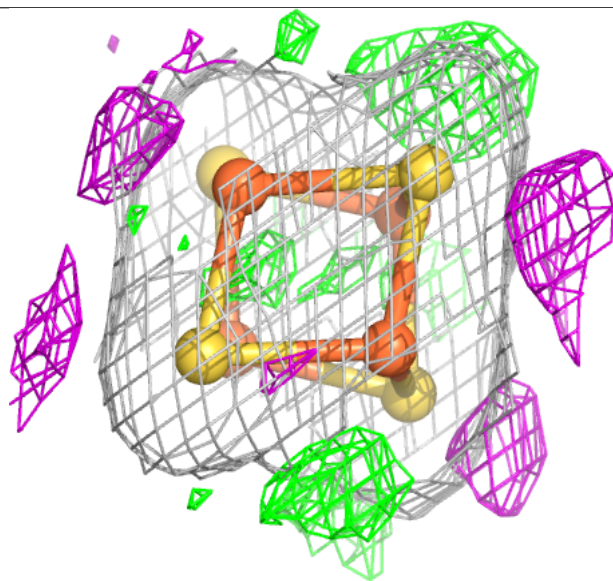
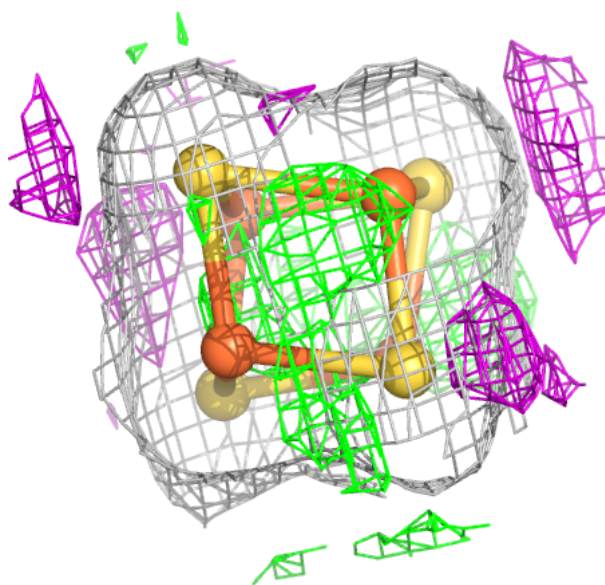
Electron density around SF4 I 401:

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and green (positive)



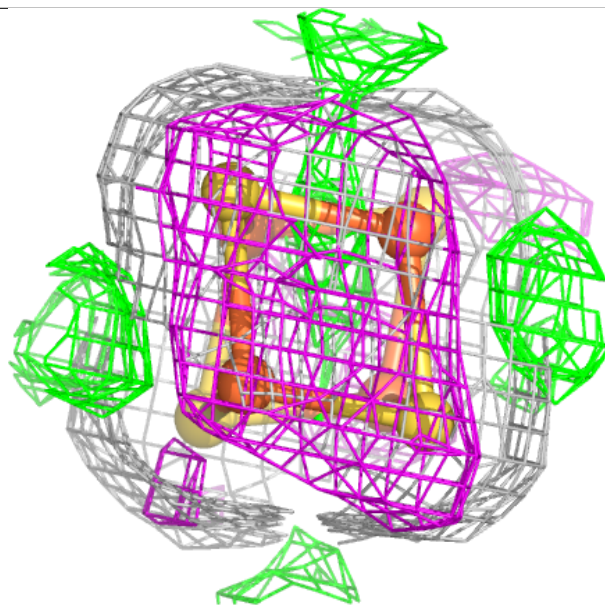
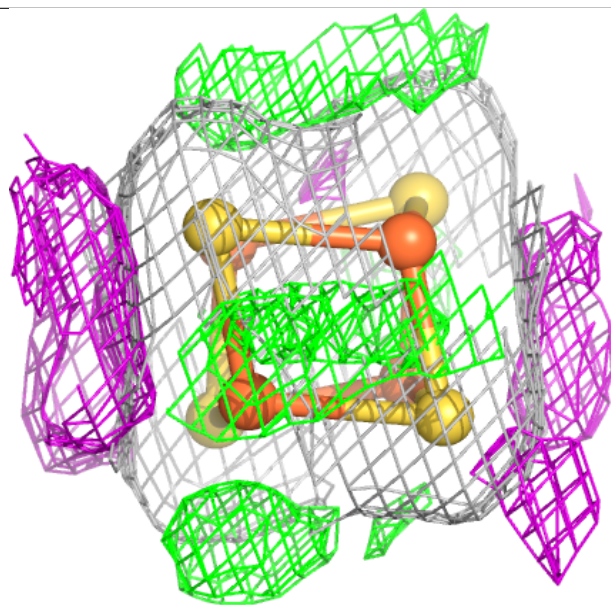
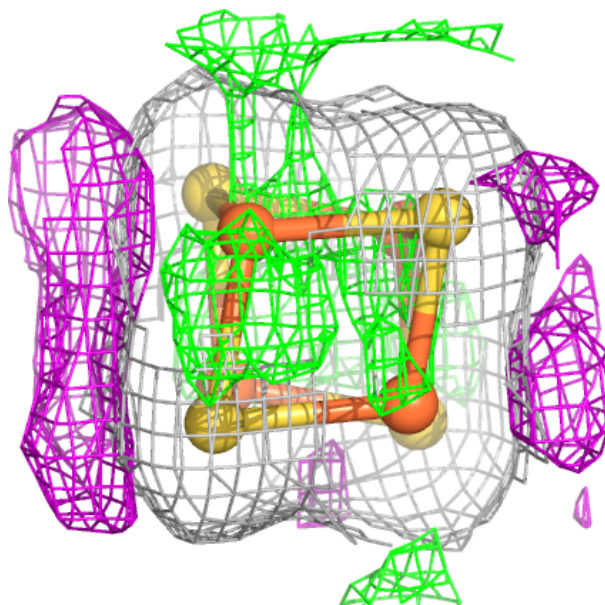
Electron density around SF4 K 301:

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



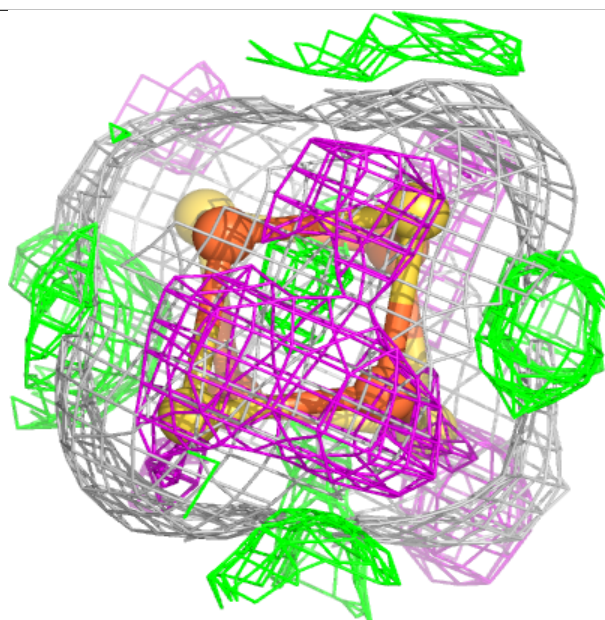
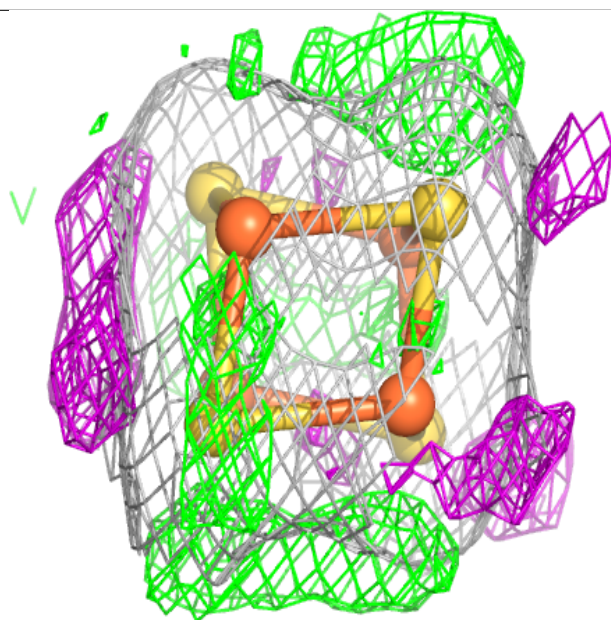
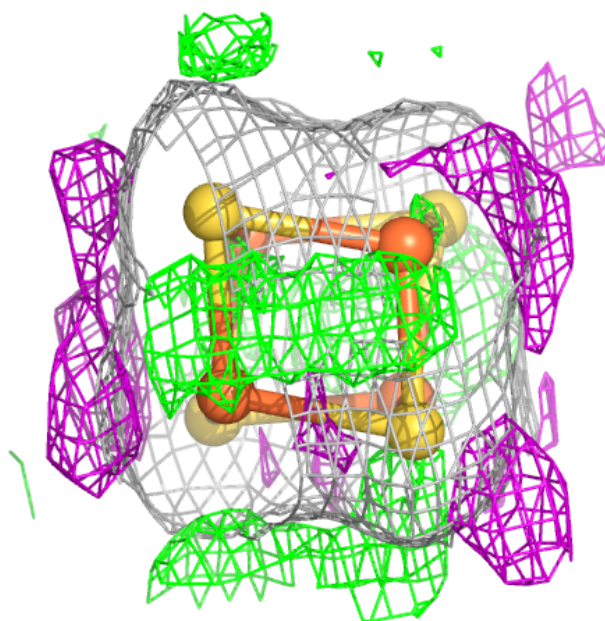
Electron density around SF4 K 302:

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and green (positive)



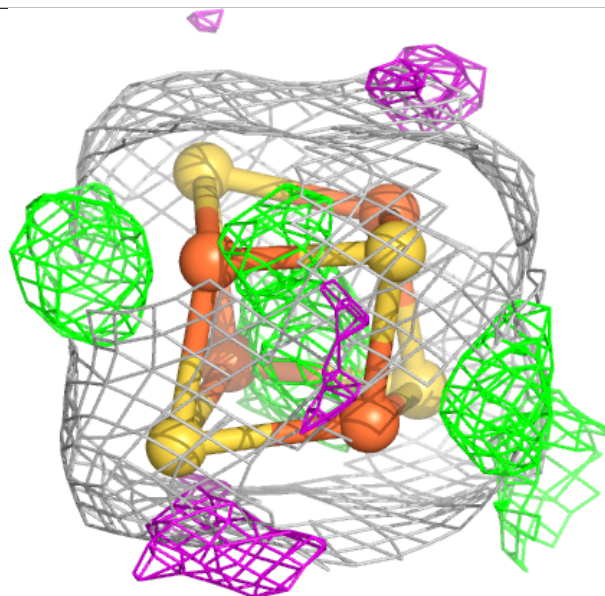
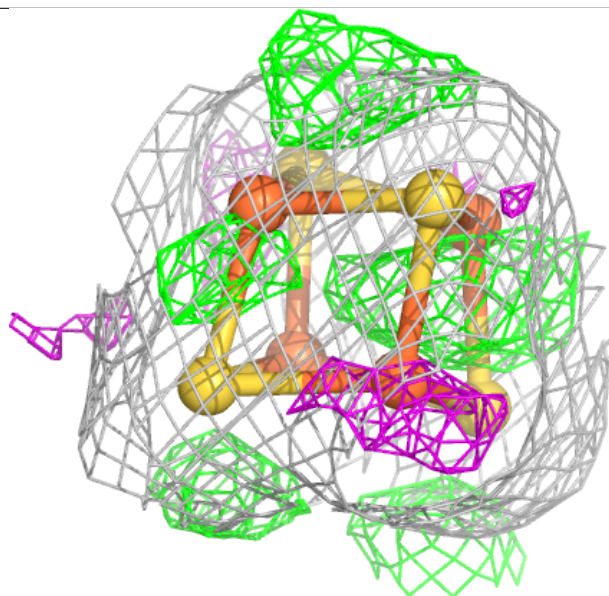
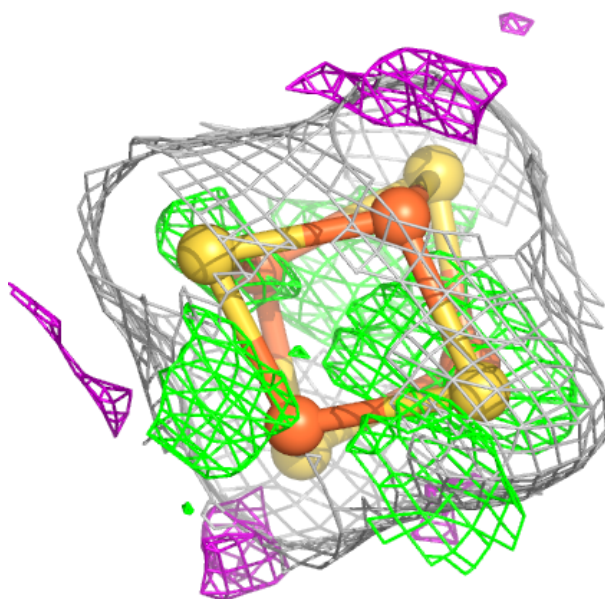
Electron density around SF4 K 303:

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



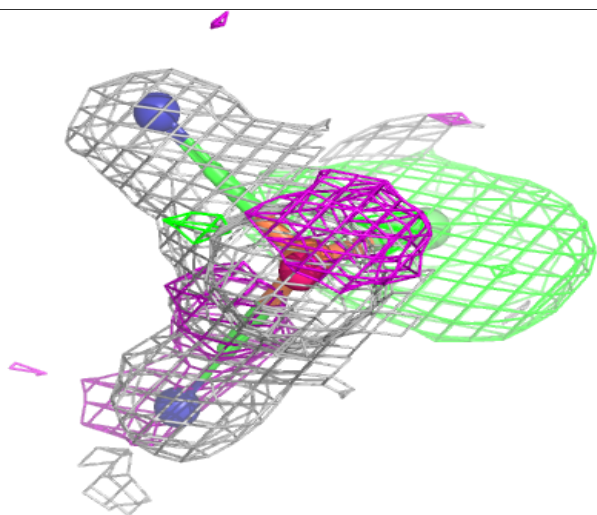
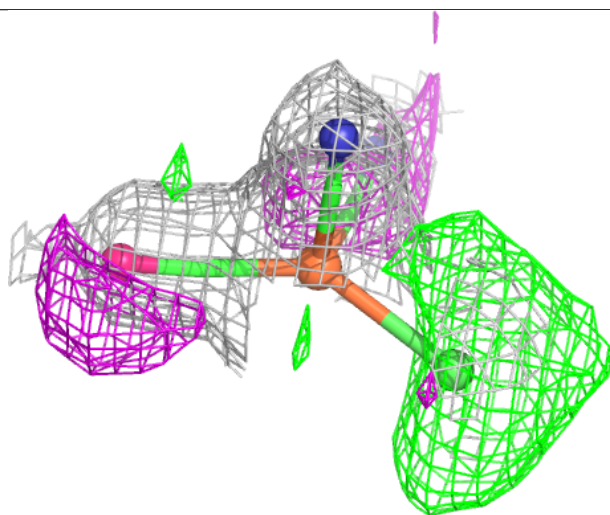
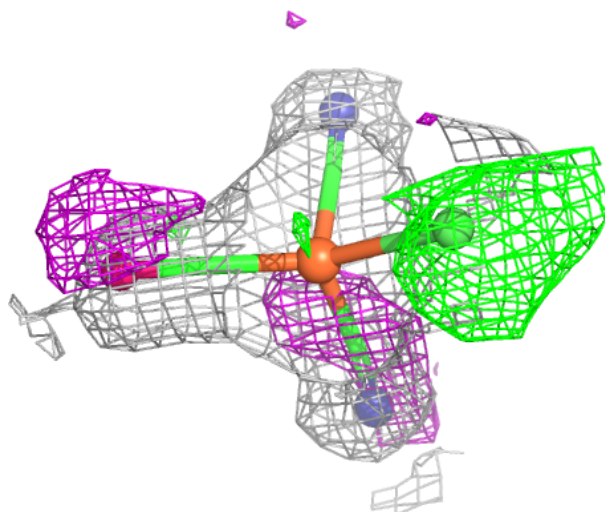
Electron density around SF4 L 401:

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



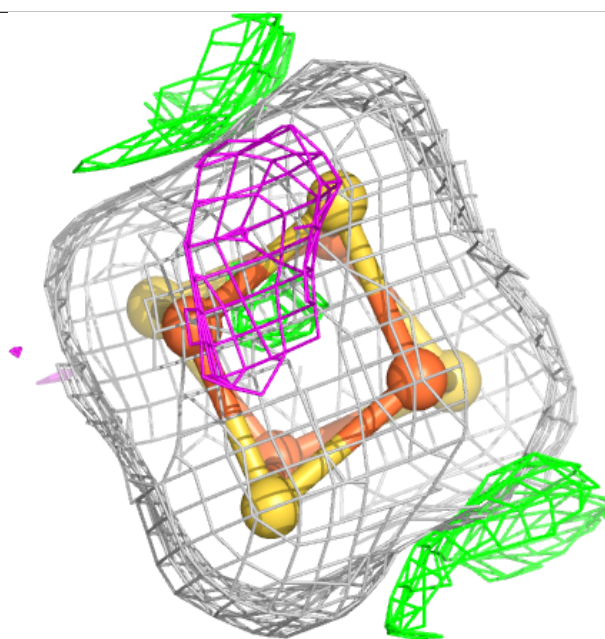
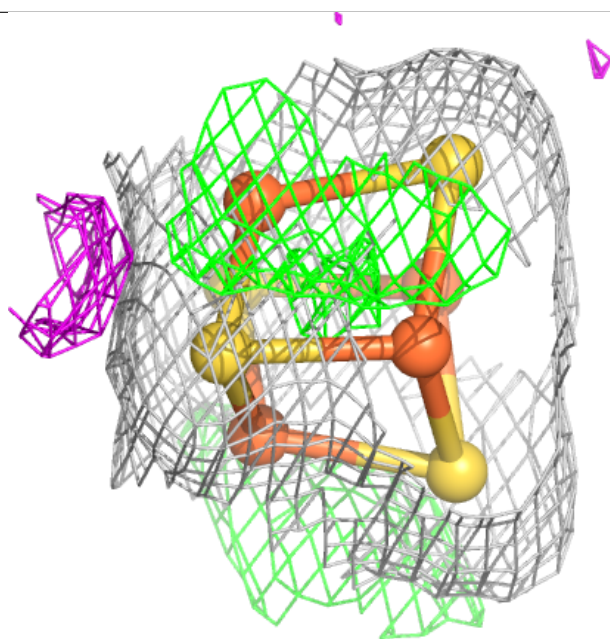
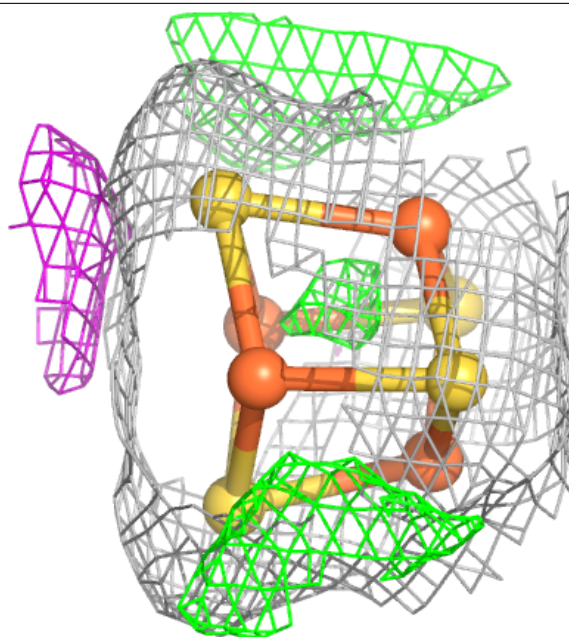
Electron density around NFU D 501:

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



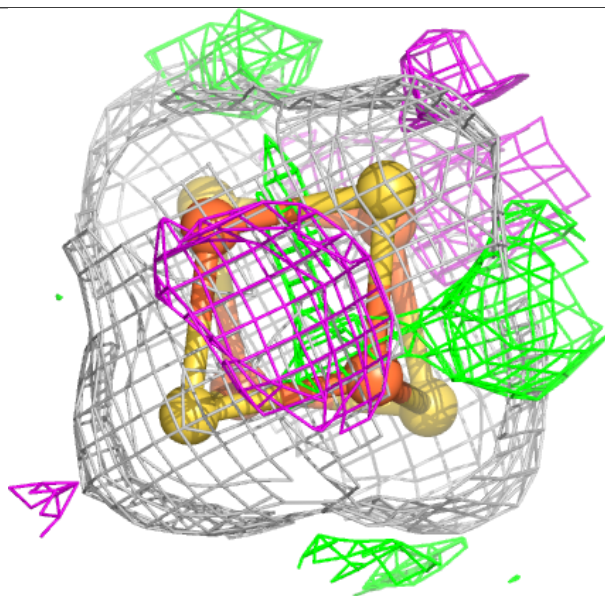
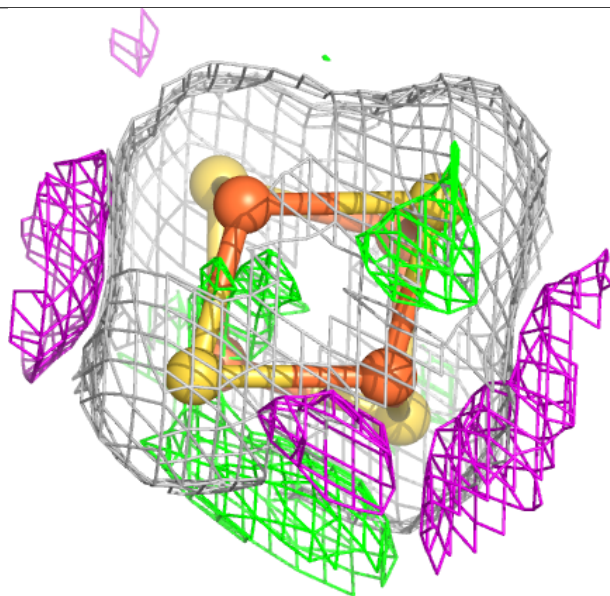
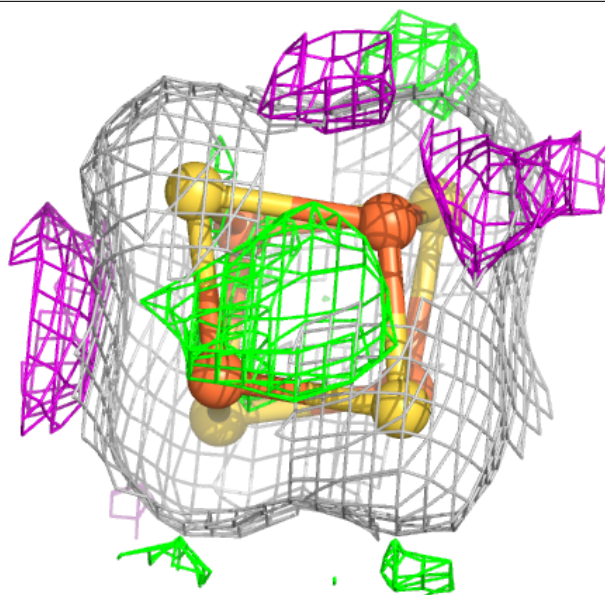
Electron density around SF4 B 401:

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



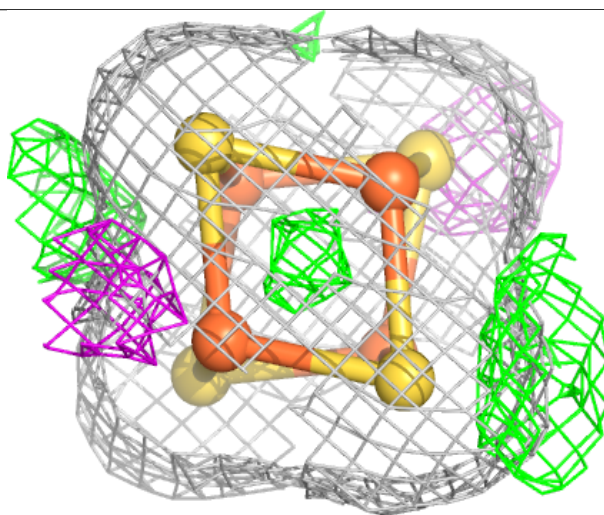
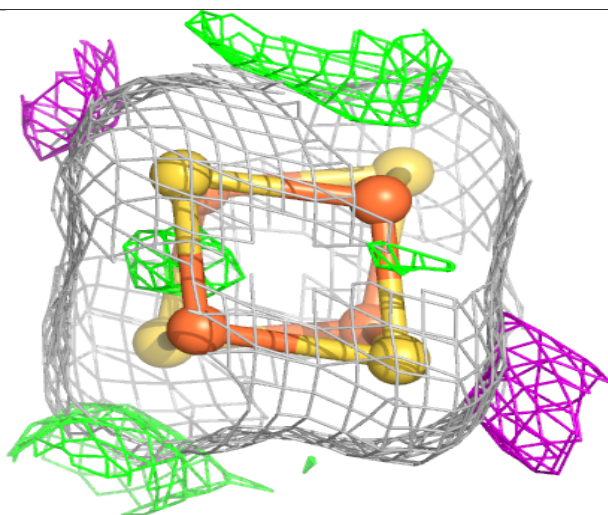
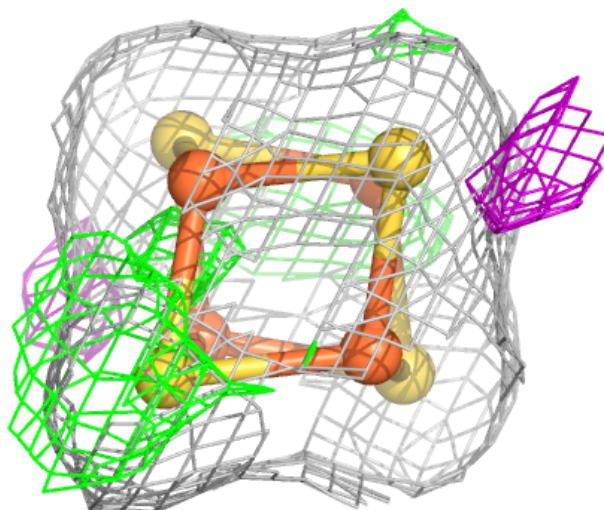
Electron density around SF4 C 301:

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



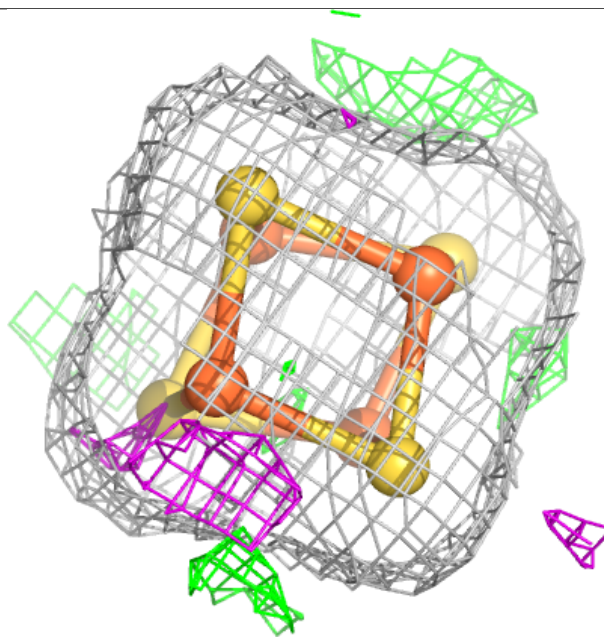
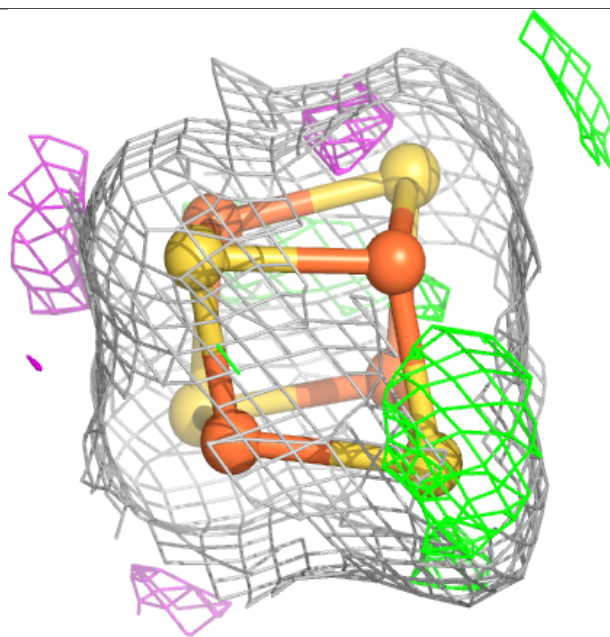
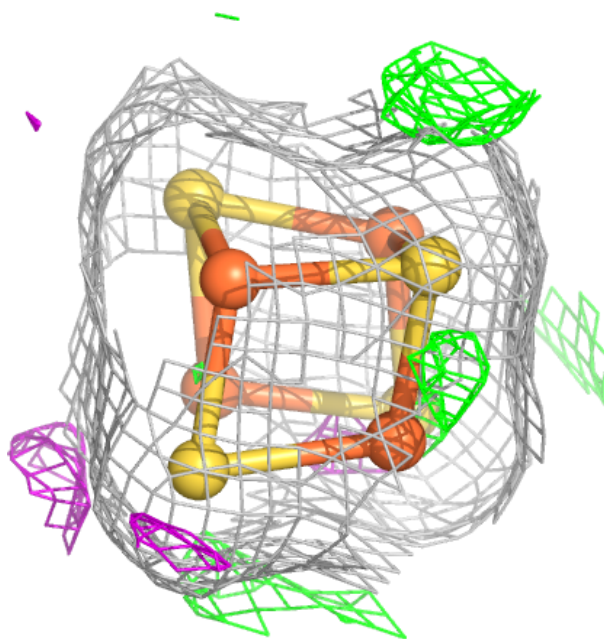
Electron density around SF4 C 302:

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



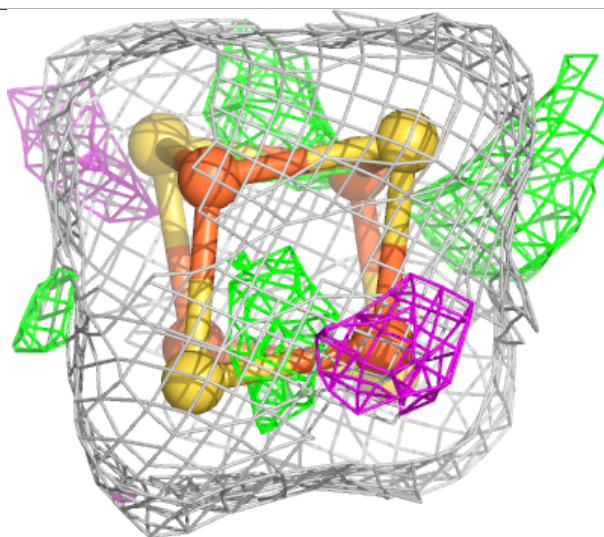
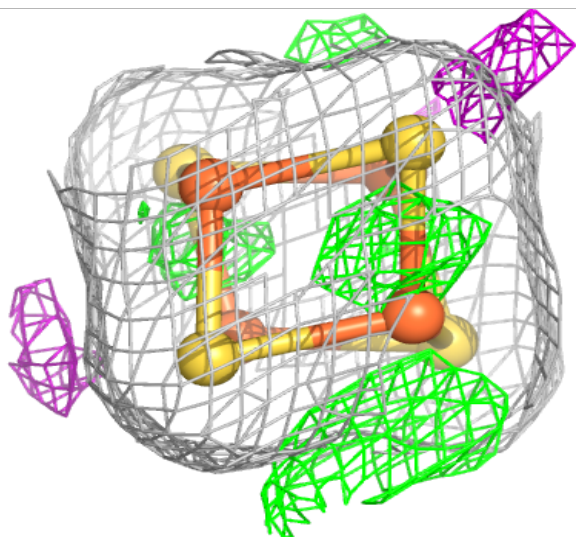
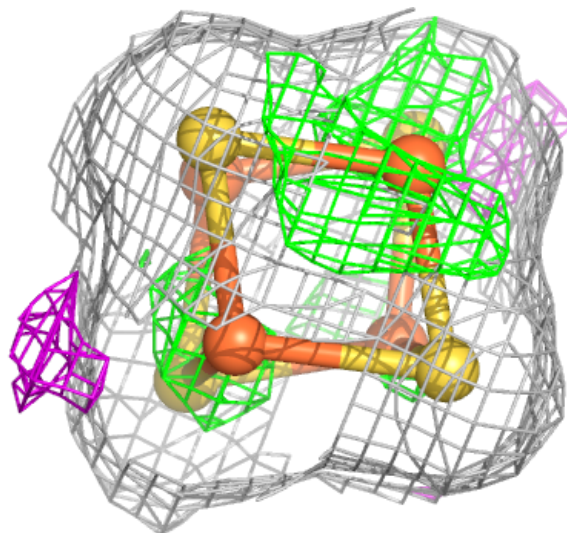
Electron density around SF4 C 303:

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



Electron density around SF4 E 301:

$2mF_o-DF_c$ (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.