



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2025 – 01:54 pm BST

PDB ID : 9R5I / pdb_00009r5i
Title : Dimeric state of the F420-reducing hydrogenase from *Methanothermococcus thermolithotrophicus* in crystalline form 3
Authors : Jespersen, M.; Lemaire, O.N.; Wagner, T.
Deposited on : 2025-05-08
Resolution : 3.13 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

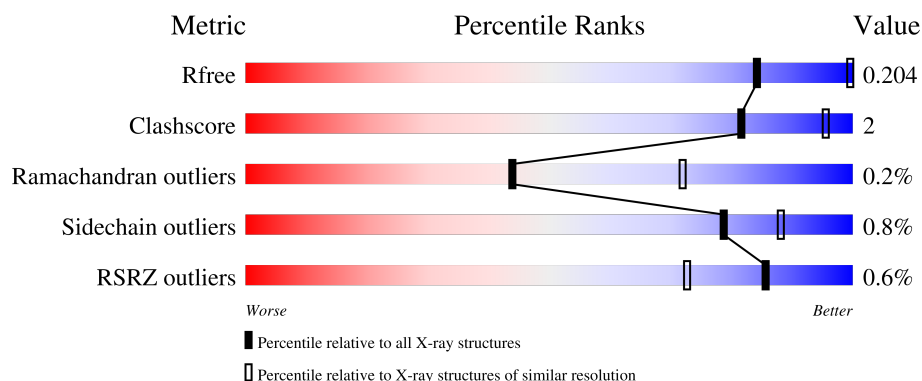
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

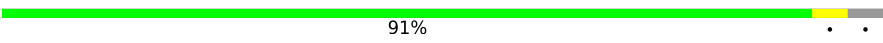
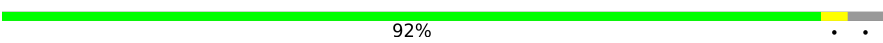


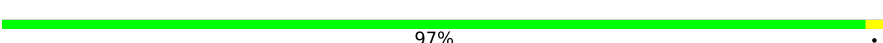
The reported resolution of this entry is 3.13 Å.

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.



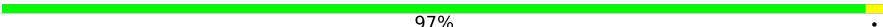
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2149 (3.18-3.10)
Clashscore	180529	2290 (3.18-3.10)
Ramachandran outliers	177936	2178 (3.18-3.10)
Sidechain outliers	177891	2178 (3.18-3.10)
RSRZ outliers	164620	2149 (3.18-3.10)

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	 91%
1	D	410	 92%
2	B	282	 2% 88% 11%
2	F	282	 2% 90% 9%
3	C	241	 97%

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Mol	Chain	Length	Quality of chain
3	E	241	 97%

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
11	SF4	B	308	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 14481 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			

- 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			

- 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	0	0
			1799	1130	299	349	21			

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



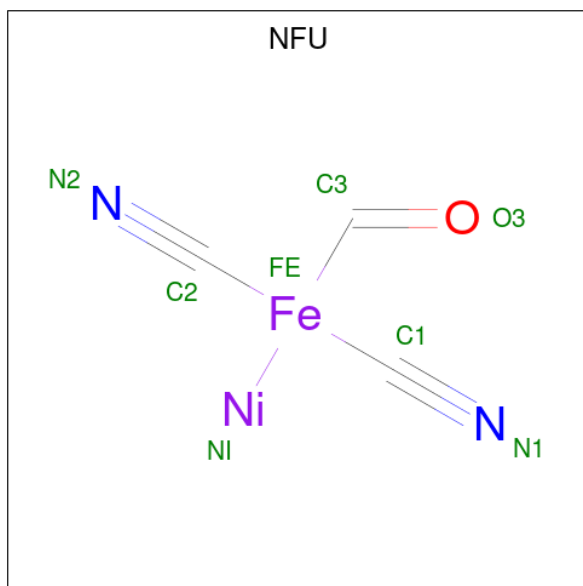
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is formyl[bis(hydrocyanato-1kappaC)]ironnickel(Fe-Ni) (CCD ID: NFU) (formula: C_3HFeN_2NiO) (labeled as "Ligand of Interest" by depositor).

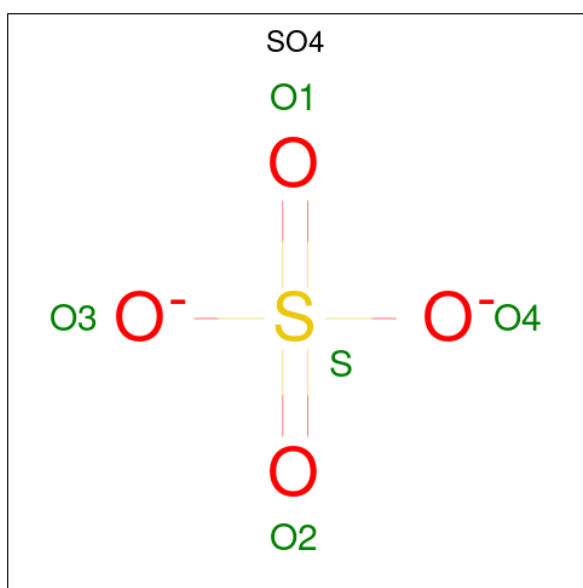


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		
6	D	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		

- Molecule 7 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Fe	0	0
			1	1		
7	D	1	Total	Fe	0	0
			1	1		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



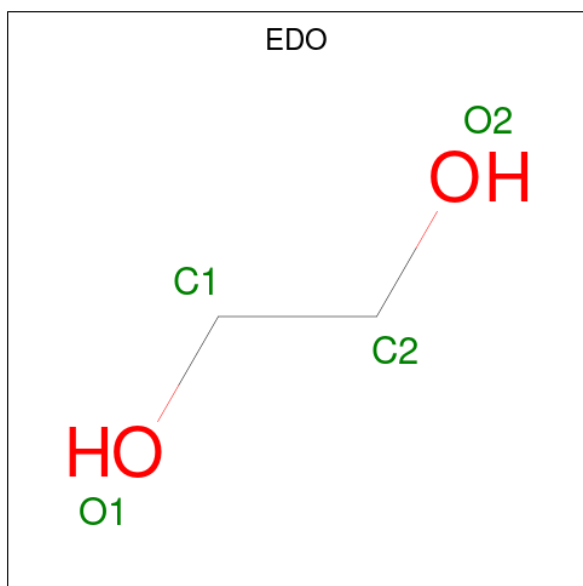
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	D	1	Total	O	S	0	0
			5	4	1		
8	F	1	Total	O	S	0	0
			5	4	1		
8	F	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

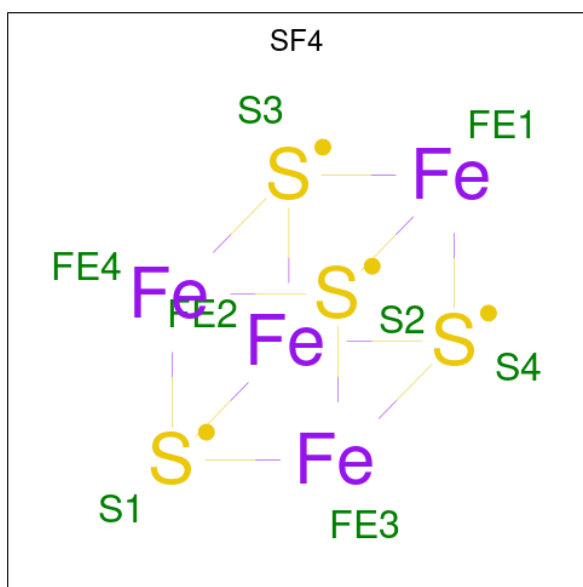
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[illegible]

- # FAD

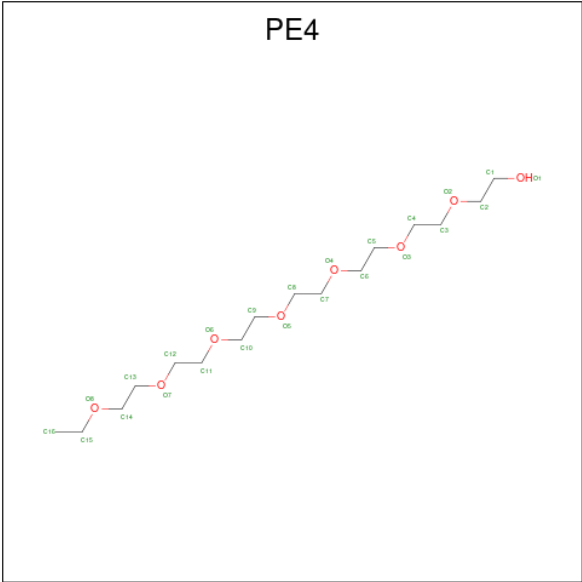
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
10	F	1	Total 53	C 27	N 9	O 15	P 2	0	0

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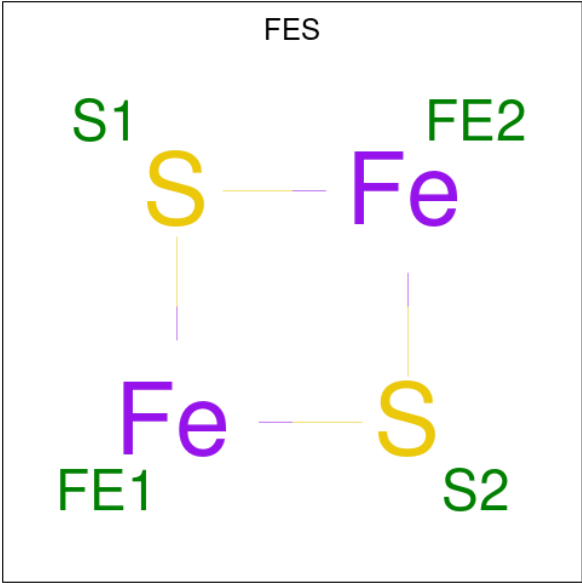
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			8	4	4		
11	C	1	Total	Fe	S	0	0
			8	4	4		
11	C	1	Total	Fe	S	0	0
			8	4	4		
11	C	1	Total	Fe	S	0	0
			8	4	4		
11	E	1	Total	Fe	S	0	0
			8	4	4		
11	E	1	Total	Fe	S	0	0
			8	4	4		
11	E	1	Total	Fe	S	0	0
			8	4	4		
11	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 12 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
12	C	1	Total	C	O	0	0
			22	14	8		

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	E	1	Total	Fe	S	0	0
			4	2	2		

3 Residue-property plots [i](#)

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

- Molecule 1: F420-reducing [NiFe]-hydrogenase from *Methanothermococcus thermolithotrophicus* subunit alpha

Chain A:  91%




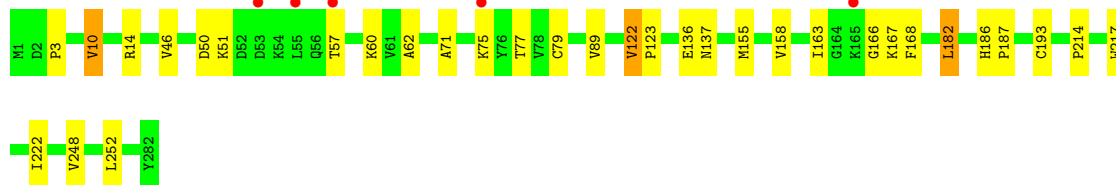
- Molecule 1: F420-reducing [NiFe]-hydrogenase from *Methanothermococcus thermolithotrophicus* subunit alpha

Chain D:  92%

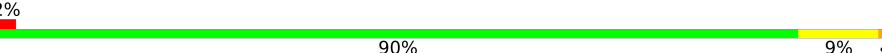


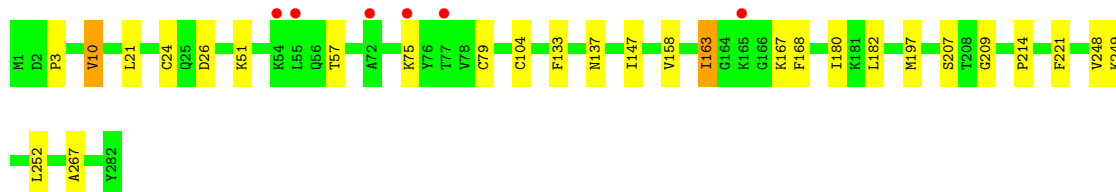
- Molecule 2: F420-reducing [NiFe]-hydrogenase from *Methanothermococcus thermolithotrophicus* subunit beta

Chain B:  88% 11% 2%



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

Chain F:  90% 9% 2%



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

Chain C:  97%



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

Chain E:  97%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.61Å 196.61Å 192.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	77.83 – 3.13 77.83 – 3.13	Depositor EDS
% Data completeness (in resolution range)	69.0 (77.83-3.13) 69.0 (77.83-3.13)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.13Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.174 , 0.206 0.175 , 0.204	Depositor DCC
R_{free} test set	2615 reflections (3.45%)	wwPDB-VP
Wilson B-factor (Å ²)	91.2	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14481	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PE4, FE, SO4, FES, NFU, SF4, MES, FAD, EDO

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	0.22	0/3140	0.40	0/4251
1	D	0.22	0/3140	0.40	0/4251
2	B	0.40	0/2219	0.63	0/2994
2	F	0.40	0/2219	0.66	0/2994
3	C	0.21	0/1821	0.40	0/2465
3	E	0.20	0/1821	0.40	0/2465
All	All	0.29	0/14360	0.49	0/19420

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3070	0	3051	13	0
1	D	3070	0	3050	11	0
2	B	2177	0	2224	21	0
2	F	2177	0	2224	18	0
3	C	1799	0	1835	3	0
3	E	1799	0	1834	5	0
4	A	18	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	6	0	8	0	0
4	D	12	0	16	0	0
4	E	18	0	24	0	0
5	A	12	0	13	0	0
6	A	8	0	0	1	0
6	D	8	0	0	1	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
8	A	5	0	0	0	0
8	B	15	0	0	0	0
8	C	5	0	0	0	0
8	D	5	0	0	0	0
8	F	15	0	0	0	0
9	A	12	0	18	0	0
9	B	12	0	18	0	0
9	C	8	0	12	0	0
9	D	32	0	48	0	0
10	B	53	0	31	1	0
10	F	53	0	31	2	0
11	B	8	0	0	2	0
11	C	24	0	0	0	0
11	E	24	0	0	0	0
11	F	8	0	0	1	0
12	C	22	0	29	0	0
13	E	4	0	0	0	0
All	All	14481	0	14490	69	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 69 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:163:ILE:HG22	2:F:168:PHE:CD1	2.28	0.68
2:F:163:ILE:HG22	2:F:168:PHE:HD1	1.62	0.64
1:D:17:THR:HG23	1:D:388:ILE:HG13	1.80	0.64
2:F:57:THR:HG21	2:F:79:CYS:HB2	1.81	0.62
2:F:167:LYS:HB2	2:F:180:ILE:O	2.01	0.61

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	373 (96%)	17 (4%)	0	100	100
1	D	390/410 (95%)	376 (96%)	14 (4%)	0	100	100
2	B	280/282 (99%)	266 (95%)	12 (4%)	2 (1%)	19	48
2	F	280/282 (99%)	264 (94%)	15 (5%)	1 (0%)	30	60
3	C	238/241 (99%)	223 (94%)	15 (6%)	0	100	100
3	E	238/241 (99%)	225 (94%)	13 (6%)	0	100	100
All	All	1816/1866 (97%)	1727 (95%)	86 (5%)	3 (0%)	44	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	122	VAL
2	F	3	PRO
2	B	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%)	328 (99%)	2 (1%)	84	91
1	D	330/347 (95%)	327 (99%)	3 (1%)	75	86
2	B	238/238 (100%)	234 (98%)	4 (2%)	56	75
2	F	238/238 (100%)	236 (99%)	2 (1%)	79	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	204/205 (100%)	203 (100%)	1 (0%)	86	92
3	E	204/205 (100%)	203 (100%)	1 (0%)	86	92
All	All	1544/1580 (98%)	1531 (99%)	13 (1%)	79	88

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	17	THR
1	D	334	ARG
2	F	163	ILE
3	E	190	MET
2	F	10	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	162	GLN
3	E	80	HIS
2	F	272	HIS
2	F	190	GLN
3	C	80	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 2 are monoatomic - leaving 49 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	$\# Z > 2$
10	FAD	B	301	-	53,58,58	0.61	0	68,89,89	0.60	1 (1%)
8	SO4	A	507	-	4,4,4	0.15	0	6,6,6	0.07	0
9	EDO	D	501	-	3,3,3	0.46	0	2,2,2	0.43	0
9	EDO	D	510	-	3,3,3	0.47	0	2,2,2	0.23	0
13	FES	E	401	3	0,4,4	-	-	-		
11	SF4	F	305	2	0,12,12	-	-	-		
6	NFU	D	504	1	2,7,7	1.22	0	-		
4	GOL	E	404	-	5,5,5	0.09	0	5,5,5	0.32	0
10	FAD	F	301	-	53,58,58	1.30	5 (9%)	68,89,89	1.33	10 (14%)
11	SF4	E	405	3	0,12,12	-	-	-		
4	GOL	A	503	-	5,5,5	0.91	0	5,5,5	0.92	0
4	GOL	D	503	-	5,5,5	0.96	0	5,5,5	0.81	0
11	SF4	E	407	3	0,12,12	-	-	-		
8	SO4	B	302	-	4,4,4	0.15	0	6,6,6	0.06	0
9	EDO	D	509	-	3,3,3	0.45	0	2,2,2	0.21	0
11	SF4	E	406	3	0,12,12	-	-	-		
4	GOL	A	501	-	5,5,5	0.89	0	5,5,5	1.00	0
9	EDO	A	508	-	3,3,3	0.45	0	2,2,2	0.26	0
9	EDO	D	511	-	3,3,3	0.46	0	2,2,2	0.32	0
9	EDO	C	304	-	3,3,3	0.44	0	2,2,2	0.40	0
4	GOL	D	502	-	5,5,5	0.92	0	5,5,5	0.78	0
4	GOL	E	403	-	5,5,5	0.92	0	5,5,5	0.91	0
9	EDO	A	509	-	3,3,3	0.44	0	2,2,2	0.39	0
11	SF4	C	306	3	0,12,12	-	-	-		
8	SO4	C	303	-	4,4,4	0.14	0	6,6,6	0.09	0
9	EDO	D	513	-	3,3,3	0.07	0	2,2,2	0.21	0
4	GOL	A	504	-	5,5,5	1.00	0	5,5,5	0.72	0
8	SO4	F	302	-	4,4,4	0.14	0	6,6,6	0.07	0
9	EDO	B	307	-	3,3,3	0.04	0	2,2,2	0.16	0
11	SF4	C	307	3	0,12,12	-	-	-		
8	SO4	F	303	-	4,4,4	0.14	0	6,6,6	0.07	0
9	EDO	A	510	-	3,3,3	0.08	0	2,2,2	0.16	0
4	GOL	C	301	-	5,5,5	0.91	0	5,5,5	0.96	0
9	EDO	C	305	-	3,3,3	0.06	0	2,2,2	0.18	0
9	EDO	B	305	-	3,3,3	0.45	0	2,2,2	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	D	512	-	3,3,3	0.47	0	2,2,2	0.24	0
11	SF4	B	308	2	0,12,12	-	-	-		
8	SO4	D	506	-	4,4,4	0.14	0	6,6,6	0.08	0
4	GOL	E	402	-	5,5,5	0.89	0	5,5,5	0.93	0
8	SO4	B	304	-	4,4,4	0.14	0	6,6,6	0.06	0
6	NFU	A	505	1	2,7,7	1.19	0	-		
9	EDO	D	507	-	3,3,3	0.46	0	2,2,2	0.29	0
9	EDO	D	508	-	3,3,3	0.45	0	2,2,2	0.36	0
8	SO4	B	303	-	4,4,4	0.13	0	6,6,6	0.08	0
11	SF4	C	308	3	0,12,12	-	-	-		
9	EDO	B	306	-	3,3,3	0.07	0	2,2,2	0.21	0
5	MES	A	502	-	12,12,12	1.69	3 (25%)	14,16,16	2.24	6 (42%)
12	PE4	C	302	-	21,21,23	0.16	0	20,20,22	0.16	0
8	SO4	F	304	-	4,4,4	0.15	0	6,6,6	0.07	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
10	FAD	B	301	-	-	4/30/50/50	0/6/6/6
9	EDO	D	501	-	-	0/1/1/1	-
9	EDO	D	510	-	-	1/1/1/1	-
13	FES	E	401	3	-	-	0/1/1/1
11	SF4	F	305	2	-	-	0/6/5/5
4	GOL	E	404	-	-	0/4/4/4	-
10	FAD	F	301	-	-	8/30/50/50	0/6/6/6
11	SF4	E	405	3	-	-	0/6/5/5
4	GOL	A	503	-	-	2/4/4/4	-
4	GOL	D	503	-	-	1/4/4/4	-
11	SF4	E	407	3	-	-	0/6/5/5
9	EDO	D	509	-	-	0/1/1/1	-
11	SF4	E	406	3	-	-	0/6/5/5
4	GOL	A	501	-	-	3/4/4/4	-
9	EDO	A	508	-	-	1/1/1/1	-
9	EDO	D	511	-	-	1/1/1/1	-
9	EDO	C	304	-	-	0/1/1/1	-
4	GOL	D	502	-	-	2/4/4/4	-
4	GOL	E	403	-	-	0/4/4/4	-
9	EDO	A	509	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SF4	C	306	3	-	-	0/6/5/5
9	EDO	D	513	-	-	1/1/1/1	-
4	GOL	A	504	-	-	4/4/4/4	-
9	EDO	B	307	-	-	0/1/1/1	-
11	SF4	C	307	3	-	-	0/6/5/5
9	EDO	A	510	-	-	0/1/1/1	-
9	EDO	C	305	-	-	1/1/1/1	-
4	GOL	C	301	-	-	0/4/4/4	-
9	EDO	B	305	-	-	0/1/1/1	-
9	EDO	D	512	-	-	1/1/1/1	-
11	SF4	B	308	2	-	-	0/6/5/5
4	GOL	E	402	-	-	1/4/4/4	-
9	EDO	D	507	-	-	0/1/1/1	-
9	EDO	D	508	-	-	0/1/1/1	-
11	SF4	C	308	3	-	-	0/6/5/5
9	EDO	B	306	-	-	1/1/1/1	-
5	MES	A	502	-	-	4/6/14/14	0/1/1/1
12	PE4	C	302	-	-	9/19/19/21	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	301	FAD	C9A-C5X	5.12	1.49	1.41
5	A	502	MES	C8-S	4.15	1.83	1.77
10	F	301	FAD	C8-C7	3.24	1.49	1.40
10	F	301	FAD	C4X-N5	2.67	1.35	1.30
10	F	301	FAD	C5A-C4A	2.57	1.47	1.40

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	MES	O2S-S-O1S	-3.85	100.64	113.95
5	A	502	MES	O1S-S-C8	3.58	111.23	106.92
5	A	502	MES	O3S-S-C8	3.29	111.09	105.77
5	A	502	MES	O2S-S-C8	3.20	110.77	106.92
10	F	301	FAD	C3B-C2B-C1B	3.20	105.80	100.98

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	GOL	C1-C2-C3-O3
4	A	504	GOL	O1-C1-C2-C3
5	A	502	MES	N4-C7-C8-S
5	A	502	MES	C7-C8-S-O2S
5	A	502	MES	C7-C8-S-O3S

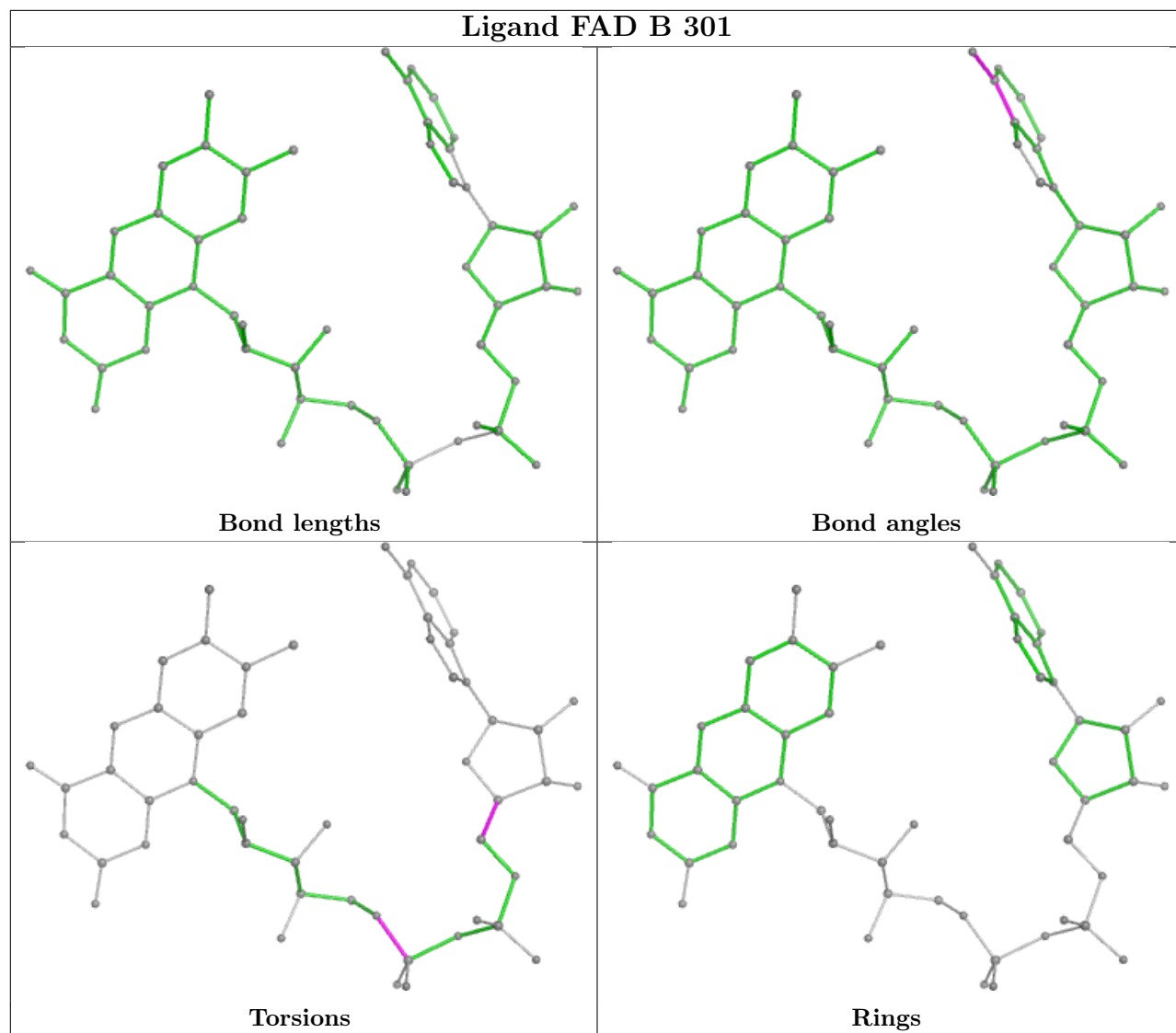
There are no ring outliers.

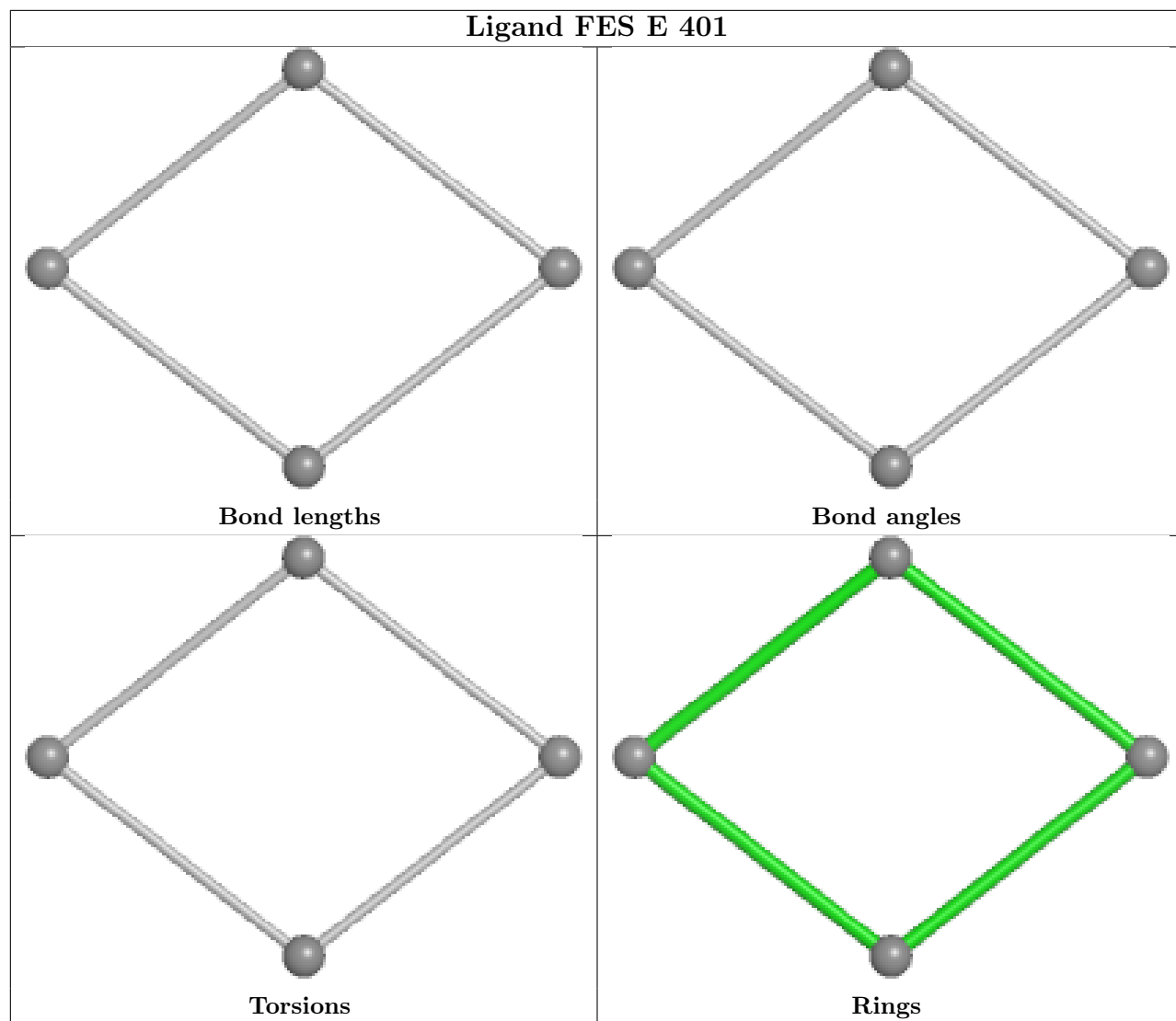
6 monomers are involved in 8 short contacts:

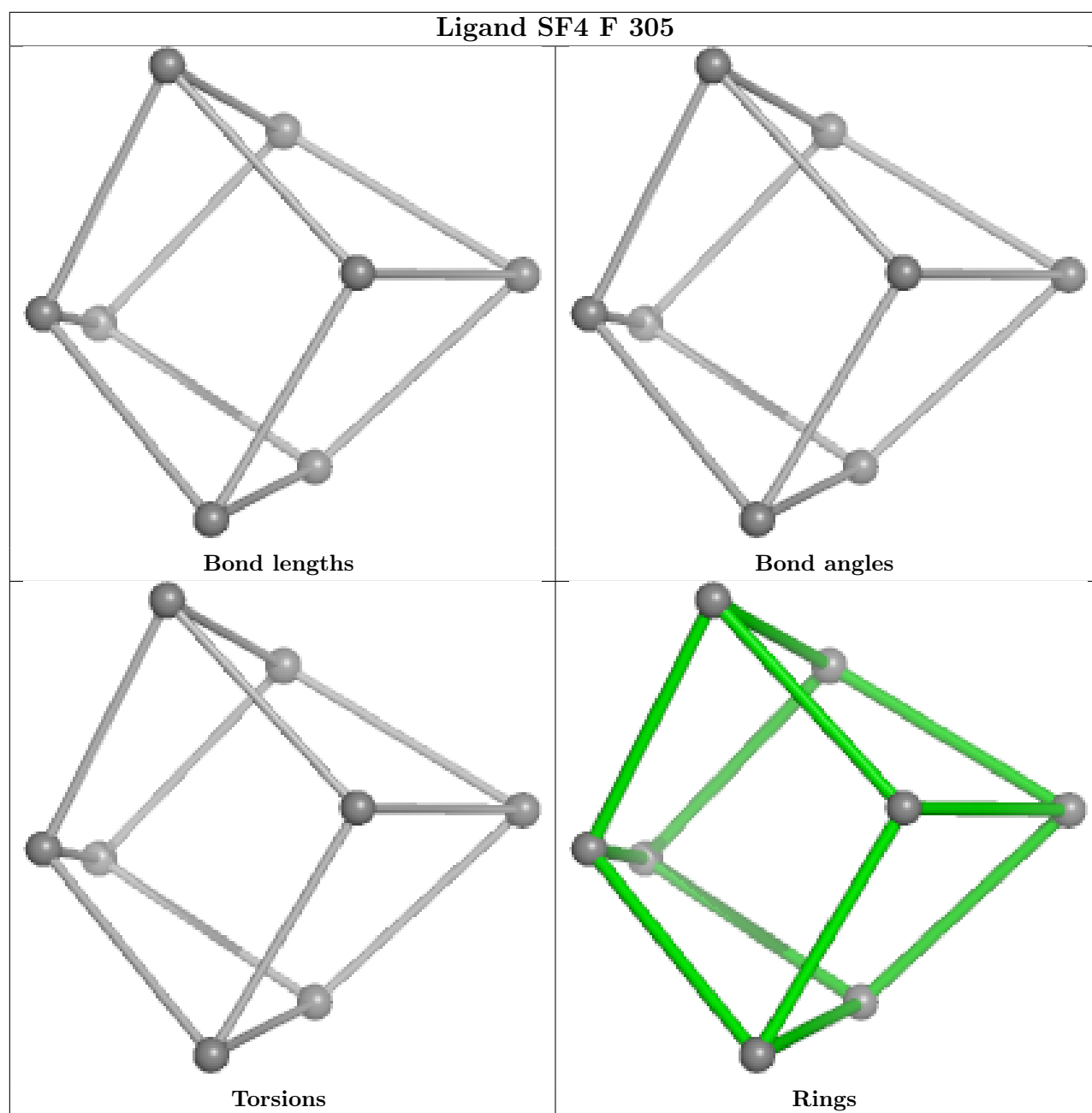
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	301	FAD	1	0
11	F	305	SF4	1	0
6	D	504	NFU	1	0
10	F	301	FAD	2	0
11	B	308	SF4	2	0
6	A	505	NFU	1	0

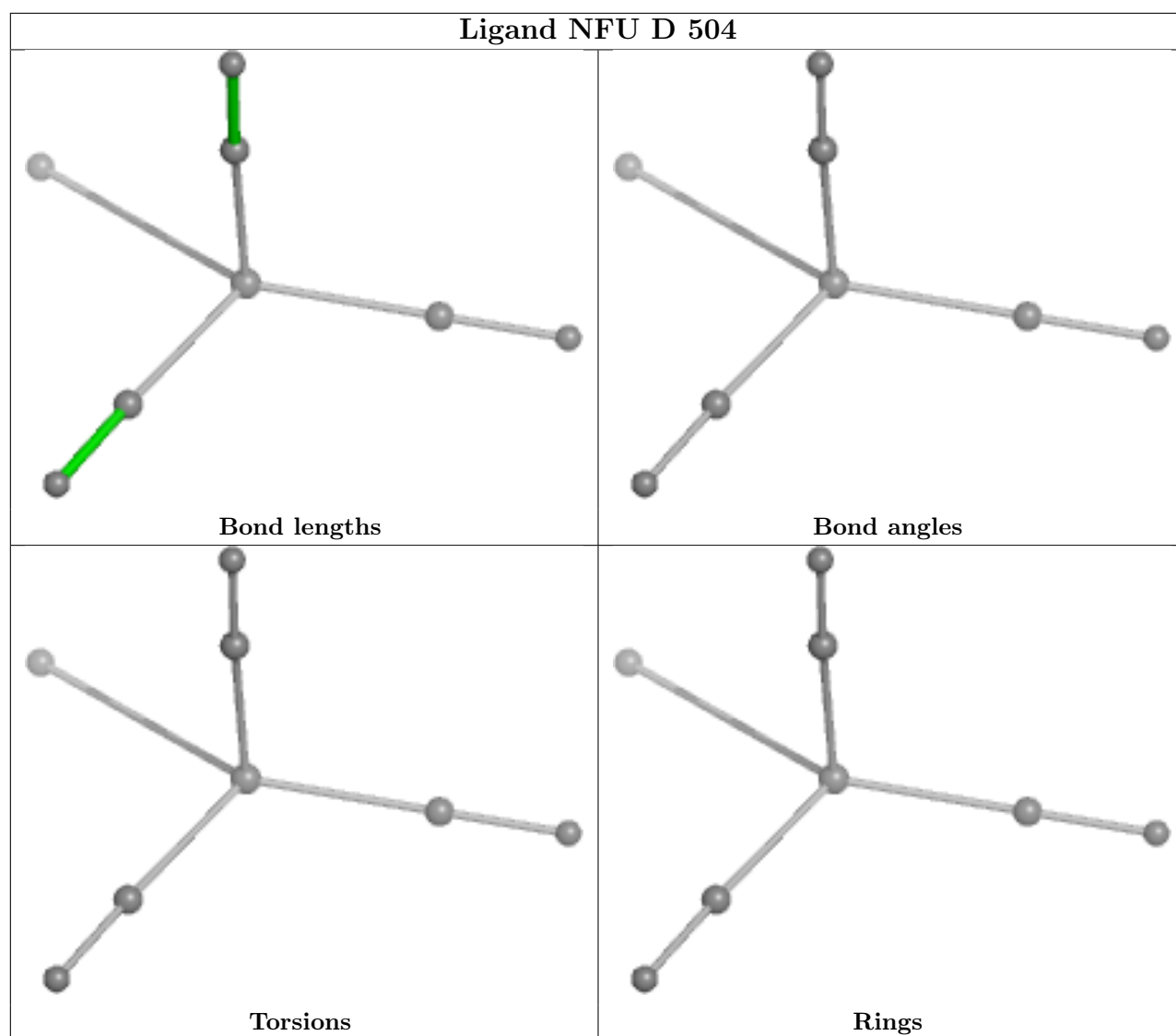
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 FAD B 301

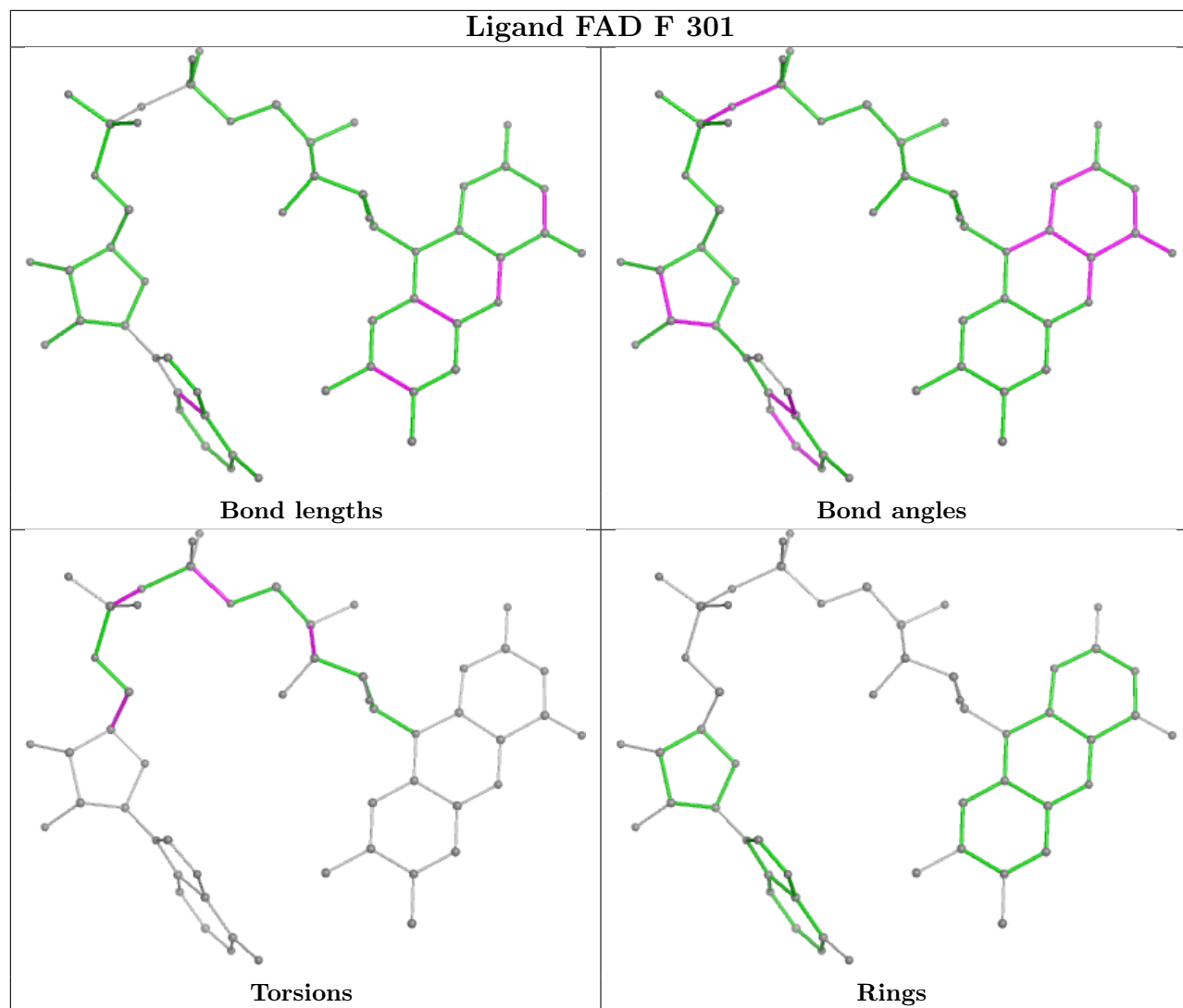


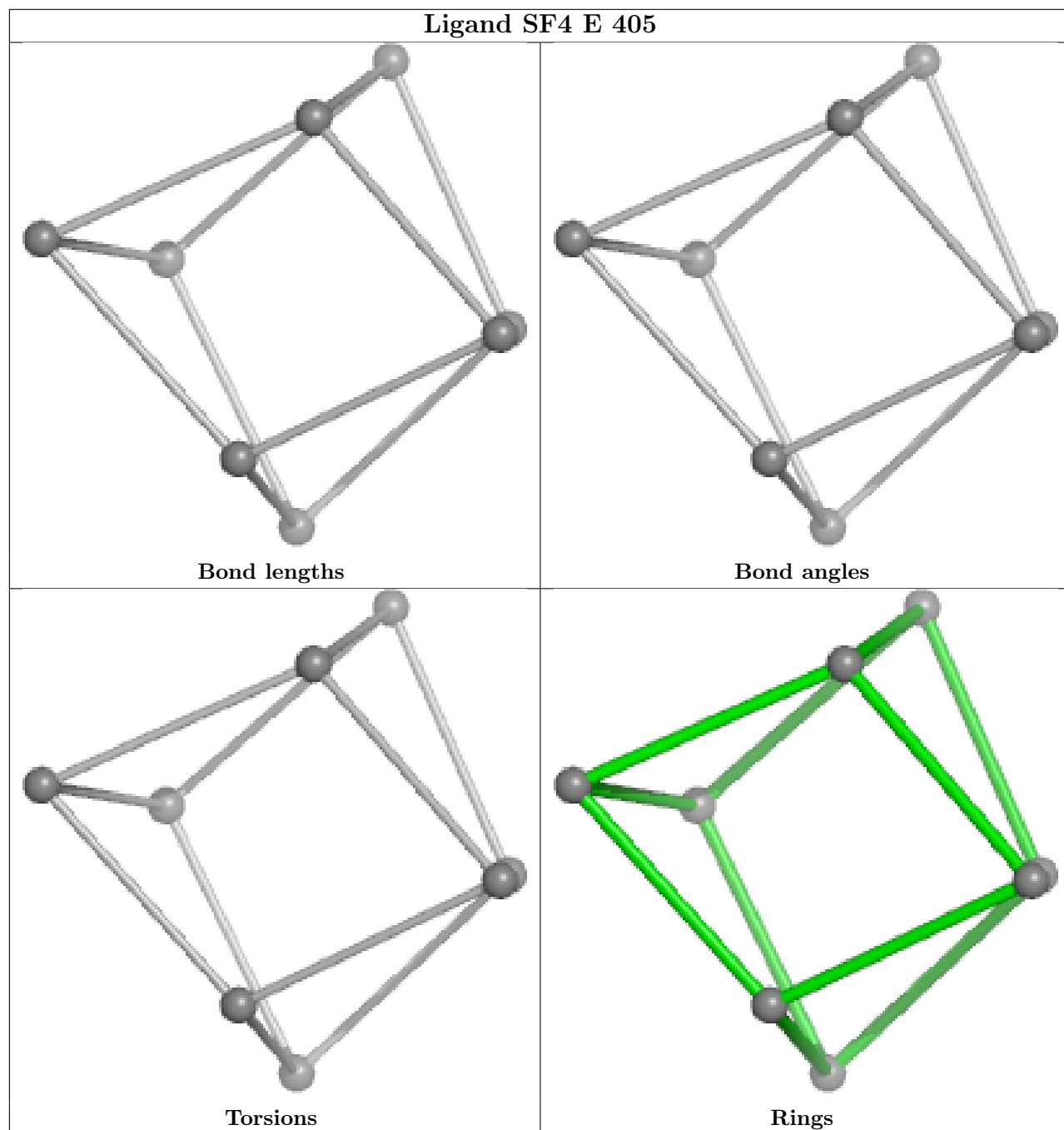




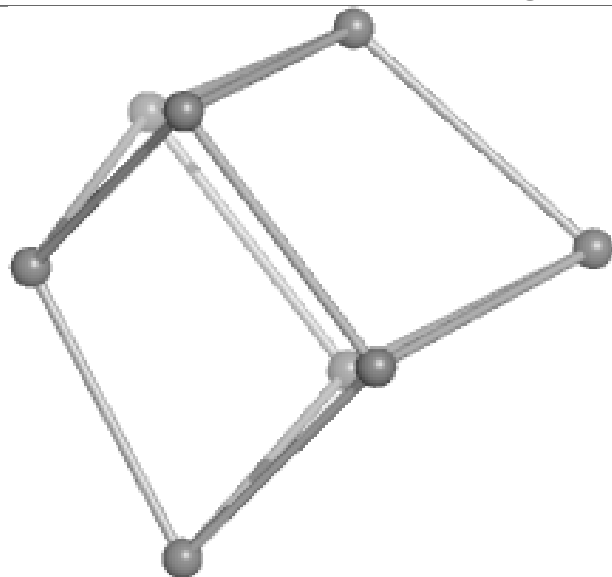


Ligand FAD F 301

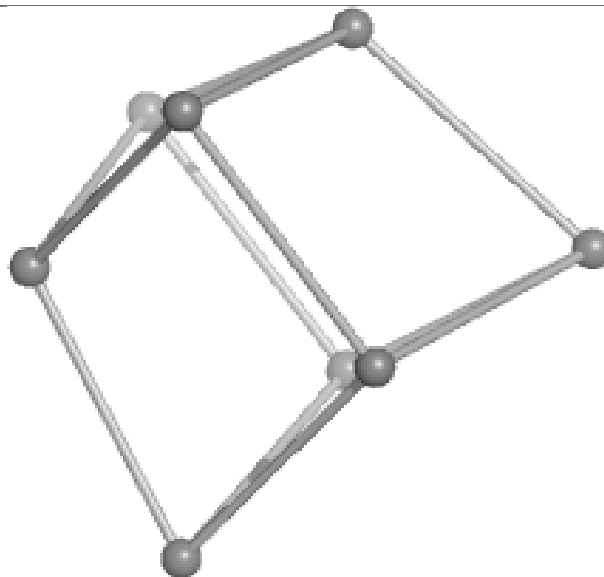




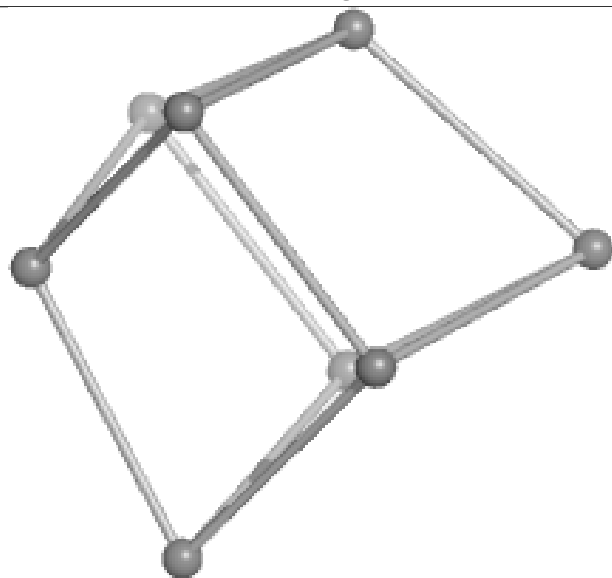
Ligand SF4 E 407



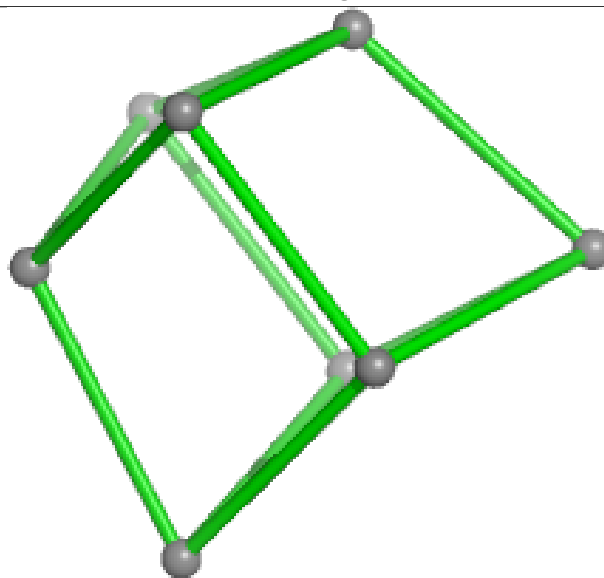
Bond lengths



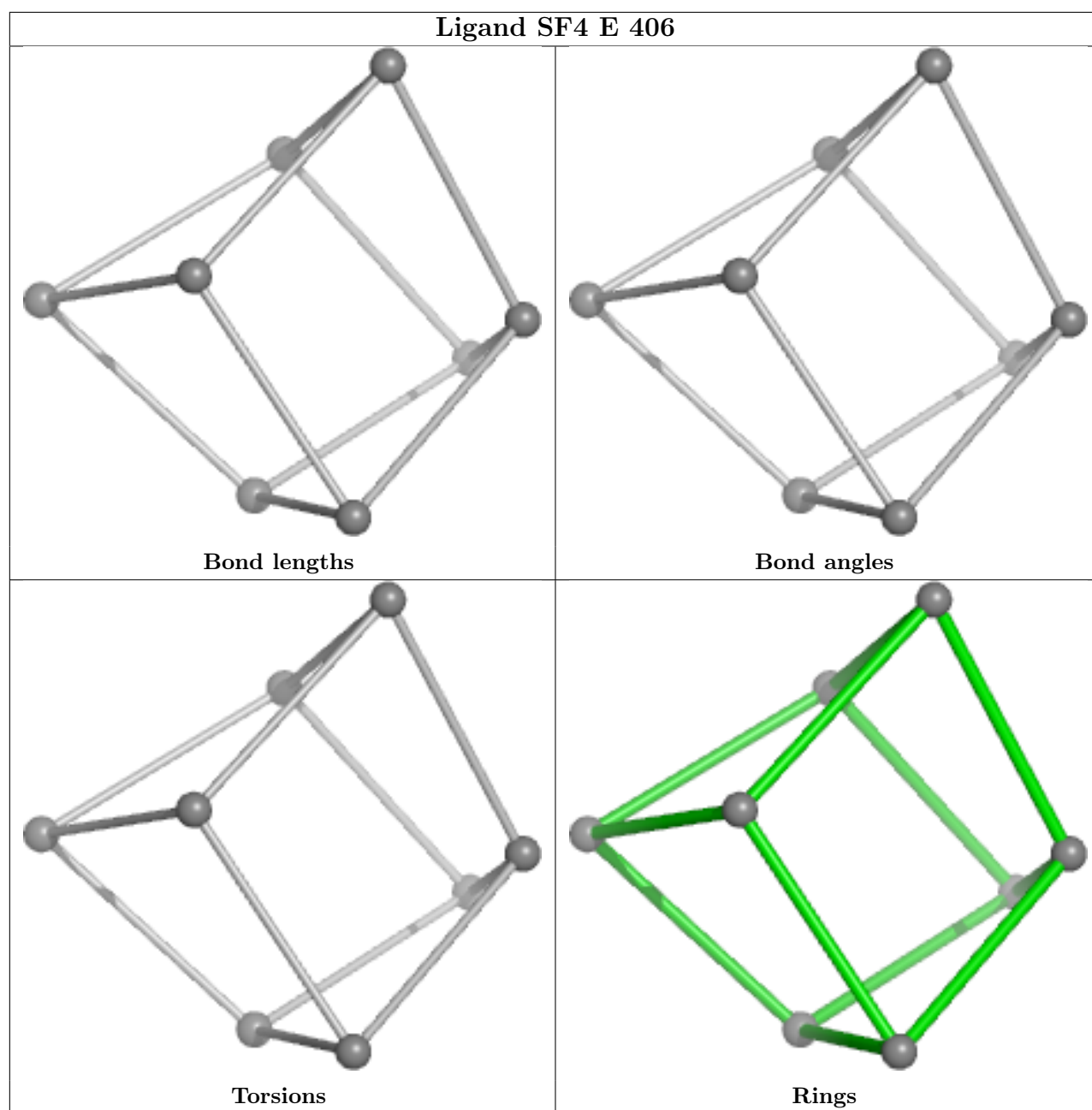
Bond angles



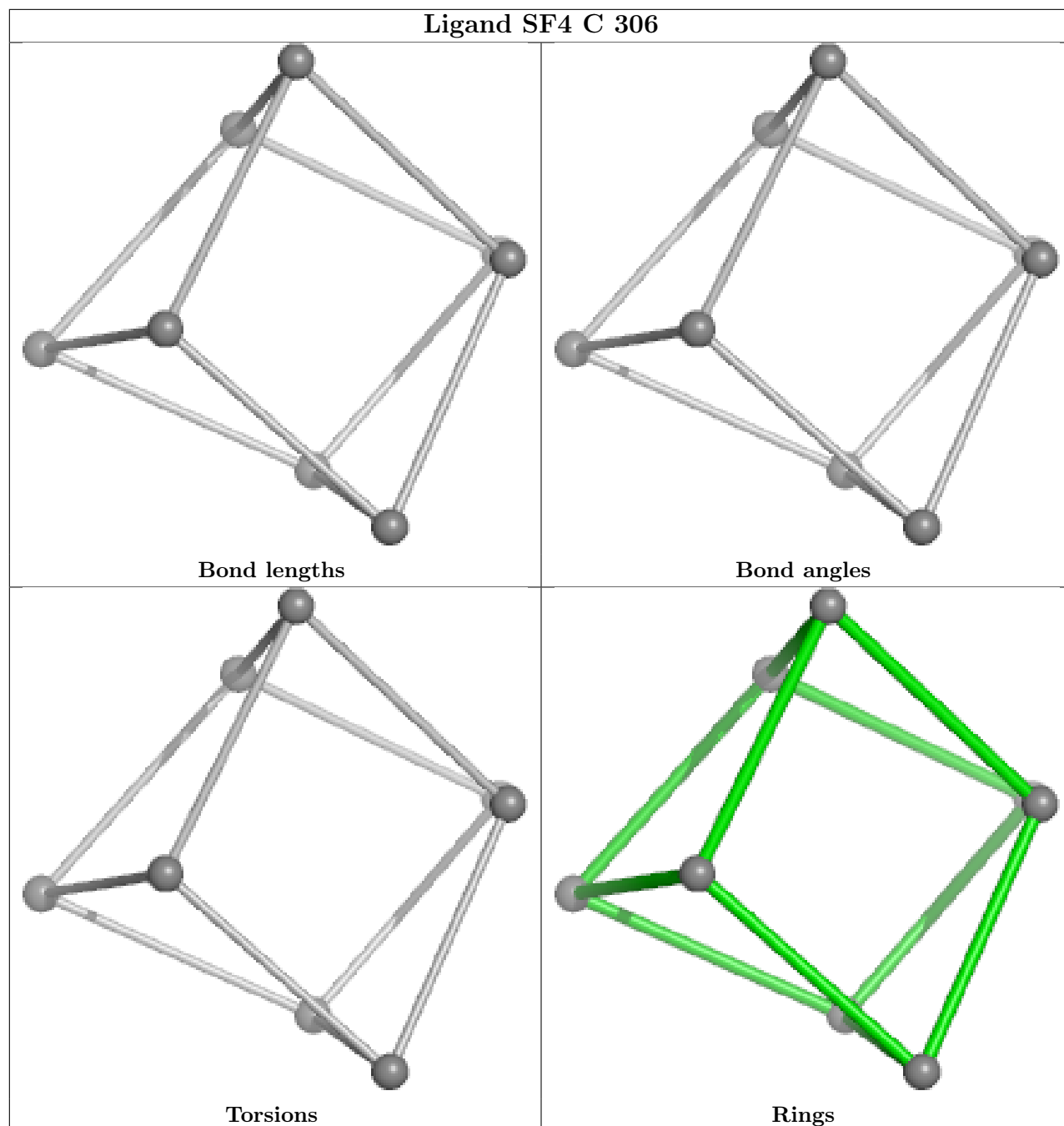
Torsions

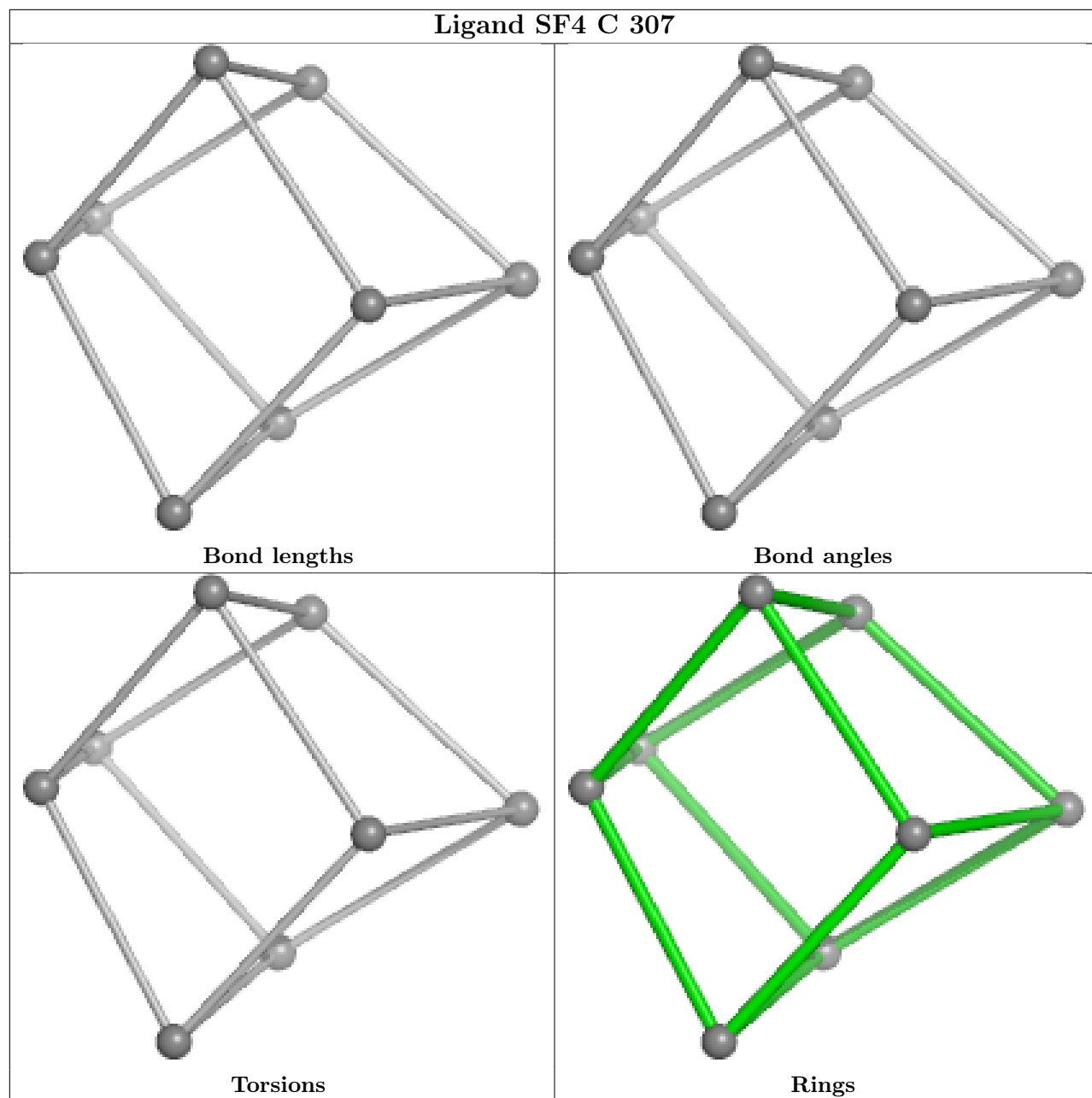


Rings

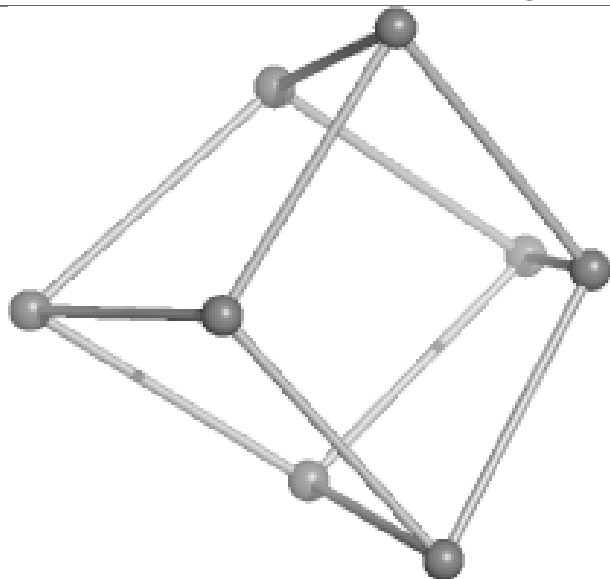


Ligand SF4 C 306

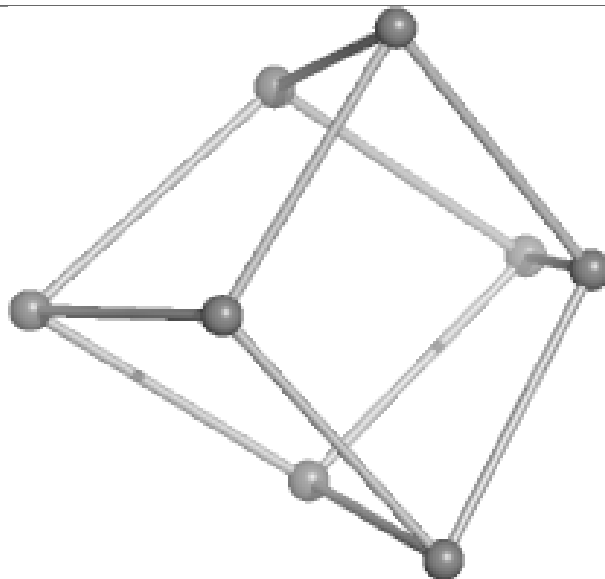




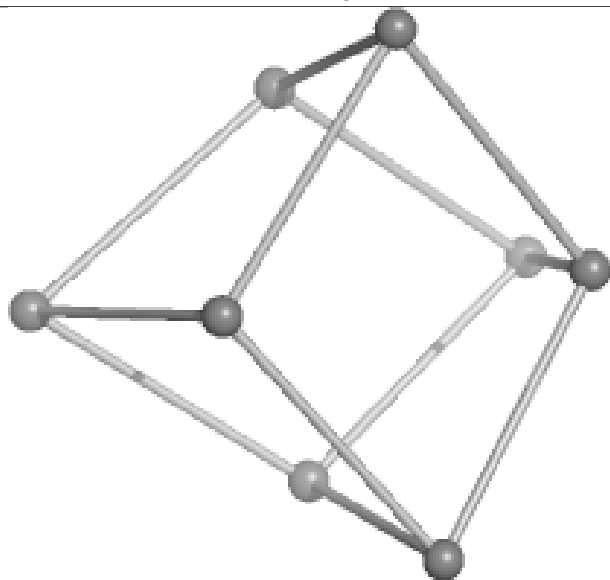
Ligand SF4 B 308



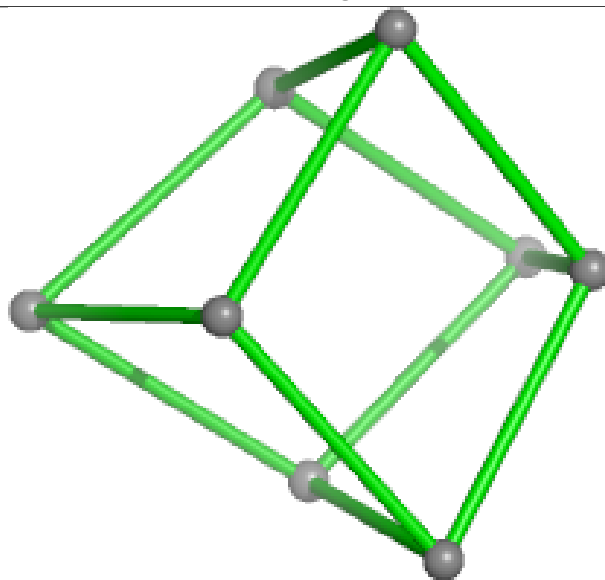
Bond lengths



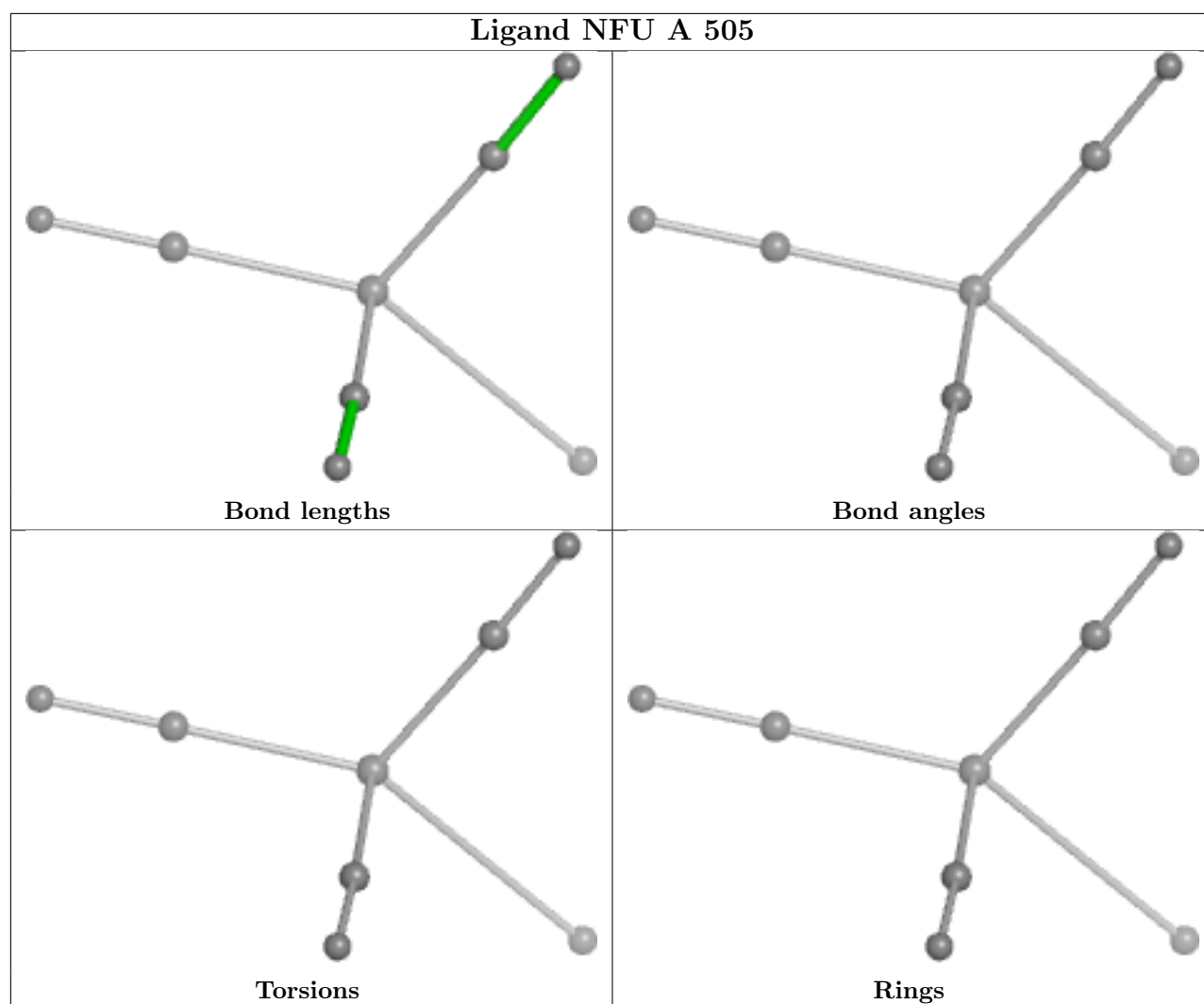
Bond angles

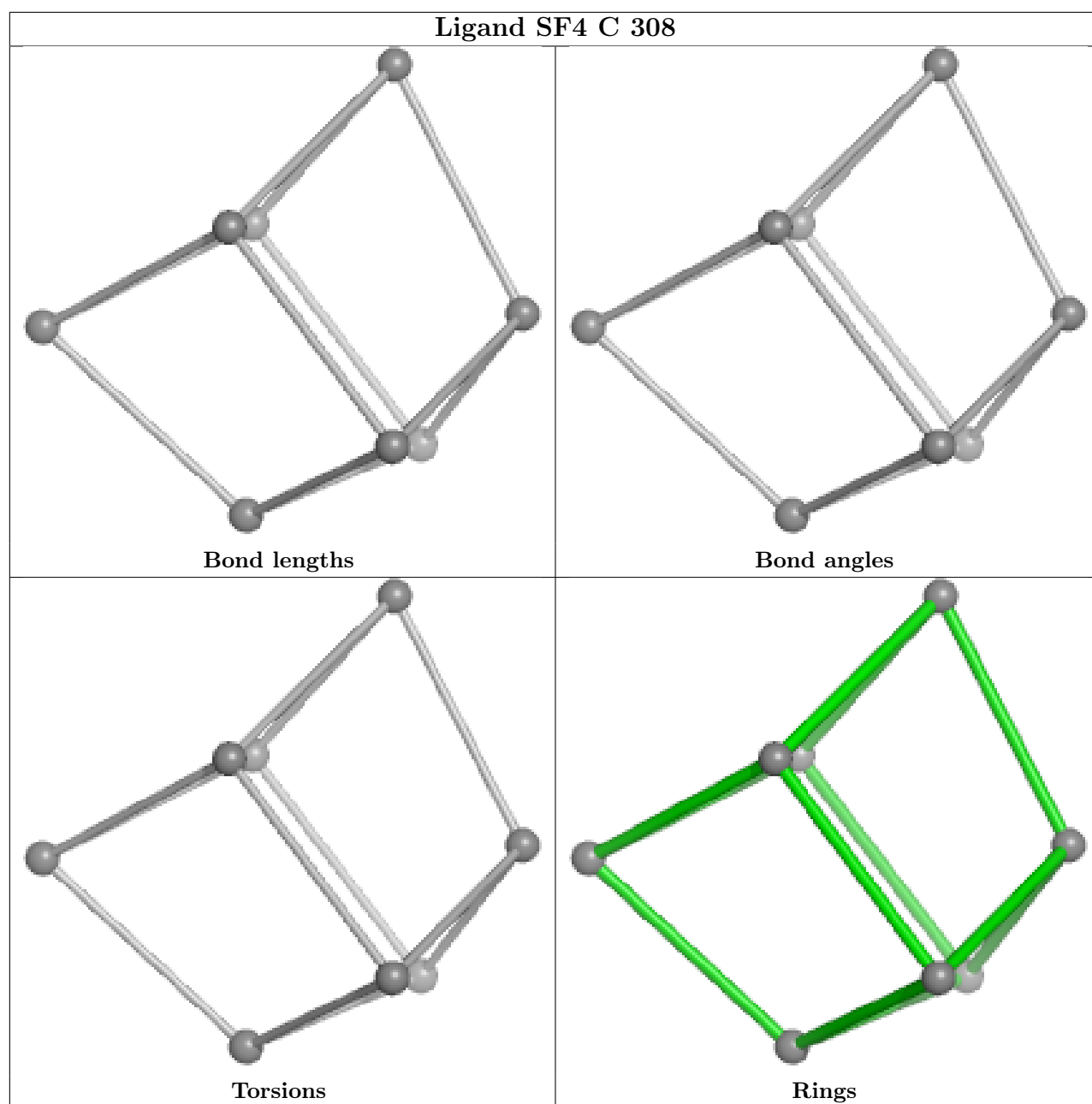


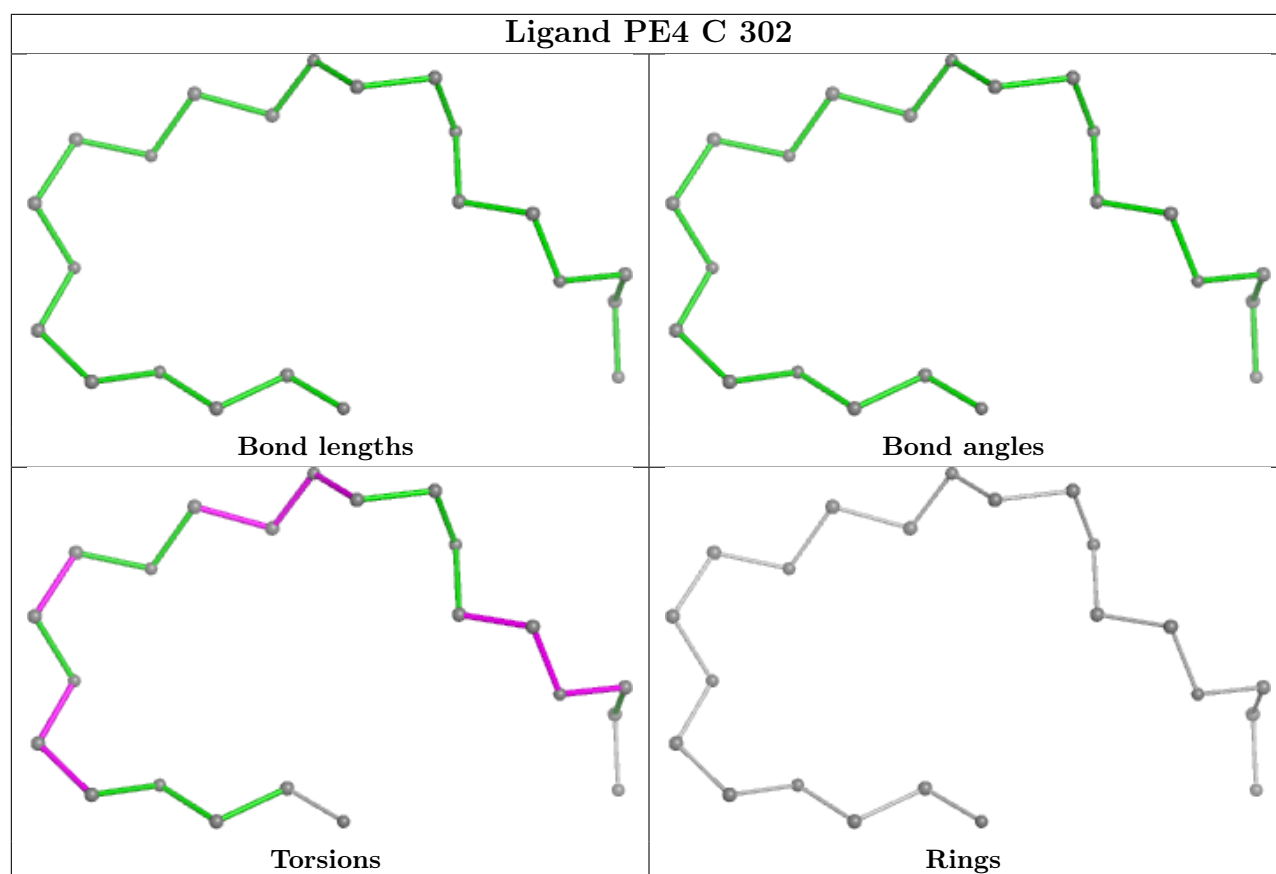
Torsions



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	392/410 (95%)	-0.73	0 100 100	52, 70, 92, 112	0
1	D	392/410 (95%)	-0.72	0 100 100	45, 70, 97, 114	0
2	B	282/282 (100%)	-0.23	5 (1%) 67 50	58, 93, 132, 169	0
2	F	282/282 (100%)	-0.16	6 (2%) 63 46	63, 99, 139, 181	0
3	C	240/241 (99%)	-0.62	0 100 100	54, 73, 105, 148	0
3	E	240/241 (99%)	-0.71	0 100 100	53, 71, 102, 144	0
All	All	1828/1866 (97%)	-0.55	11 (0%) 85 73	45, 76, 121, 181	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	55	LEU	4.4
2	F	72	ALA	3.2
2	B	75	LYS	2.8
2	B	165	LYS	2.5
2	F	165	LYS	2.4

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
9	EDO	C	305	4/4	0.51	0.17	106,108,114,116	0
8	SO4	C	303	5/5	0.53	0.11	129,143,163,179	0
8	SO4	A	507	5/5	0.58	0.10	131,150,168,172	0
9	EDO	C	304	4/4	0.62	0.21	84,84,89,90	0
8	SO4	B	304	5/5	0.64	0.08	152,153,165,168	0
8	SO4	F	304	5/5	0.70	0.07	149,155,158,166	0
4	GOL	E	404	6/6	0.71	0.18	94,104,110,116	0
8	SO4	D	506	5/5	0.72	0.09	131,141,154,159	0
4	GOL	E	402	6/6	0.72	0.16	74,92,109,115	0
9	EDO	D	511	4/4	0.72	0.19	70,74,84,98	0
9	EDO	B	305	4/4	0.74	0.19	85,89,92,95	0
9	EDO	D	509	4/4	0.75	0.29	99,105,105,108	0
9	EDO	A	509	4/4	0.76	0.17	84,88,90,97	0
9	EDO	D	512	4/4	0.76	0.23	79,86,94,102	0
8	SO4	B	303	5/5	0.77	0.32	108,115,142,166	0
8	SO4	F	303	5/5	0.77	0.11	117,118,155,166	0
9	EDO	D	513	4/4	0.77	0.28	94,99,100,101	0
9	EDO	A	510	4/4	0.81	0.27	91,101,104,105	0
9	EDO	B	306	4/4	0.82	0.20	79,97,98,109	0
5	MES	A	502	12/12	0.83	0.19	93,109,168,177	0
8	SO4	F	302	5/5	0.85	0.18	103,107,137,161	0
9	EDO	A	508	4/4	0.85	0.19	81,83,84,85	0
4	GOL	A	504	6/6	0.85	0.17	77,100,109,111	0
4	GOL	D	503	6/6	0.86	0.20	82,94,112,113	0
4	GOL	A	501	6/6	0.87	0.13	77,90,94,94	0
10	FAD	B	301	53/53	0.87	0.18	97,131,147,156	0
10	FAD	F	301	53/53	0.87	0.17	95,142,159,163	0
12	PE4	C	302	22/24	0.87	0.20	80,113,126,129	0
9	EDO	B	307	4/4	0.88	0.17	79,83,83,84	0
4	GOL	A	503	6/6	0.88	0.19	77,95,108,115	0
9	EDO	D	508	4/4	0.89	0.25	74,75,79,84	0
8	SO4	B	302	5/5	0.91	0.26	115,120,153,157	0
7	FE	A	506	1/1	0.92	0.24	67,67,67,67	0
4	GOL	E	403	6/6	0.92	0.13	74,83,100,112	0
9	EDO	D	510	4/4	0.92	0.20	66,72,84,91	0
9	EDO	D	501	4/4	0.93	0.14	70,70,77,85	0
7	FE	D	505	1/1	0.93	0.27	74,74,74,74	0

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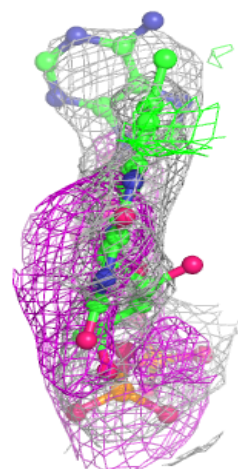
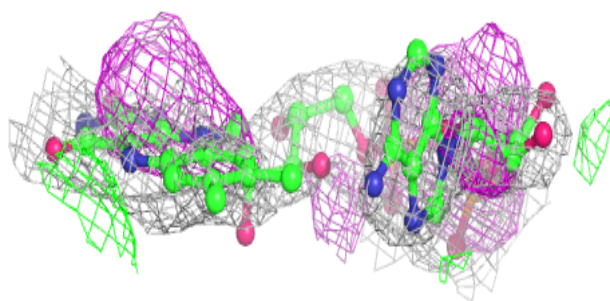
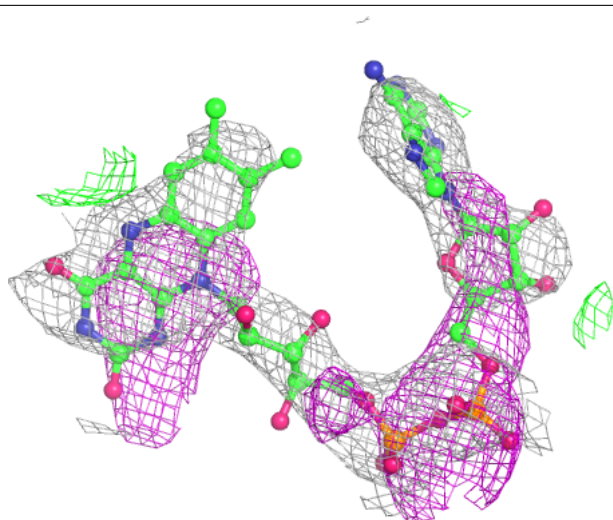
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	D	502	6/6	0.94	0.12	55,78,83,98	0
4	GOL	C	301	6/6	0.94	0.13	66,84,93,97	0
9	EDO	D	507	4/4	0.94	0.22	73,77,80,87	0
13	FES	E	401	4/4	0.94	0.14	87,96,106,111	0
11	SF4	F	305	8/8	0.97	0.08	68,104,133,135	0
11	SF4	E	406	8/8	0.98	0.09	84,97,99,126	0
11	SF4	E	407	8/8	0.98	0.07	82,94,108,132	0
11	SF4	C	306	8/8	0.98	0.08	71,92,107,114	0
11	SF4	C	307	8/8	0.98	0.09	83,93,111,124	0
11	SF4	C	308	8/8	0.98	0.08	77,93,116,118	0
6	NFU	A	505	8/8	0.99	0.14	51,67,75,81	0
11	SF4	B	308	8/8	0.99	0.06	65,102,111,112	0
11	SF4	E	405	8/8	0.99	0.08	67,93,110,111	0
6	NFU	D	504	8/8	0.99	0.12	51,68,86,90	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.

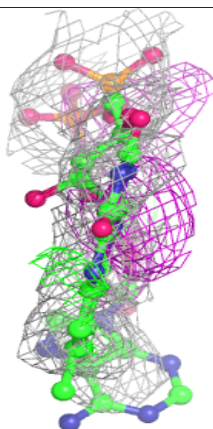
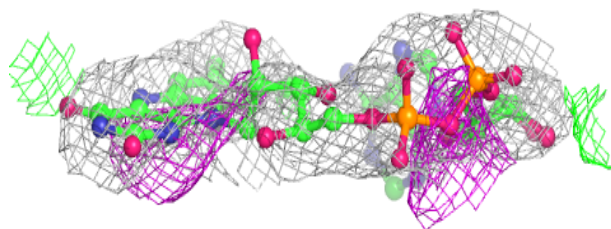
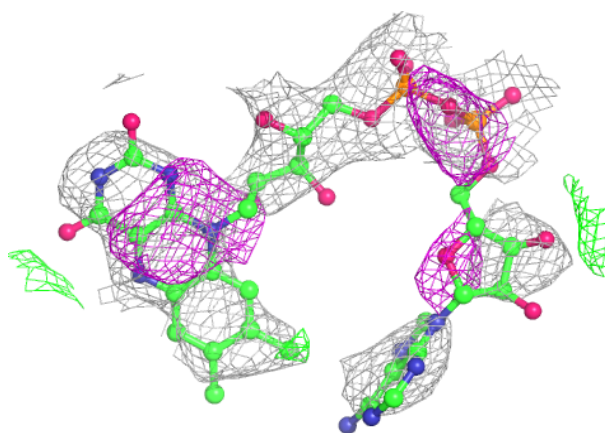
Electron density around FAD B 301:

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

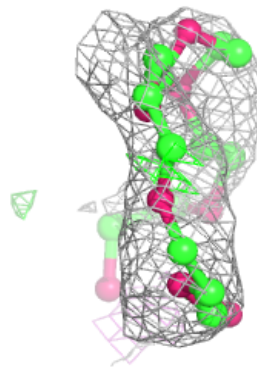
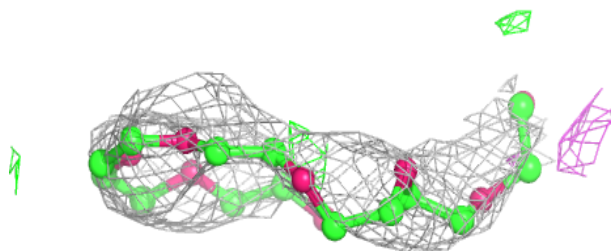
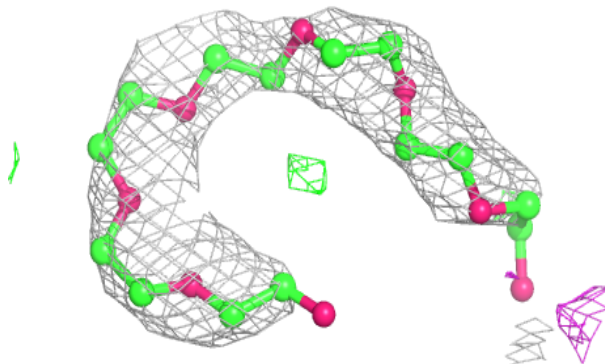


Electron density around FAD F 301:

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

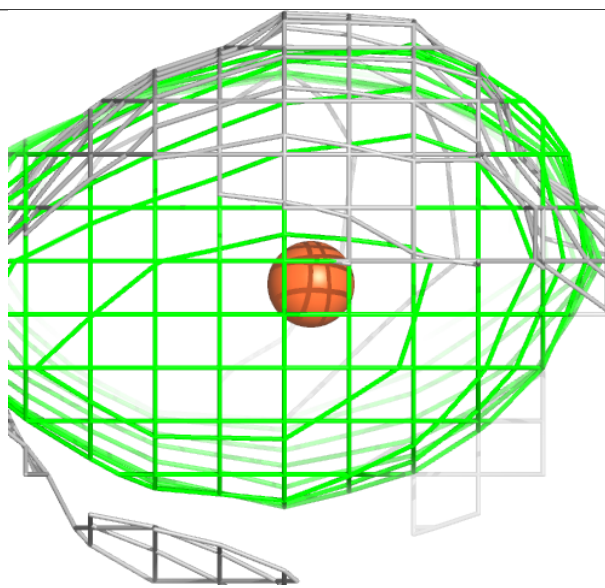
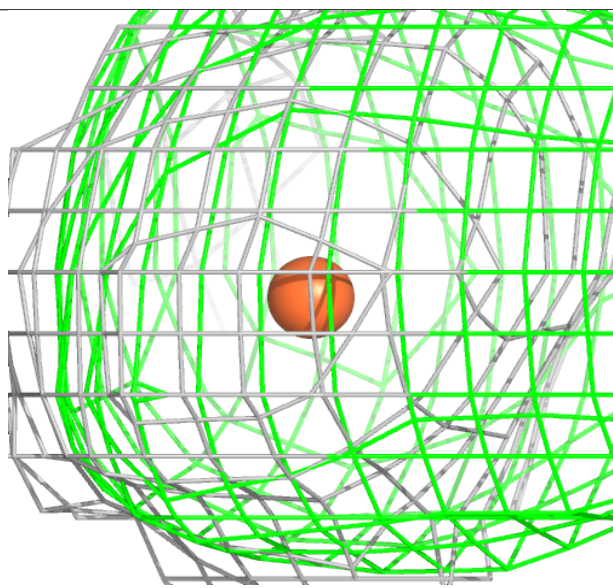
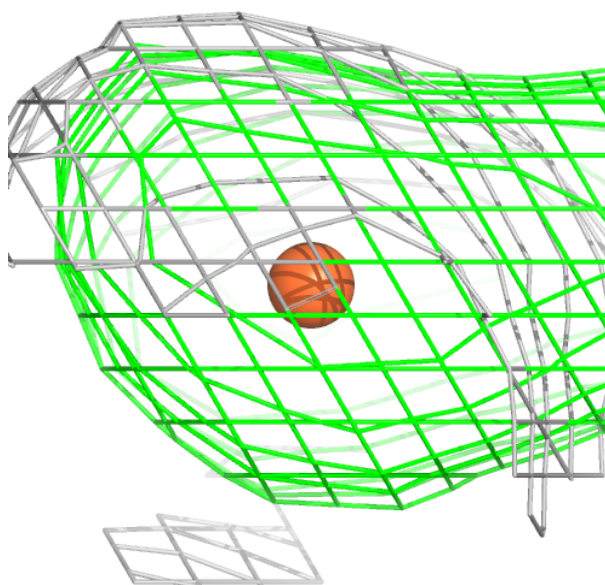
**Electron density around PE4 C 302:**

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



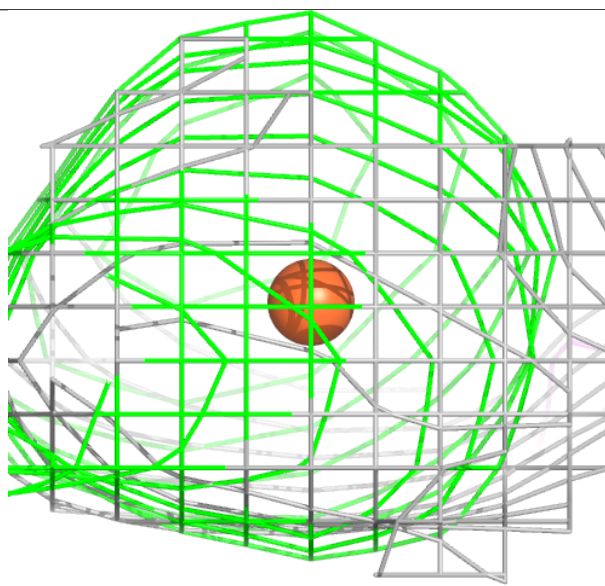
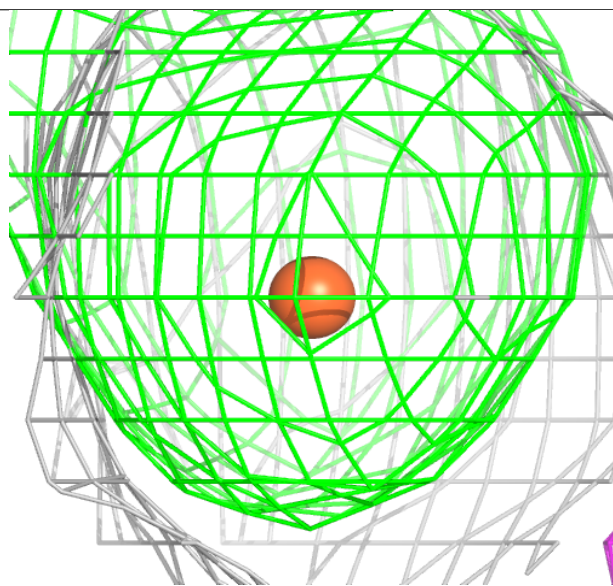
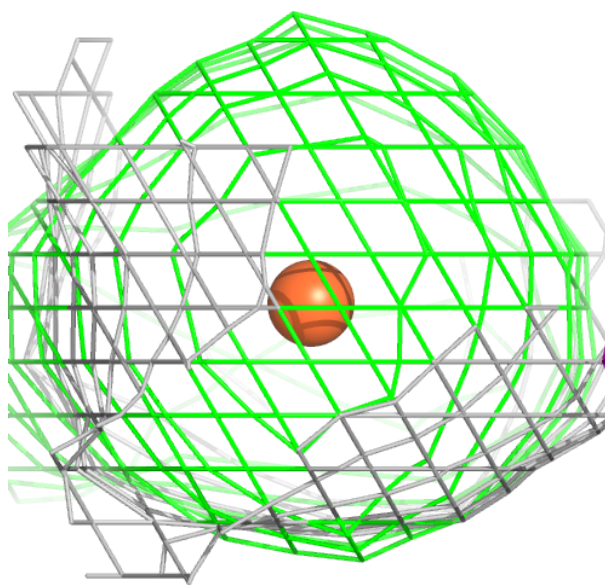
Electron density around FE A 506:

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



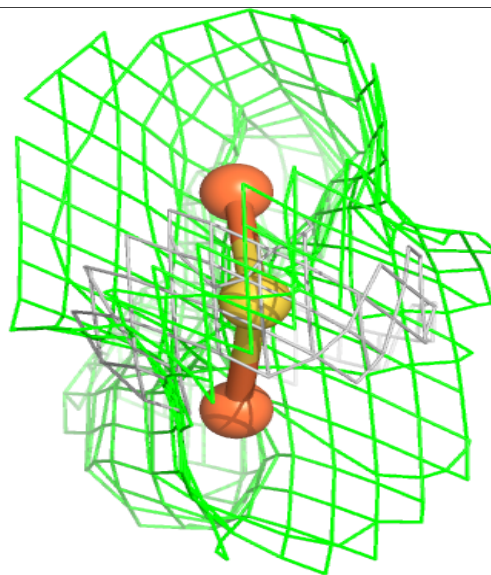
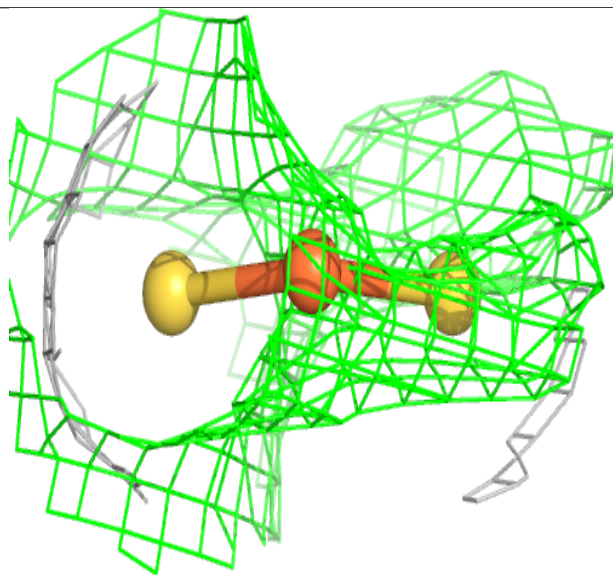
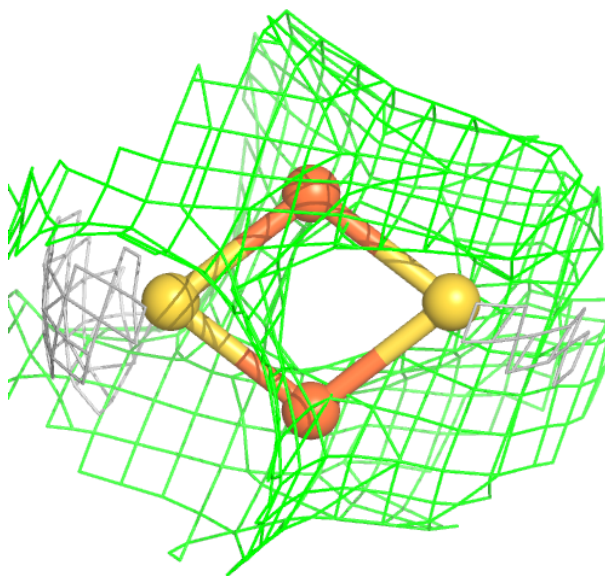
Electron density around FE D 505:

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



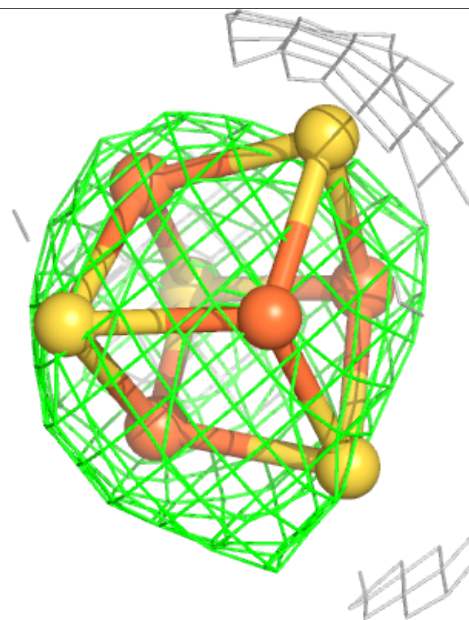
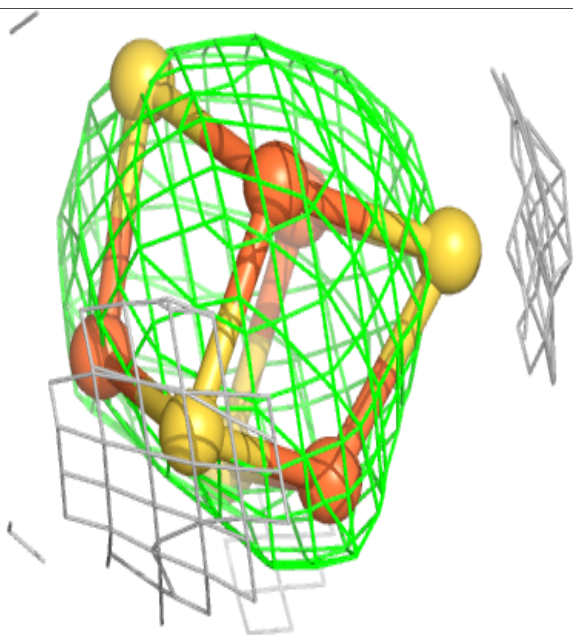
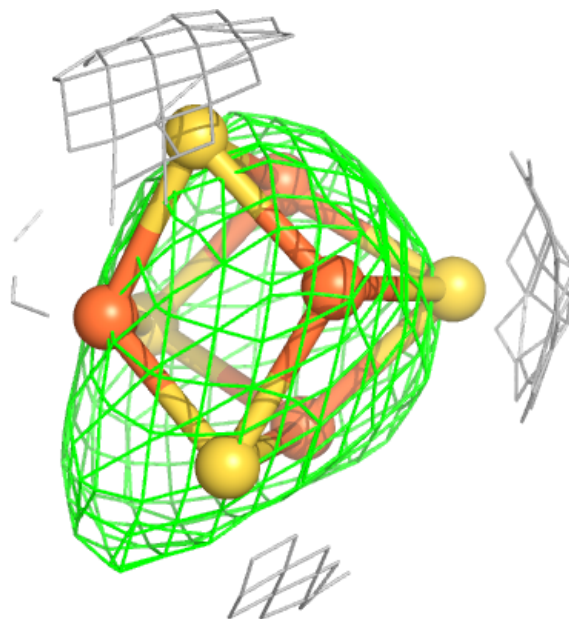
Electron density around FES E 401:

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



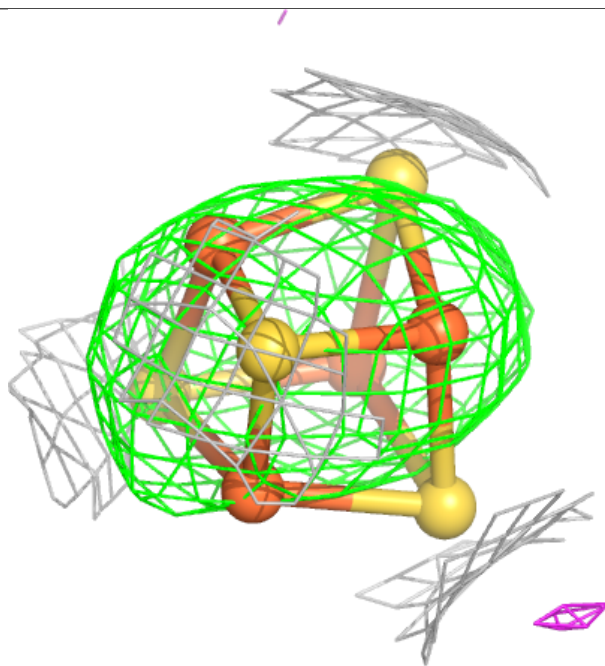
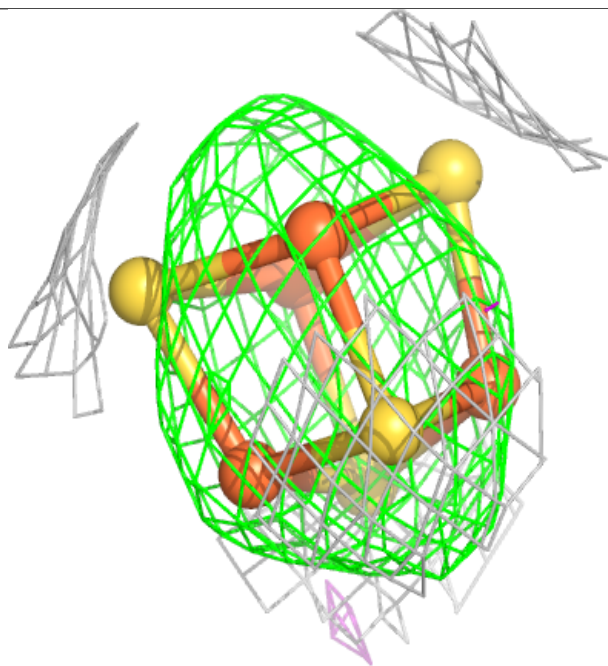
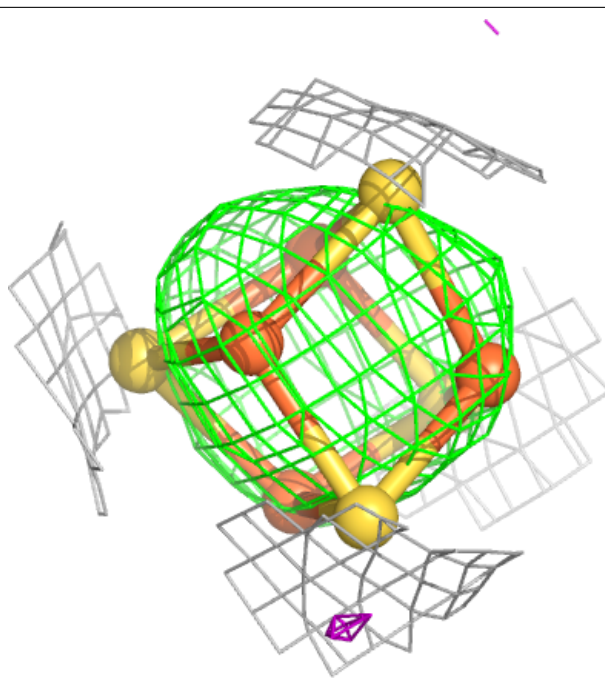
Electron density around SF4 F 305:

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



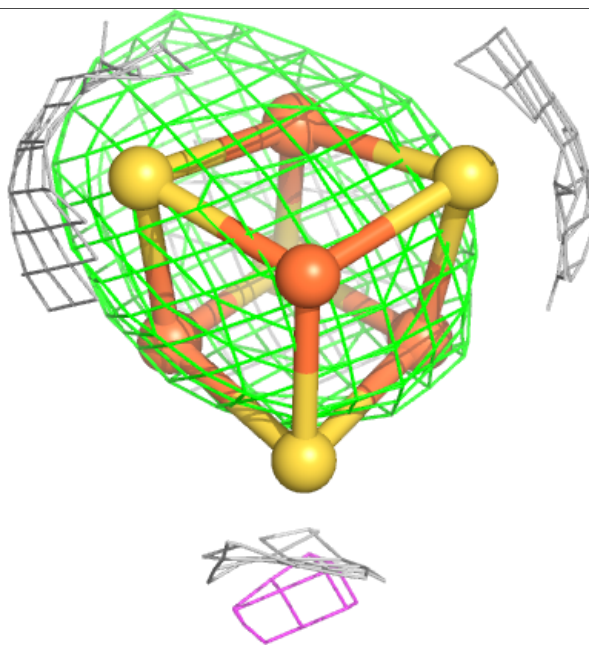
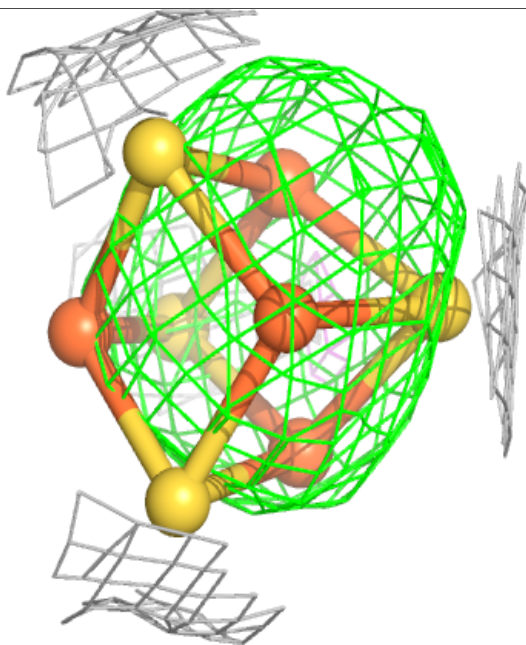
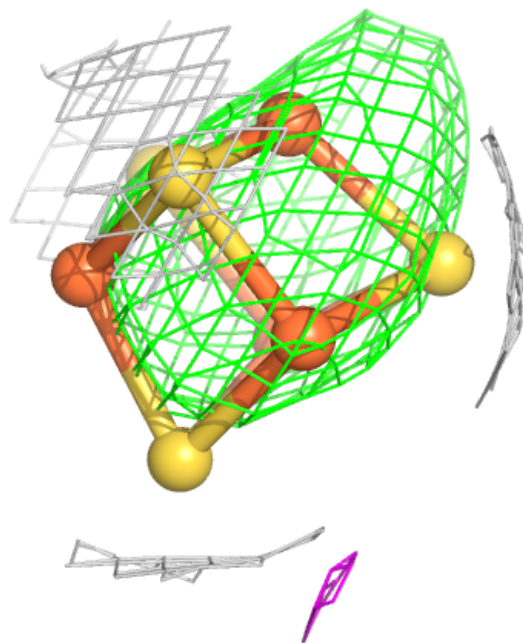
Electron density around SF4 E 406:

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



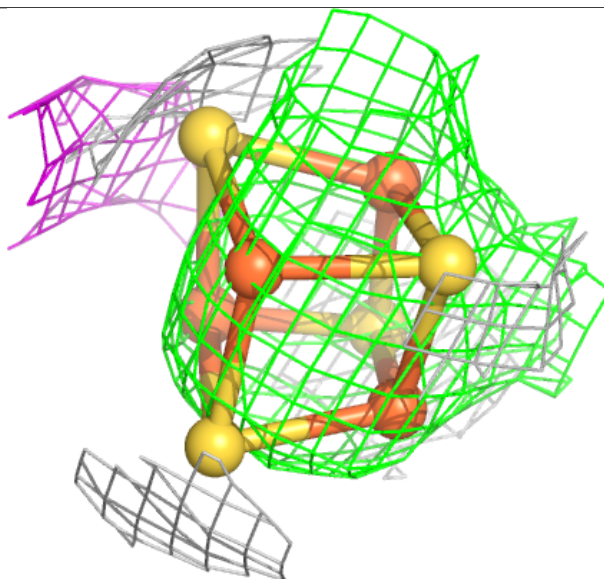
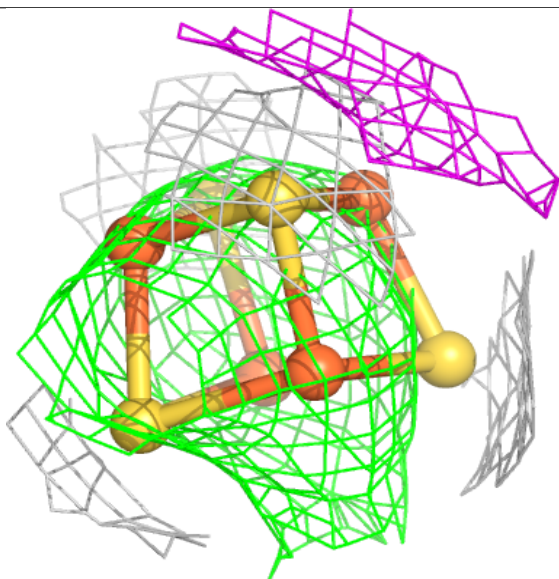
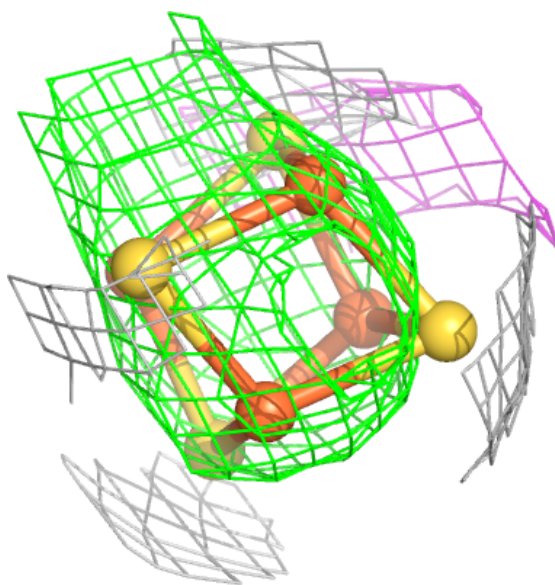
Electron density around SF4 E 407:

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



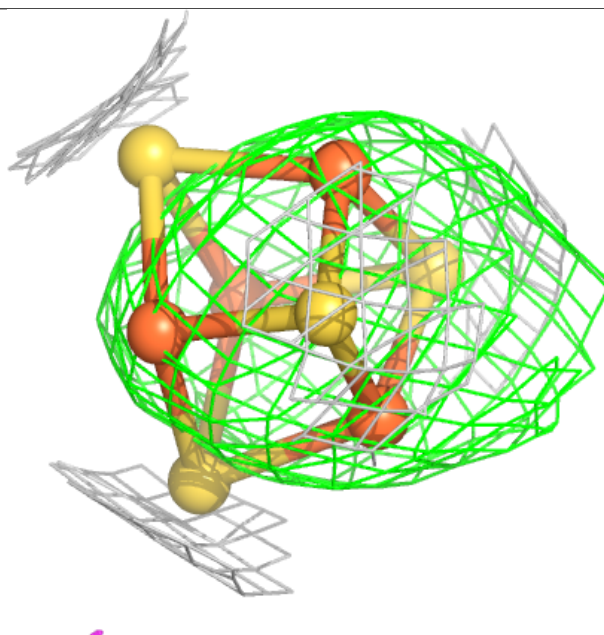
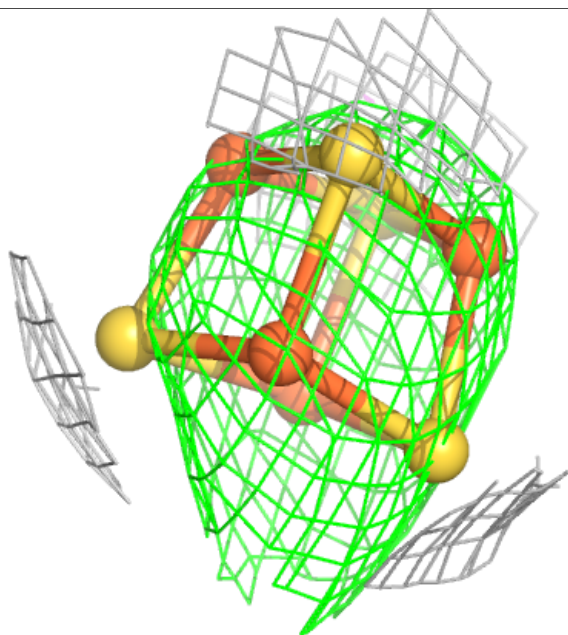
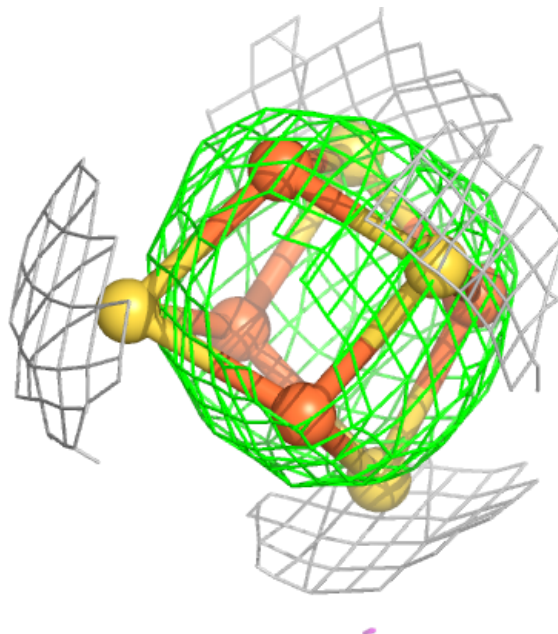
Electron density around SF4 C 306:

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



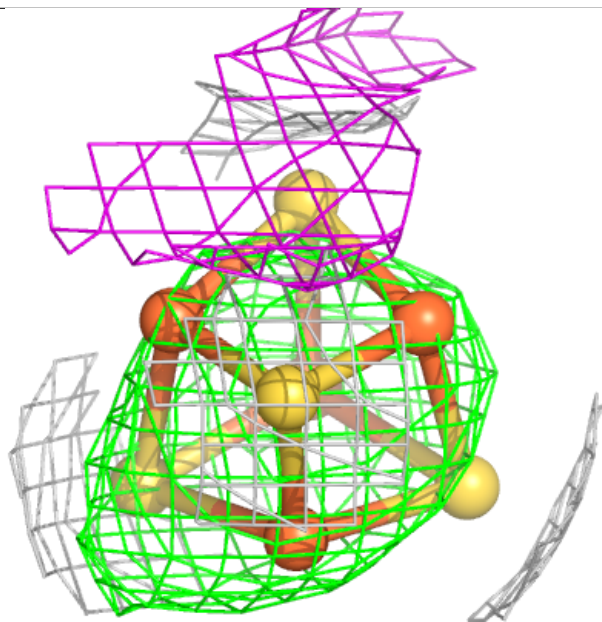
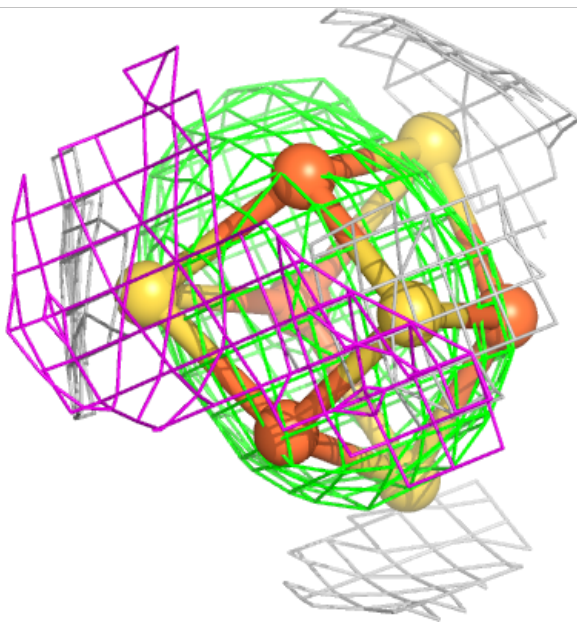
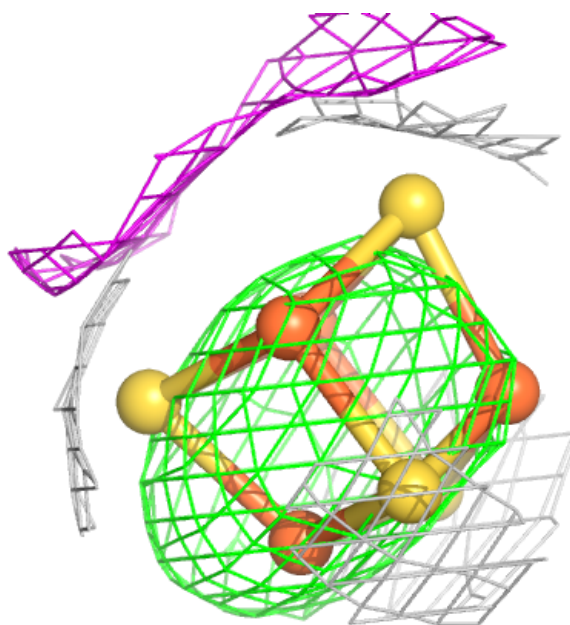
Electron density around SF4 C 307:

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



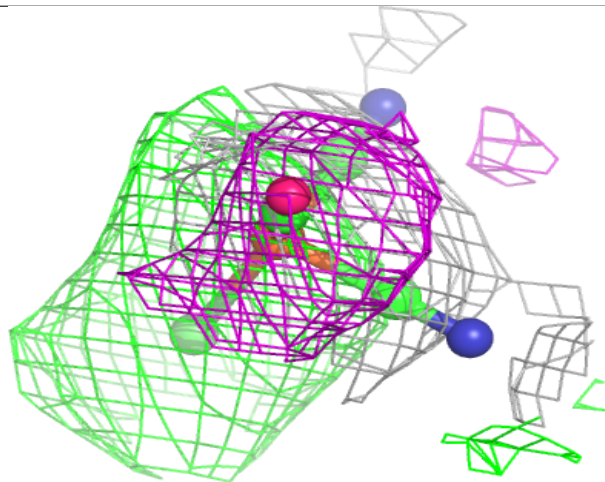
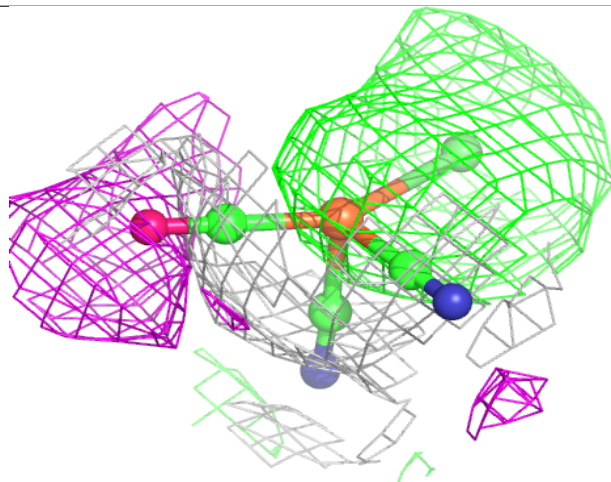
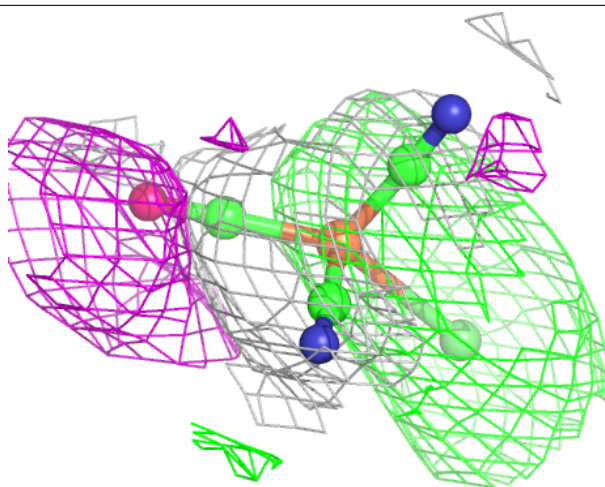
Electron density around SF4 C 308:

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



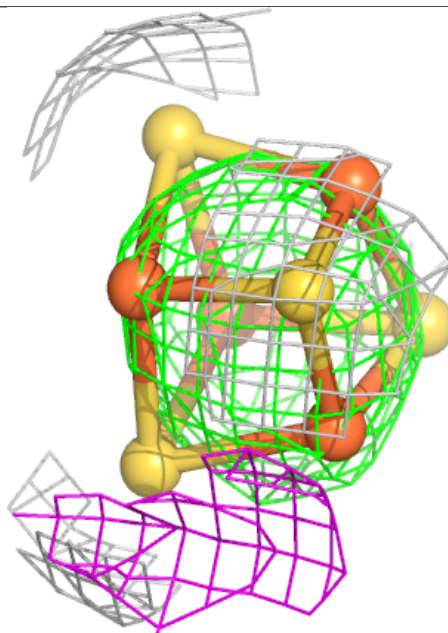
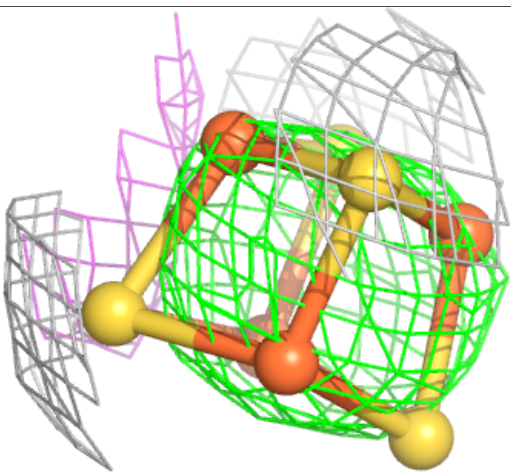
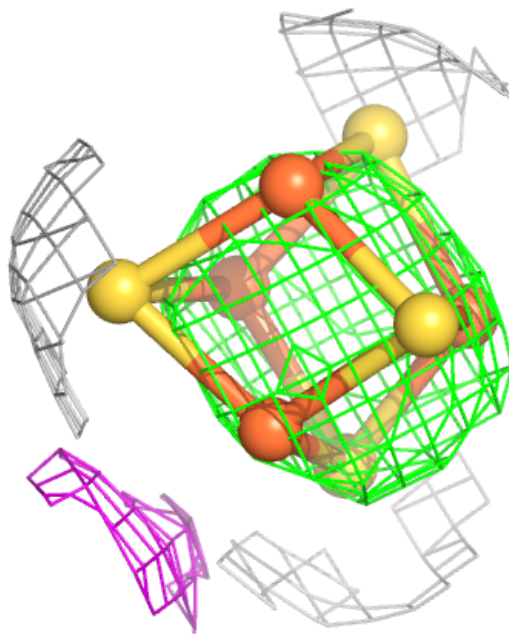
Electron density around NFU A 505:

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



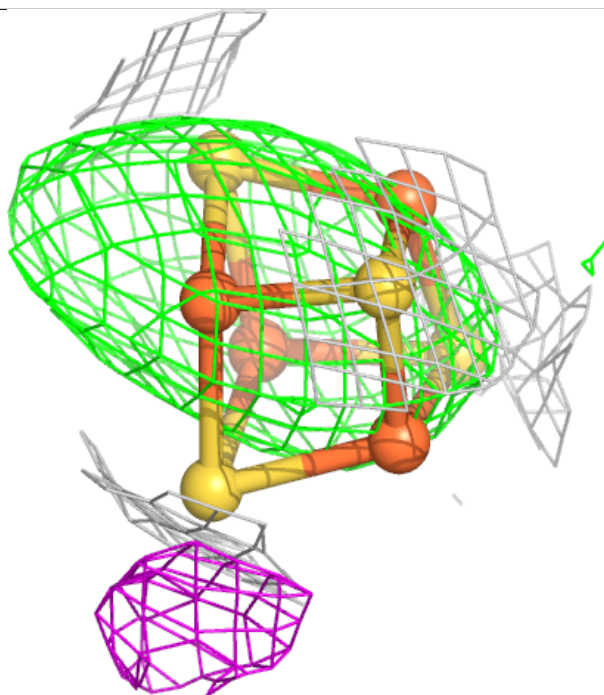
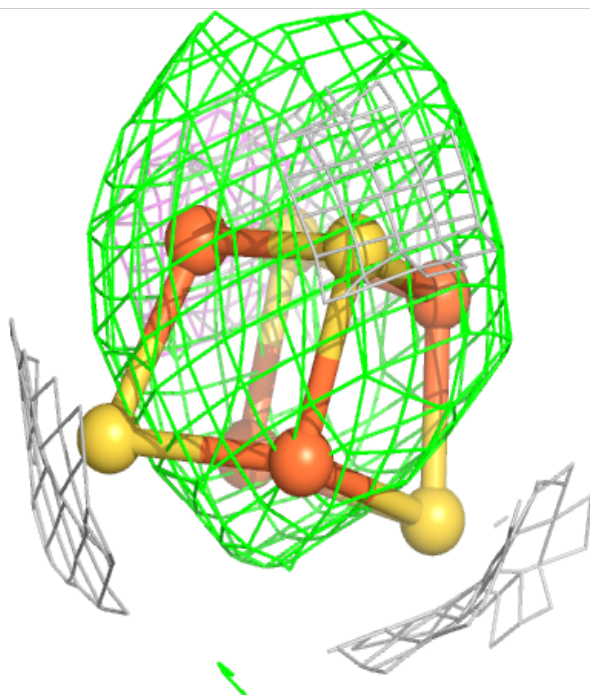
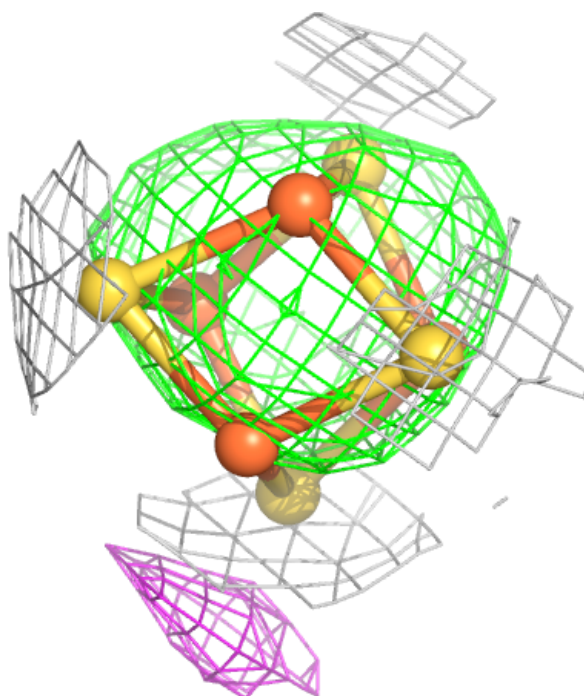
Electron density around SF4 B 308:

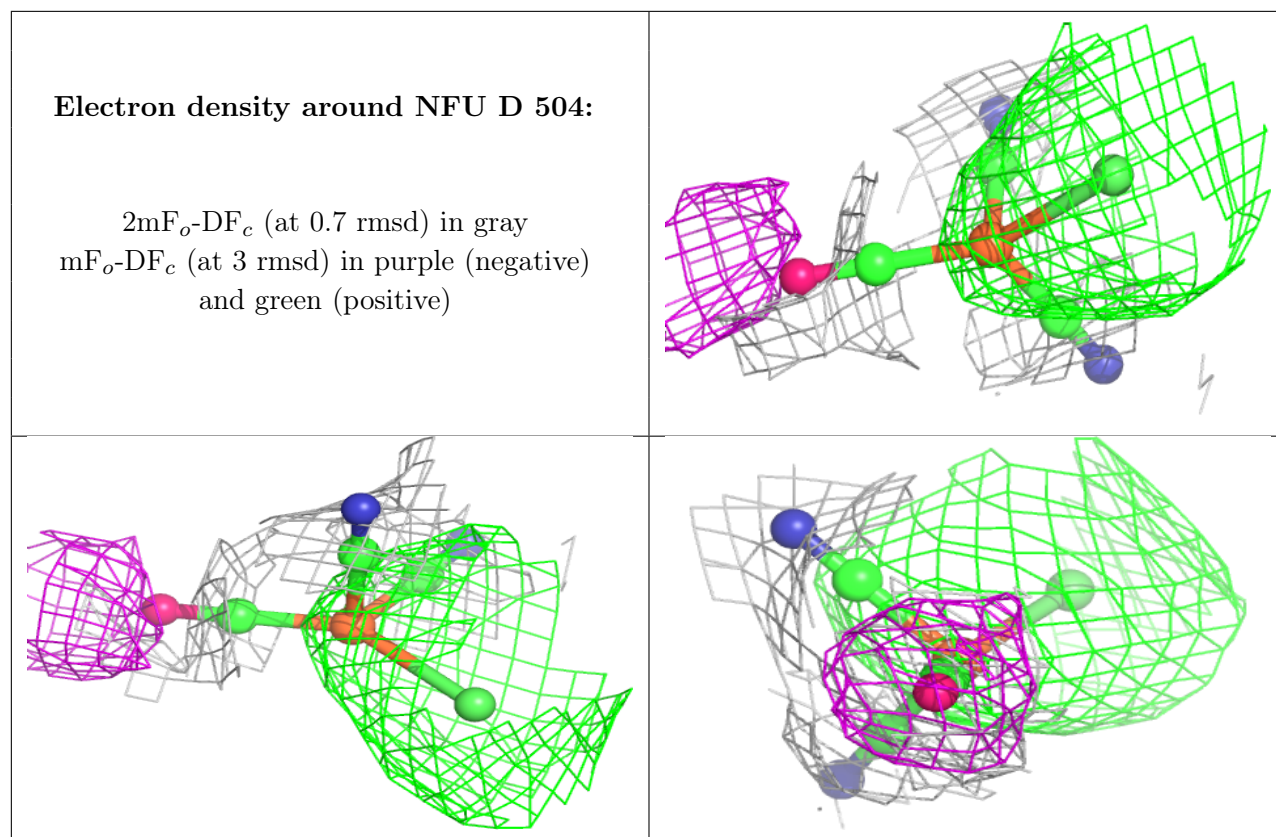
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SF4 E 405:

$2mF_o - DF_c$ (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.