



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:57 PM UTC

PDB ID : 9R6Z / pdb_00009r6z
Title : Cubic state of the F420-reducing hydrogenase from *Methanothermococcus thermolithotrophicus*
Authors : Jespersen, M.; Lemaire, O.N.; Wagner, T.
Deposited on : 2025-05-13
Resolution : 2.85 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

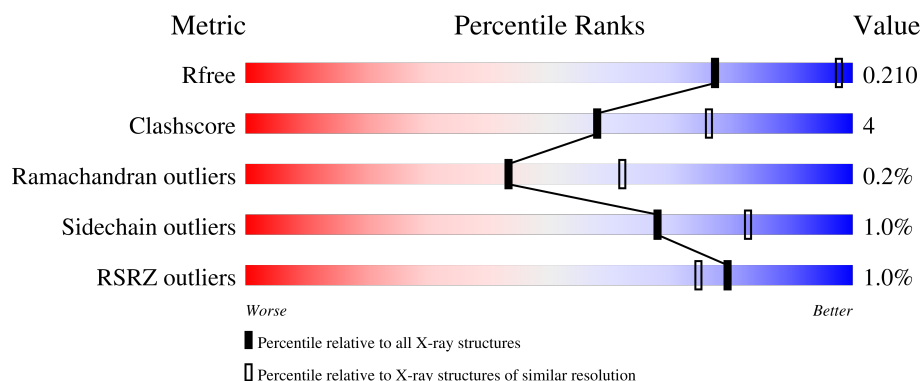
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	
1	D	410	
1	G	410	
1	J	410	
2	B	282	

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Mol	Chain	Length	Quality of chain
2	E	282	 82% 18%
2	H	282	 91% 9%
2	K	282	 91% 9%
3	C	241	 4% 85% 14%
3	F	241	 4% 87% 11%
3	I	241	 4% 88% 11%
3	L	241	 2% 90% 8%

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
5	NFU	D	511	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28822 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 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 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	E	282	Total	C	N	O	S	0	0	0
			2177	1394	356	412	15			
2	H	282	Total	C	N	O	S	0	0	0
			2177	1394	356	412	15			
2	K	282	Total	C	N	O	S	0	0	0
			2177	1394	356	412	15			

- Molecule 3 is a protein called F420-reducing [NiFe]-hydrogenase 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	F	240	Total	C	N	O	S	0	0	0
			1799	1130	299	349	21			
3	I	240	Total	C	N	O	S	0	1	0
			1802	1132	299	349	22			
3	L	240	Total	C	N	O	S	0	1	0
			1802	1132	299	349	22			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



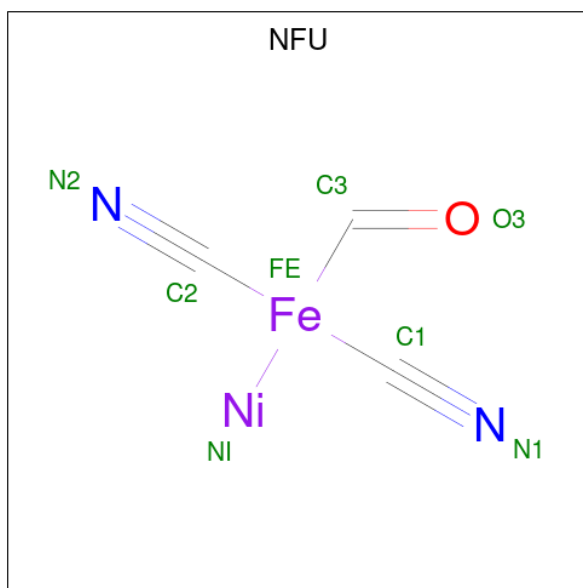
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total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

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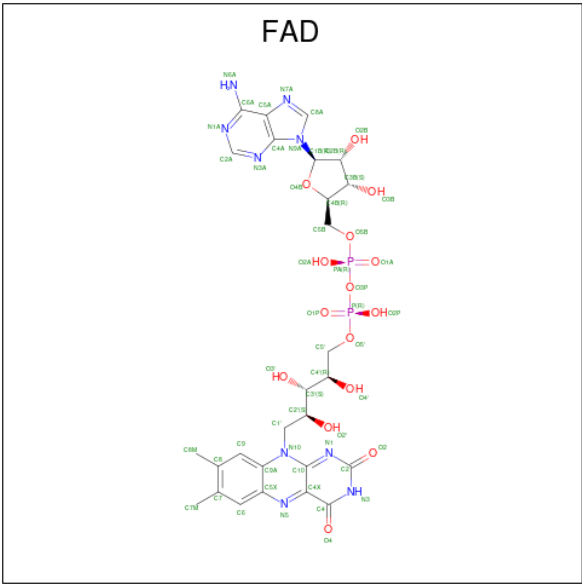
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 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
5	A	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		
5	D	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		
5	G	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		
5	J	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

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



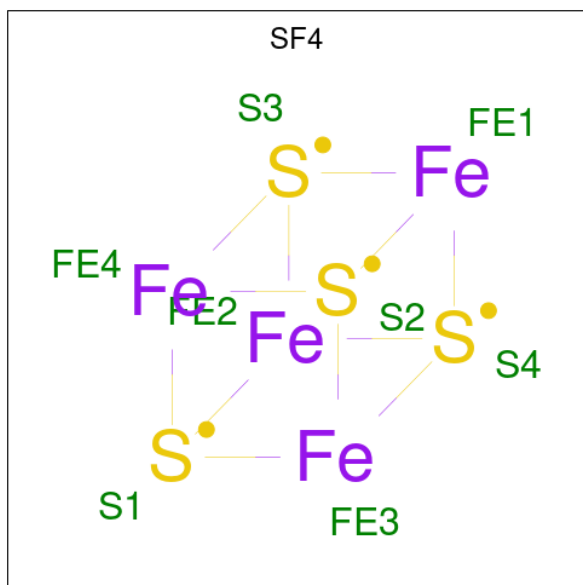
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total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

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

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

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

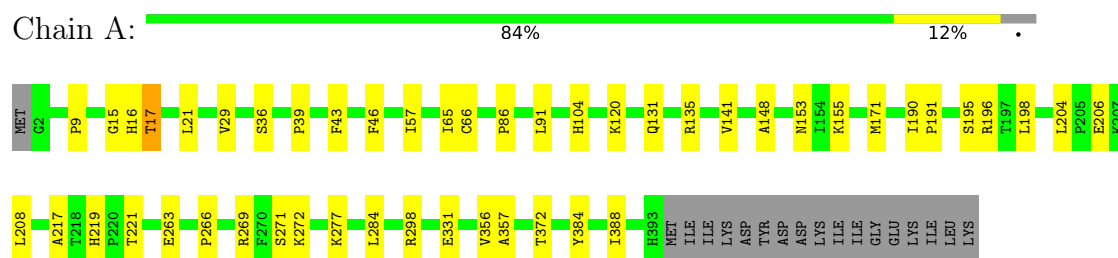
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total	O	0	0
			2	2		
9	B	3	Total	O	0	0
			3	3		
9	C	1	Total	O	0	0
			1	1		
9	D	15	Total	O	0	0
			15	15		
9	E	2	Total	O	0	0
			2	2		
9	G	21	Total	O	0	0
			21	21		
9	H	1	Total	O	0	0
			1	1		
9	I	3	Total	O	0	0
			3	3		
9	J	19	Total	O	0	0
			19	19		
9	K	1	Total	O	0	0
			1	1		
9	L	2	Total	O	0	0
			2	2		

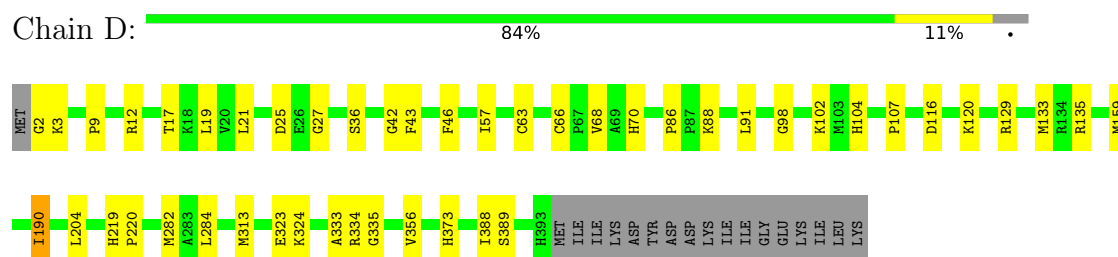
3 Residue-property plots

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

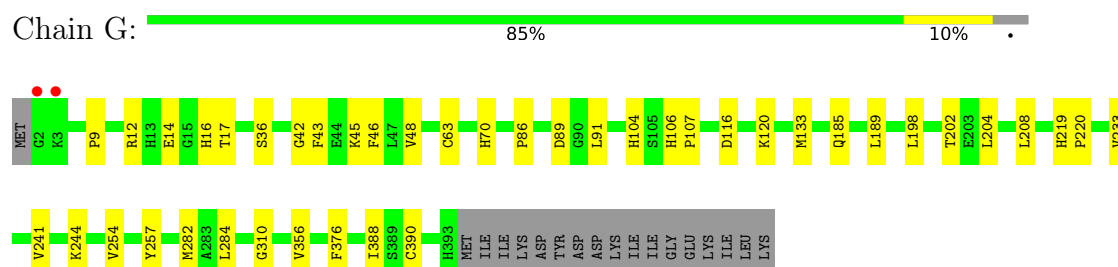
- Molecule 1: F420-reducing [NiFe]-hydrogenase subunit alpha



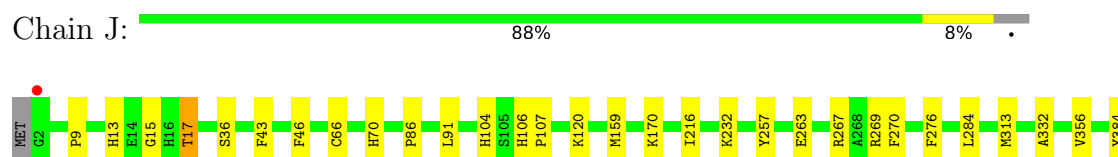
- Molecule 1: F420-reducing [NiFe]-hydrogenase subunit alpha

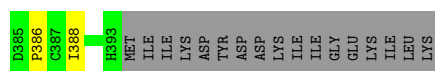


- Molecule 1: F420-reducing [NiFe]-hydrogenase subunit alpha



- Molecule 1: F420-reducing [NiFe]-hydrogenase subunit alpha





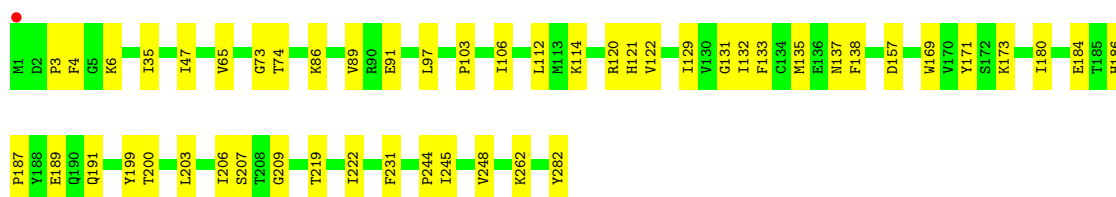
- Molecule 2: F420-reducing [NiFe]-hydrogenase subunit beta

Chain B: 87% 12%



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

Chain E: 82% 18%



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

Chain H: 91% 9%



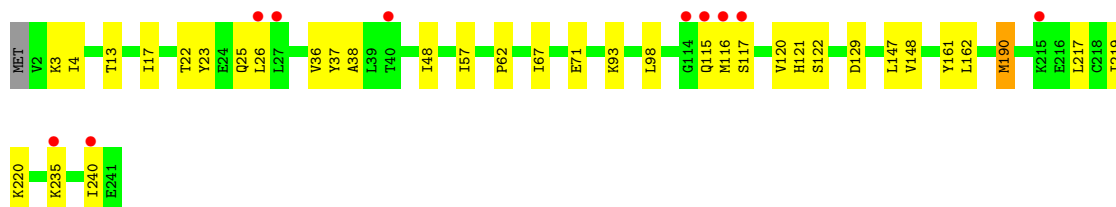
- Molecule 2: F420-reducing [NiFe]-hydrogenase subunit beta

Chain K: 91% 9%



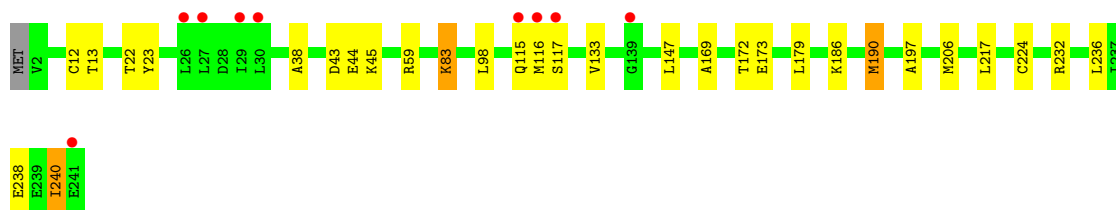
- Molecule 3: F420-reducing [NiFe]-hydrogenase subunit gamma

Chain C: 4% 85% 14%



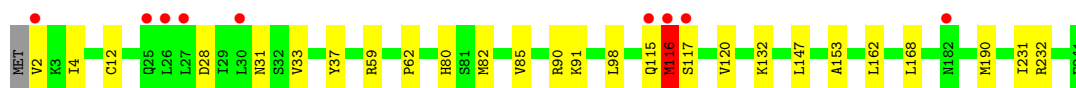
- Molecule 3: F420-reducing [NiFe]-hydrogenase subunit gamma

Chain F:  4% 87% 11%

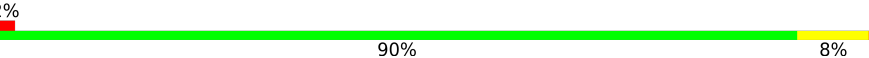


- Molecule 3: F420-reducing [NiFe]-hydrogenase subunit gamma

Chain I:  4% 88% 11%



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

Chain L:  2% 90% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	282.07 Å 282.07 Å 282.07 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.34 – 2.85 31.34 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.34-2.85) 99.8 (31.34-2.85)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.86 Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???), BUSTER	Depositor
R, R_{free}	0.182 , 0.210 0.183 , 0.210	Depositor DCC
R_{free} test set	8771 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	73.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28822	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: SF4, NFU, FAD, SO4, GOL

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	0.34	0/3140	0.51	0/4251
1	D	0.31	0/3140	0.48	1/4251 (0.0%)
1	G	0.30	0/3140	0.46	0/4251
1	J	0.33	0/3140	0.50	0/4251
2	B	0.34	0/2219	0.56	0/2994
2	E	0.33	0/2219	0.54	0/2994
2	H	0.31	0/2219	0.50	0/2994
2	K	0.29	0/2219	0.46	0/2994
3	C	0.44	0/1821	0.61	0/2465
3	F	0.38	0/1821	0.53	0/2465
3	I	0.41	0/1827	0.60	1/2473 (0.0%)
3	L	0.40	1/1827 (0.1%)	0.54	1/2473 (0.0%)
All	All	0.35	1/28732 (0.0%)	0.52	3/38856 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	115	GLN	CA-C	-5.81	1.45	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	335	GLY	N-CA-C	7.33	121.38	110.97
3	L	116	MET	N-CA-C	-7.11	101.16	110.33
3	I	116	MET	N-CA-C	-5.48	103.25	110.43

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	3051	33	0
1	D	3070	0	3049	30	0
1	G	3070	0	3050	30	0
1	J	3070	0	3050	20	0
2	B	2177	0	2224	20	0
2	E	2177	0	2224	38	0
2	H	2177	0	2224	15	0
2	K	2177	0	2224	16	0
3	C	1799	0	1836	22	0
3	F	1799	0	1836	27	0
3	I	1802	0	1841	20	0
3	L	1802	0	1841	14	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	D	15	0	0	0	0
4	E	15	0	0	0	0
4	G	10	0	0	0	0
4	H	5	0	0	0	0
4	J	25	0	0	0	0
4	K	5	0	0	0	0
5	A	8	0	0	1	0
5	D	8	0	0	2	0
5	G	8	0	0	0	0
5	J	8	0	0	1	0
6	B	53	0	31	1	0
6	E	53	0	31	6	0
6	H	53	0	31	2	0
6	K	53	0	31	1	0
7	B	6	0	8	0	0
7	D	42	0	56	2	0
7	G	18	0	24	0	0
7	J	24	0	32	0	0
8	B	8	0	0	1	0
8	C	24	0	0	0	0
8	E	8	0	0	1	0
8	F	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	8	0	0	1	0
8	I	24	0	0	0	0
8	K	8	0	0	1	0
8	L	24	0	0	0	0
9	A	2	0	0	0	0
9	B	3	0	0	0	0
9	C	1	0	0	0	0
9	D	15	0	0	0	0
9	E	2	0	0	0	0
9	G	21	0	0	0	0
9	H	1	0	0	0	0
9	I	3	0	0	0	0
9	J	19	0	0	0	0
9	K	1	0	0	0	0
9	L	2	0	0	0	0
All	All	28822	0	28694	256	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 4.

All (256) 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)
3:F:116:MET:HB3	3:F:117:SER:HA	1.71	0.73
1:G:17:THR:HG23	1:G:388:ILE:HG13	1.71	0.72
1:G:14:GLU:O	1:G:388:ILE:HG12	2.00	0.61
3:F:116:MET:CB	3:F:117:SER:HA	2.31	0.61
1:G:356:VAL:HG11	1:G:390:CYS:HB3	1.84	0.60
2:E:74:THR:HG23	6:E:301:FAD:HM82	1.84	0.59
3:F:98:LEU:HD11	3:F:147:LEU:HD21	1.84	0.59
1:D:135:ARG:HG3	3:F:23:TYR:CE2	2.39	0.57
1:A:17:THR:HG22	1:A:36:SER:HA	1.85	0.57
1:D:42:GLY:HA2	3:F:115:GLN:CD	2.29	0.57
1:D:17:THR:HG23	1:D:388:ILE:HG13	1.85	0.57
3:C:120:VAL:HG22	2:E:191:GLN:HG3	1.88	0.56
3:L:116:MET:HB3	3:L:117:SER:HA	1.89	0.55
1:A:66:CYS:SG	5:A:503:NFU:C1	2.96	0.54
1:J:120:LYS:H	1:J:120:LYS:HD2	1.73	0.54
3:L:4:ILE:HG12	3:L:33:VAL:CG2	2.37	0.53
1:D:334:ARG:HD2	5:D:511:NFU:C1	2.40	0.51
2:E:135:MET:HE1	2:E:262:LYS:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:109:THR:O	2:H:112:LEU:HG	2.10	0.51
2:E:203:LEU:HD22	3:F:240:ILE:HD11	1.92	0.51
1:G:120:LYS:H	1:G:120:LYS:HD3	1.75	0.51
2:E:138:PHE:CE2	2:E:189:GLU:HG2	2.46	0.51
3:I:82:MET:O	3:I:85:VAL:HG12	2.11	0.51
1:J:15:GLY:HA3	1:J:388:ILE:HB	1.93	0.51
2:K:17:ASP:C	2:K:17:ASP:OD1	2.54	0.50
3:C:22:THR:OG1	3:C:26:LEU:HB2	2.11	0.50
1:A:263:GLU:HG3	1:A:384:TYR:HE2	1.75	0.50
3:I:90:ARG:HG3	3:I:91:LYS:HG3	1.92	0.50
1:A:141:VAL:HG23	1:A:148:ALA:HA	1.94	0.50
1:D:66:CYS:SG	5:D:511:NFU:C1	3.00	0.50
2:K:197:MET:HE1	2:K:267:ALA:N	2.27	0.50
1:D:17:THR:HG22	1:D:36:SER:HA	1.92	0.50
1:G:63:CYS:HA	3:I:12:CYS:HB2	1.93	0.50
3:I:98:LEU:HD11	3:I:147:LEU:HD21	1.94	0.50
1:G:43:PHE:HA	1:G:46:PHE:CE2	2.47	0.49
3:I:120:VAL:CG2	2:K:191:GLN:HG2	2.42	0.49
1:J:9:PRO:HD2	3:L:59:ARG:HB2	1.93	0.49
3:L:13:THR:O	3:L:13:THR:HG22	2.12	0.49
1:A:131:GLN:HE21	3:C:23:TYR:HA	1.78	0.49
3:C:98:LEU:HD11	3:C:147:LEU:HD21	1.93	0.49
1:A:135:ARG:HG3	3:C:23:TYR:CE2	2.48	0.49
3:F:133:VAL:HG13	3:F:169:ALA:HB1	1.94	0.49
3:I:2:VAL:HA	3:I:33:VAL:HG22	1.93	0.49
1:A:271:SER:OG	1:A:277:LYS:NZ	2.44	0.49
2:E:199:TYR:HB2	2:E:262:LYS:HD2	1.95	0.49
2:E:219:THR:HG23	2:E:245:ILE:HD13	1.95	0.49
2:E:222:ILE:HD11	2:E:231:PHE:CD2	2.48	0.49
2:B:37:GLY:HA2	2:B:42:LEU:HB2	1.94	0.49
3:L:115:GLN:C	3:L:116:MET:O	2.52	0.49
1:A:153:ASN:O	1:A:155:LYS:HG3	2.12	0.49
1:J:66:CYS:SG	5:J:510:NFU:C1	3.01	0.49
1:J:43:PHE:HA	1:J:46:PHE:CE2	2.48	0.48
1:J:170:LYS:NZ	2:K:95:GLU:OE1	2.46	0.48
2:E:132:ILE:HD12	6:E:301:FAD:H9	1.95	0.48
2:E:133:PHE:CD2	2:E:209:GLY:HA3	2.49	0.48
3:C:37:TYR:HB2	3:C:62:PRO:HD2	1.96	0.48
2:K:245:ILE:HA	2:K:248:VAL:HG22	1.95	0.48
1:J:13:HIS:CG	1:J:386:PRO:HG2	2.48	0.48
1:G:185:GLN:HG3	1:G:189:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ILE:HD12	3:C:217:LEU:HD22	1.95	0.48
1:D:120:LYS:H	7:D:509:GOL:H11	1.79	0.48
2:H:137:ASN:HB2	8:H:303:SF4:S2	2.53	0.48
3:L:116:MET:CB	3:L:117:SER:HA	2.42	0.48
1:A:39:PRO:HA	3:C:121:HIS:CE1	2.48	0.48
2:B:35:ILE:O	2:B:39:GLU:HG3	2.14	0.48
1:A:43:PHE:HA	1:A:46:PHE:CE2	2.49	0.47
1:A:198:LEU:HD21	1:A:204:LEU:HD11	1.96	0.47
1:D:68:VAL:HG11	1:D:98:GLY:HA2	1.95	0.47
2:E:133:PHE:HB2	6:E:301:FAD:C2	2.44	0.47
1:G:244:LYS:HE2	2:K:150:HIS:CE1	2.49	0.47
1:D:43:PHE:HA	1:D:46:PHE:CE2	2.48	0.47
1:D:12:ARG:NH2	1:D:116:ASP:OD2	2.46	0.47
2:E:114:LYS:HE3	3:F:236:LEU:HD12	1.96	0.47
2:E:73:GLY:O	6:E:301:FAD:H8A	2.13	0.47
1:J:70:HIS:HE1	1:J:356:VAL:HG13	1.78	0.47
2:K:137:ASN:HB2	8:K:303:SF4:S2	2.55	0.47
1:D:42:GLY:HA2	3:F:115:GLN:NE2	2.30	0.47
3:C:116:MET:CB	3:C:117:SER:HA	2.44	0.47
2:E:4:PHE:HD1	2:E:200:THR:HG21	1.78	0.47
3:F:98:LEU:CD1	3:F:147:LEU:HD21	2.44	0.47
1:J:267:ARG:HB2	1:J:284:LEU:HD23	1.96	0.47
3:F:206:MET:HE3	3:F:206:MET:HA	1.96	0.47
3:I:153:ALA:HB3	3:I:162:LEU:HD21	1.97	0.47
2:B:137:ASN:HB2	8:B:305:SF4:S2	2.54	0.46
1:D:12:ARG:HD3	3:F:43:ASP:OD1	2.15	0.46
2:E:86:LYS:HE2	3:F:197:ALA:O	2.15	0.46
1:G:89:ASP:OD2	1:G:310:GLY:HA3	2.15	0.46
1:G:198:LEU:HD12	1:G:202:THR:HB	1.97	0.46
2:H:54:LYS:O	2:H:55:LEU:HB2	2.16	0.46
1:A:196:ARG:NH1	1:A:206:GLU:HA	2.31	0.46
2:B:47:ILE:HG13	2:B:97:LEU:HD11	1.98	0.46
2:K:133:PHE:CD2	2:K:209:GLY:HA3	2.51	0.46
1:D:63:CYS:HA	3:F:12:CYS:HB2	1.98	0.46
1:D:102:LYS:HG2	1:D:333:ALA:HB2	1.97	0.46
2:K:100:VAL:HA	2:K:130:VAL:O	2.16	0.46
1:A:171:MET:HE2	1:A:171:MET:HB3	1.87	0.46
1:G:17:THR:HG22	1:G:36:SER:HA	1.98	0.46
1:J:17:THR:HG22	1:J:36:SER:HA	1.96	0.46
2:E:206:ILE:HG12	2:E:222:ILE:HD12	1.97	0.46
1:G:9:PRO:HD2	3:I:59:ARG:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:270:PHE:HB3	1:J:276:PHE:HB3	1.98	0.46
2:E:244:PRO:O	2:E:248:VAL:HG23	2.16	0.46
1:G:86:PRO:HG2	1:G:91:LEU:HG	1.98	0.46
3:L:137:LEU:CD1	3:L:147:LEU:HD23	2.46	0.46
1:A:120:LYS:H	1:A:120:LYS:HD3	1.80	0.46
1:A:208:LEU:HD12	1:A:372:THR:HG21	1.98	0.46
2:B:54:LYS:O	2:B:55:LEU:HB2	2.16	0.46
3:L:2:VAL:HB	3:L:33:VAL:HG12	1.98	0.46
2:H:230:PHE:O	2:H:234:MET:HG3	2.16	0.45
3:I:4:ILE:HD12	3:I:33:VAL:HG11	1.98	0.45
2:B:10:VAL:HG21	2:B:252:LEU:HD13	1.98	0.45
3:C:48:ILE:HG23	3:C:57:ILE:HG12	1.99	0.45
2:K:135:MET:HE2	2:K:199:TYR:CE1	2.51	0.45
3:L:175[B]:CYS:SG	3:L:177:CYS:HB2	2.56	0.45
2:B:62:ALA:HB1	2:B:67:GLU:HB3	1.97	0.45
2:E:47:ILE:HD11	2:E:97:LEU:HD21	1.99	0.45
2:H:113:MET:HE3	2:H:126:LEU:HD12	1.97	0.45
1:D:86:PRO:HG2	1:D:91:LEU:HG	1.97	0.45
1:J:46:PHE:HA	3:L:112:ARG:CZ	2.46	0.45
6:B:301:FAD:H9	6:B:301:FAD:H1'1	1.72	0.45
2:E:89:VAL:HG21	2:E:122:VAL:HG22	1.99	0.45
3:I:116:MET:HB3	3:I:117:SER:HA	1.99	0.45
1:A:21:LEU:HD23	1:A:29:VAL:HG11	1.99	0.45
2:E:282:TYR:CZ	3:F:232:ARG:HD3	2.52	0.45
1:G:107:PRO:HG3	1:G:133:MET:HE2	1.98	0.45
2:H:30:VAL:HG11	6:H:301:FAD:H4B	1.99	0.45
3:C:129:ASP:OD2	3:F:186:LYS:HE2	2.17	0.44
1:D:107:PRO:HG3	1:D:133:MET:HE2	1.99	0.44
1:D:159:MET:O	1:D:313:MET:HG2	2.17	0.44
1:A:356:VAL:HG12	1:A:357:ALA:H	1.82	0.44
3:L:183:VAL:HG12	3:L:189:CYS:HB2	1.98	0.44
2:B:35:ILE:HG12	2:B:65:VAL:HG22	2.00	0.44
1:D:70:HIS:HE1	1:D:356:VAL:HG13	1.81	0.44
1:D:323:GLU:OE1	1:D:323:GLU:HA	2.18	0.44
2:E:35:ILE:HD13	2:E:65:VAL:HG13	1.98	0.44
2:E:169:TRP:HB3	2:E:171:TYR:HE1	1.82	0.44
1:G:70:HIS:HE1	1:G:356:VAL:HG13	1.82	0.44
2:B:141:ASN:HB3	3:F:116:MET:HG3	1.99	0.44
2:E:169:TRP:HB3	2:E:171:TYR:CE1	2.53	0.44
2:B:26:ASP:CG	2:B:210:SER:HB2	2.43	0.44
3:C:25:GLN:HG2	3:C:148:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:180:ILE:HD12	2:E:184:GLU:OE2	2.18	0.44
3:C:235:LYS:H	3:C:235:LYS:HD3	1.82	0.44
2:K:74:THR:HG23	6:K:301:FAD:HM83	2.00	0.44
1:D:129:ARG:O	1:D:133:MET:HG3	2.16	0.44
2:H:103:PRO:HD3	2:H:132:ILE:O	2.18	0.44
1:D:2:GLY:N	1:D:25:ASP:OD1	2.50	0.44
1:D:19:LEU:HD22	1:D:21:LEU:HD21	2.00	0.44
1:D:57:ILE:HD12	3:F:217:LEU:HD22	2.00	0.44
1:D:204:LEU:HD13	1:D:282:MET:HE3	2.00	0.44
1:D:324:LYS:HA	7:D:506:GOL:H11	2.00	0.43
1:G:42:GLY:HA2	3:I:115:GLN:CD	2.43	0.43
1:G:45:LYS:O	1:G:48:VAL:HG12	2.18	0.43
1:G:241:VAL:HG11	1:G:254:VAL:HG11	2.00	0.43
2:K:53:ASP:OD1	2:K:53:ASP:N	2.51	0.43
2:H:15:ALA:HA	2:H:240:LEU:HD23	1.99	0.43
3:I:28:ASP:O	3:I:31:ASN:OD1	2.35	0.43
3:I:116:MET:CB	3:I:117:SER:HA	2.47	0.43
2:K:54:LYS:O	2:K:55:LEU:HB2	2.18	0.43
3:L:28:ASP:OD1	3:L:28:ASP:C	2.61	0.43
1:D:388:ILE:O	1:D:389:SER:C	2.61	0.43
1:G:16:HIS:HE1	3:I:80:HIS:CD2	2.36	0.43
1:J:263:GLU:HG3	1:J:384:TYR:HE2	1.84	0.43
2:B:100:VAL:HA	2:B:130:VAL:O	2.18	0.43
2:E:103:PRO:HD3	2:E:132:ILE:O	2.19	0.43
3:F:22:THR:O	3:F:23:TYR:C	2.61	0.43
1:G:120:LYS:H	1:G:120:LYS:CD	2.32	0.43
3:I:115:GLN:C	3:I:116:MET:O	2.61	0.43
1:A:9:PRO:HB3	1:A:16:HIS:HD2	1.84	0.43
1:A:15:GLY:HA3	1:A:388:ILE:HB	2.01	0.43
2:E:132:ILE:HD12	6:E:301:FAD:C9	2.49	0.43
2:E:203:LEU:HD21	3:F:238:GLU:HA	1.99	0.43
1:G:63:CYS:HB3	1:G:390:CYS:SG	2.59	0.43
2:H:148:GLU:OE2	2:H:155:MET:HG2	2.19	0.43
2:B:249:LYS:HA	2:B:250:PRO:C	2.44	0.42
3:C:13:THR:O	3:C:17:ILE:HD12	2.19	0.42
1:A:266:PRO:HA	1:A:269:ARG:NH1	2.35	0.42
3:C:115:GLN:HG2	3:C:116:MET:O	2.20	0.42
3:F:44:GLU:HA	3:F:45:LYS:HA	1.80	0.42
2:K:154:LYS:HE2	2:K:156:GLU:OE1	2.20	0.42
1:D:9:PRO:HD2	3:F:59:ARG:HB2	2.01	0.42
2:H:186:HIS:N	2:H:187:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:301:FAD:H9	6:H:301:FAD:H1'1	1.75	0.42
3:I:82:MET:HE2	3:I:82:MET:HB3	1.92	0.42
1:A:17:THR:HG23	1:A:388:ILE:HG13	2.01	0.42
1:G:219:HIS:CG	1:G:220:PRO:HD2	2.55	0.42
1:A:21:LEU:HB3	1:A:29:VAL:HG13	2.01	0.42
1:A:36:SER:HB2	1:A:388:ILE:HG23	2.00	0.42
1:A:195:SER:C	1:A:196:ARG:HG3	2.45	0.42
3:C:120:VAL:CG2	2:E:191:GLN:HG3	2.49	0.42
3:F:13:THR:HG22	3:F:13:THR:O	2.20	0.42
3:I:37:TYR:HB2	3:I:62:PRO:CD	2.50	0.42
1:J:86:PRO:HG2	1:J:91:LEU:HG	2.02	0.42
1:A:217:ALA:HB3	1:A:272:LYS:HG3	2.02	0.42
2:B:18:LYS:HA	2:B:21:LEU:HD12	2.01	0.42
2:H:55:LEU:HD12	2:H:155:MET:HE3	2.02	0.42
1:A:219:HIS:O	1:A:331:GLU:HG3	2.19	0.42
1:G:42:GLY:HA2	3:I:115:GLN:OE1	2.20	0.42
1:G:46:PHE:CD1	1:G:46:PHE:C	2.98	0.42
3:C:219:ILE:C	3:C:220:LYS:HG3	2.45	0.42
2:E:35:ILE:CD1	2:E:65:VAL:HG13	2.50	0.42
2:B:4:PHE:HE1	2:B:256:GLU:HA	1.85	0.41
2:E:157:ASP:O	2:E:173:LYS:HG3	2.19	0.41
3:F:179:LEU:HD11	3:F:224:CYS:HB2	2.02	0.41
1:J:232:LYS:HD3	1:J:232:LYS:N	2.34	0.41
1:G:106:HIS:HB2	1:G:107:PRO:HD3	2.02	0.41
1:J:216:ILE:HD11	1:J:257:TYR:HB2	2.02	0.41
2:B:14:ARG:HD3	2:B:217:TRP:CE2	2.56	0.41
2:H:245:ILE:HA	2:H:248:VAL:CG2	2.50	0.41
1:A:221:THR:HG21	1:A:298:ARG:HG2	2.03	0.41
1:J:269:ARG:NH2	1:J:332:ALA:O	2.53	0.41
2:H:249:LYS:HA	2:H:250:PRO:C	2.46	0.41
1:D:27:GLY:HA3	1:D:373:HIS:CD2	2.56	0.41
1:D:190:ILE:HD13	1:D:190:ILE:HA	1.86	0.41
2:E:112:LEU:C	2:E:112:LEU:HD23	2.45	0.41
2:E:131:GLY:O	2:E:207:SER:HA	2.21	0.41
3:F:83:LYS:HD3	3:F:83:LYS:HA	1.60	0.41
3:F:190:MET:H	3:F:190:MET:HG3	1.62	0.41
3:L:184:ILE:HD11	3:L:211:PRO:HG2	2.03	0.41
1:A:86:PRO:HG2	1:A:91:LEU:HG	2.03	0.41
2:E:186:HIS:N	2:E:187:PRO:HD2	2.36	0.41
3:F:172:THR:C	3:F:173:GLU:OE1	2.63	0.41
1:J:106:HIS:HB2	1:J:107:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:159:MET:O	1:J:313:MET:HG2	2.20	0.41
3:L:153:ALA:HB1	3:L:158:ASP:HB3	2.02	0.41
2:B:135:MET:HG3	2:B:136:GLU:HG3	2.02	0.41
2:B:239:ALA:O	2:B:240:LEU:HD23	2.21	0.41
2:E:106:ILE:HD12	2:E:129:ILE:HG22	2.02	0.41
1:J:17:THR:HG23	1:J:388:ILE:HG13	2.02	0.41
1:A:46:PHE:CD1	1:A:46:PHE:C	2.99	0.41
1:A:190:ILE:N	1:A:191:PRO:HD2	2.36	0.41
3:C:161:TYR:HD1	3:C:162:LEU:HD12	1.86	0.41
1:D:219:HIS:CG	1:D:220:PRO:HD2	2.56	0.41
2:E:180:ILE:HD12	2:E:184:GLU:HG2	2.03	0.41
1:G:204:LEU:HD13	1:G:282:MET:HE3	2.03	0.41
2:H:22:LYS:HA	2:H:22:LYS:HD2	1.86	0.41
3:I:231:ILE:HG22	3:I:232:ARG:HG2	2.02	0.41
1:A:65:ILE:HG13	3:C:17:ILE:HD11	2.03	0.41
2:E:120:ARG:HG2	2:E:121:HIS:CD2	2.56	0.41
1:G:233:VAL:HG22	1:G:257:TYR:HD1	1.84	0.41
1:A:198:LEU:N	1:A:198:LEU:HD23	2.36	0.40
2:E:137:ASN:HB2	8:E:305:SF4:S2	2.61	0.40
2:H:207:SER:HB2	2:H:221:PHE:HB2	2.02	0.40
2:B:103:PRO:HD3	2:B:132:ILE:O	2.20	0.40
3:C:4:ILE:HG22	3:C:67:ILE:HB	2.03	0.40
1:G:208:LEU:HD11	1:G:376:PHE:HB3	2.03	0.40
2:K:232:ASN:HA	2:K:235:VAL:HG22	2.04	0.40
3:C:190:MET:H	3:C:190:MET:HG3	1.75	0.40
1:G:12:ARG:NH2	1:G:116:ASP:OD2	2.54	0.40
3:C:3:LYS:HB2	3:C:36:VAL:CG1	2.52	0.40
2:B:103:PRO:HD2	2:B:134:CYS:HB3	2.03	0.40
2:B:207:SER:O	2:B:220:VAL:HA	2.21	0.40
2:E:231:PHE:CD1	2:E:231:PHE:C	3.00	0.40
6:E:301:FAD:H9	6:E:301:FAD:H1'1	1.88	0.40
1:G:16:HIS:CE1	3:I:80:HIS:CD2	3.09	0.40
2:K:26:ASP:CG	2:K:210:SER:HB3	2.46	0.40

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%)	375 (96%)	15 (4%)	0	100	100
1	D	390/410 (95%)	378 (97%)	12 (3%)	0	100	100
1	G	390/410 (95%)	383 (98%)	7 (2%)	0	100	100
1	J	390/410 (95%)	377 (97%)	13 (3%)	0	100	100
2	B	280/282 (99%)	266 (95%)	13 (5%)	1 (0%)	30	48
2	E	280/282 (99%)	268 (96%)	11 (4%)	1 (0%)	30	48
2	H	280/282 (99%)	268 (96%)	11 (4%)	1 (0%)	30	48
2	K	280/282 (99%)	270 (96%)	10 (4%)	0	100	100
3	C	238/241 (99%)	224 (94%)	12 (5%)	2 (1%)	16	31
3	F	238/241 (99%)	226 (95%)	11 (5%)	1 (0%)	30	48
3	I	239/241 (99%)	225 (94%)	14 (6%)	0	100	100
3	L	239/241 (99%)	225 (94%)	13 (5%)	1 (0%)	30	48
All	All	3634/3732 (97%)	3485 (96%)	142 (4%)	7 (0%)	43	62

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	38	ALA
3	C	122	SER
3	F	38	ALA
3	L	38	ALA
2	B	3	PRO
2	E	3	PRO
2	H	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%)	327 (99%)	3 (1%)	70	84
1	D	330/347 (95%)	325 (98%)	5 (2%)	57	77
1	G	330/347 (95%)	328 (99%)	2 (1%)	78	89
1	J	330/347 (95%)	328 (99%)	2 (1%)	78	89
2	B	238/238 (100%)	236 (99%)	2 (1%)	73	86
2	E	238/238 (100%)	236 (99%)	2 (1%)	73	86
2	H	238/238 (100%)	238 (100%)	0	100	100
2	K	238/238 (100%)	238 (100%)	0	100	100
3	C	204/205 (100%)	200 (98%)	4 (2%)	48	71
3	F	204/205 (100%)	201 (98%)	3 (2%)	57	77
3	I	205/205 (100%)	201 (98%)	4 (2%)	48	71
3	L	205/205 (100%)	202 (98%)	3 (2%)	57	77
All	All	3090/3160 (98%)	3060 (99%)	30 (1%)	68	83

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	104	HIS
1	A	284	LEU
2	B	10	VAL
2	B	35	ILE
3	C	71	GLU
3	C	93	LYS
3	C	190	MET
3	C	240	ILE
1	D	3	LYS
1	D	88	LYS
1	D	104	HIS
1	D	190	ILE
1	D	284	LEU

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Mol	Chain	Res	Type
2	E	6	LYS
2	E	91	GLU
3	F	83	LYS
3	F	190	MET
3	F	240	ILE
1	G	104	HIS
1	G	284	LEU
3	I	116	MET
3	I	132	LYS
3	I	168	LEU
3	I	190	MET
1	J	17	THR
1	J	104	HIS
3	L	4	ILE
3	L	116	MET
3	L	190	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	A	340	GLN
1	A	353	ASN
2	B	40	ASN
2	B	105	GLN
3	C	8	HIS
3	C	115	GLN
1	D	101	ASN
1	D	124	ASN
1	D	336	HIS
2	E	105	GLN
2	E	190	GLN
3	F	115	GLN
1	G	340	GLN
1	G	353	ASN
2	H	190	GLN
1	J	307	ASN
1	J	353	ASN
1	J	379	HIS
2	K	40	ASN
3	L	25	GLN

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 ⓘ

59 ligands are modelled in this entry.

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	J	507	-	5,5,5	0.09	0	5,5,5	0.31	0
7	GOL	J	506	-	5,5,5	0.30	0	5,5,5	0.39	0
4	SO4	B	302	-	4,4,4	0.68	0	6,6,6	0.06	0
7	GOL	G	504	-	5,5,5	0.09	0	5,5,5	0.33	0
7	GOL	D	507	-	5,5,5	0.09	0	5,5,5	0.31	0
7	GOL	J	508	-	5,5,5	0.08	0	5,5,5	0.32	0
6	FAD	H	301	-	58,58,58	1.48	9 (15%)	85,89,89	1.56	14 (16%)
4	SO4	G	502	-	4,4,4	0.71	0	6,6,6	0.09	0
7	GOL	B	304	-	5,5,5	0.09	0	5,5,5	0.32	0
4	SO4	H	302	-	4,4,4	0.67	0	6,6,6	0.07	0
4	SO4	D	501	-	4,4,4	0.36	0	6,6,6	0.08	0
5	NFU	J	510	1	2,7,7	1.06	0	-	-	-
7	GOL	D	506	-	5,5,5	0.08	0	5,5,5	0.33	0
7	GOL	D	505	-	5,5,5	0.09	0	5,5,5	0.34	0
7	GOL	D	508	-	5,5,5	0.08	0	5,5,5	0.31	0
4	SO4	J	502	-	4,4,4	0.69	0	6,6,6	0.09	0
8	SF4	F	301	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SF4	L	302	3	0,12,12	-	-	-		
4	SO4	J	503	-	4,4,4	0.69	0	6,6,6	0.08	0
7	GOL	J	509	-	5,5,5	0.08	0	5,5,5	0.33	0
4	SO4	K	302	-	4,4,4	0.68	0	6,6,6	0.07	0
7	GOL	G	503	-	5,5,5	0.35	0	5,5,5	0.34	0
8	SF4	I	302	3	0,12,12	-	-	-		
5	NFU	A	503	1	2,7,7	0.91	0	-		
7	GOL	D	504	-	5,5,5	0.08	0	5,5,5	0.32	0
4	SO4	A	501	-	4,4,4	0.68	0	6,6,6	0.09	0
4	SO4	C	301	-	4,4,4	0.68	0	6,6,6	0.10	0
5	NFU	D	511	1	2,7,7	1.34	0	-		
6	FAD	K	301	-	58,58,58	1.46	9 (15%)	85,89,89	1.52	15 (17%)
8	SF4	E	305	2	0,12,12	-	-	-		
7	GOL	D	510	-	5,5,5	0.08	0	5,5,5	0.32	0
4	SO4	D	502	-	4,4,4	0.69	0	6,6,6	0.09	0
4	SO4	E	304	-	4,4,4	0.67	0	6,6,6	0.09	0
5	NFU	G	506	1	2,7,7	0.75	0	-		
8	SF4	H	303	2	0,12,12	-	-	-		
4	SO4	J	505	-	4,4,4	0.34	0	6,6,6	0.08	0
7	GOL	G	505	-	5,5,5	0.08	0	5,5,5	0.31	0
8	SF4	B	305	2	0,12,12	-	-	-		
8	SF4	I	303	3	0,12,12	-	-	-		
4	SO4	J	501	-	4,4,4	0.69	0	6,6,6	0.07	0
8	SF4	C	303	3	0,12,12	-	-	-		
4	SO4	A	502	-	4,4,4	0.69	0	6,6,6	0.09	0
6	FAD	B	301	-	58,58,58	1.50	11 (18%)	85,89,89	1.51	13 (15%)
4	SO4	J	504	-	4,4,4	0.69	0	6,6,6	0.11	0
4	SO4	E	303	-	4,4,4	0.34	0	6,6,6	0.07	0
7	GOL	D	509	-	5,5,5	0.09	0	5,5,5	0.32	0
8	SF4	K	303	2	0,12,12	-	-	-		
4	SO4	B	303	-	4,4,4	0.68	0	6,6,6	0.06	0
4	SO4	G	501	-	4,4,4	0.67	0	6,6,6	0.13	0
4	SO4	D	503	-	4,4,4	0.69	0	6,6,6	0.10	0
8	SF4	F	303	3	0,12,12	-	-	-		
8	SF4	C	304	3	0,12,12	-	-	-		
6	FAD	E	301	-	58,58,58	1.47	9 (15%)	85,89,89	1.51	15 (17%)
4	SO4	E	302	-	4,4,4	0.68	0	6,6,6	0.10	0
8	SF4	C	302	3	0,12,12	-	-	-		
8	SF4	L	303	3	0,12,12	-	-	-		
8	SF4	F	302	3	0,12,12	-	-	-		
8	SF4	I	301	3	0,12,12	-	-	-		
8	SF4	L	301	3	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	J	507	-	-	0/4/4/4	-
7	GOL	J	506	-	-	2/4/4/4	-
7	GOL	G	504	-	-	4/4/4/4	-
7	GOL	D	507	-	-	2/4/4/4	-
7	GOL	J	508	-	-	2/4/4/4	-
6	FAD	H	301	-	-	2/34/50/50	0/6/6/6
7	GOL	B	304	-	-	2/4/4/4	-
7	GOL	D	506	-	-	2/4/4/4	-
7	GOL	D	505	-	-	2/4/4/4	-
7	GOL	D	508	-	-	3/4/4/4	-
8	SF4	F	301	3	-	-	0/6/5/5
8	SF4	L	302	3	-	-	0/6/5/5
7	GOL	J	509	-	-	4/4/4/4	-
7	GOL	G	503	-	-	1/4/4/4	-
8	SF4	I	302	3	-	-	0/6/5/5
7	GOL	D	504	-	-	0/4/4/4	-
8	SF4	E	305	2	-	-	0/6/5/5
6	FAD	K	301	-	-	2/34/50/50	0/6/6/6
7	GOL	D	510	-	-	2/4/4/4	-
8	SF4	H	303	2	-	-	0/6/5/5
7	GOL	G	505	-	-	0/4/4/4	-
8	SF4	B	305	2	-	-	0/6/5/5
8	SF4	I	303	3	-	-	0/6/5/5
8	SF4	C	303	3	-	-	0/6/5/5
7	GOL	D	509	-	-	3/4/4/4	-
6	FAD	B	301	-	-	1/34/50/50	0/6/6/6
8	SF4	K	303	2	-	-	0/6/5/5
8	SF4	F	303	3	-	-	0/6/5/5
8	SF4	C	304	3	-	-	0/6/5/5
6	FAD	E	301	-	-	0/34/50/50	0/6/6/6
8	SF4	C	302	3	-	-	0/6/5/5
8	SF4	L	303	3	-	-	0/6/5/5
8	SF4	F	302	3	-	-	0/6/5/5
8	SF4	I	301	3	-	-	0/6/5/5
8	SF4	L	301	3	-	-	0/6/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	301	FAD	C9A-C5X	5.28	1.49	1.41
6	H	301	FAD	C9A-C5X	5.18	1.49	1.41
6	E	301	FAD	C9A-C5X	5.14	1.49	1.41
6	K	301	FAD	C9A-C5X	5.13	1.49	1.41
6	H	301	FAD	C5A-C4A	4.72	1.47	1.39
6	K	301	FAD	C5A-C4A	4.63	1.47	1.39
6	B	301	FAD	C5A-C4A	4.61	1.47	1.39
6	E	301	FAD	C5A-C4A	4.60	1.47	1.39
6	B	301	FAD	C8-C7	3.50	1.49	1.40
6	H	301	FAD	C8-C7	3.39	1.49	1.40
6	E	301	FAD	C8-C7	3.38	1.49	1.40
6	K	301	FAD	C8-C7	3.34	1.49	1.40
6	K	301	FAD	C5A-C6A	2.73	1.48	1.41
6	E	301	FAD	C5A-C6A	2.71	1.48	1.41
6	H	301	FAD	C5A-C6A	2.68	1.48	1.41
6	E	301	FAD	C4-N3	-2.60	1.34	1.38
6	B	301	FAD	C5A-C6A	2.57	1.48	1.41
6	B	301	FAD	C4-N3	-2.51	1.34	1.38
6	K	301	FAD	C4-N3	-2.51	1.34	1.38
6	E	301	FAD	C8A-N7A	2.40	1.36	1.31
6	H	301	FAD	C4-N3	-2.39	1.34	1.38
6	H	301	FAD	C8A-N7A	2.37	1.36	1.31
6	B	301	FAD	C8A-N7A	2.37	1.36	1.31
6	K	301	FAD	C8A-N7A	2.35	1.36	1.31
6	B	301	FAD	C5A-N7A	-2.32	1.34	1.39
6	H	301	FAD	C5A-N7A	-2.31	1.34	1.39
6	H	301	FAD	PA-O3P	2.27	1.61	1.59
6	B	301	FAD	C4X-N5	2.27	1.35	1.30
6	E	301	FAD	C5A-N7A	-2.24	1.35	1.39
6	H	301	FAD	C4X-N5	2.24	1.35	1.30
6	K	301	FAD	C5A-N7A	-2.21	1.35	1.39
6	E	301	FAD	C5X-N5	-2.18	1.35	1.39
6	K	301	FAD	C5X-N5	-2.14	1.35	1.39
6	K	301	FAD	C4X-N5	2.13	1.35	1.30
6	E	301	FAD	C4X-N5	2.10	1.35	1.30
6	B	301	FAD	C5X-N5	-2.06	1.35	1.39
6	B	301	FAD	PA-O3P	2.03	1.61	1.59
6	B	301	FAD	C10-N10	2.01	1.41	1.37

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	301	FAD	C5A-C4A-N3A	-5.84	118.67	126.72
6	H	301	FAD	C5A-C4A-N3A	-5.77	118.77	126.72
6	E	301	FAD	C5A-C4A-N3A	-5.66	118.93	126.72
6	K	301	FAD	C5A-C4A-N3A	-5.64	118.96	126.72
6	B	301	FAD	N3A-C4A-N9A	4.57	134.93	127.17
6	H	301	FAD	N3A-C4A-N9A	4.49	134.80	127.17
6	E	301	FAD	N3A-C4A-N9A	4.45	134.74	127.17
6	K	301	FAD	N3A-C4A-N9A	4.39	134.63	127.17
6	E	301	FAD	C2A-N3A-C4A	3.70	120.87	111.83
6	H	301	FAD	C2A-N3A-C4A	3.67	120.80	111.83
6	K	301	FAD	C2A-N3A-C4A	3.67	120.79	111.83
6	B	301	FAD	C2A-N3A-C4A	3.63	120.70	111.83
6	K	301	FAD	C4A-C5A-N7A	-3.55	106.52	110.58
6	H	301	FAD	C4A-C5A-N7A	-3.48	106.60	110.58
6	E	301	FAD	C4A-C5A-N7A	-3.41	106.68	110.58
6	B	301	FAD	C4A-C5A-N7A	-3.36	106.74	110.58
6	E	301	FAD	N3A-C2A-N1A	-3.31	123.58	128.58
6	K	301	FAD	N3A-C2A-N1A	-3.24	123.68	128.58
6	H	301	FAD	N3A-C2A-N1A	-3.16	123.79	128.58
6	H	301	FAD	C4-C4X-N5	3.08	122.47	118.21
6	B	301	FAD	N3A-C2A-N1A	-3.07	123.94	128.58
6	E	301	FAD	C4A-N9A-C8A	2.77	108.65	105.74
6	K	301	FAD	C4A-N9A-C8A	2.70	108.57	105.74
6	B	301	FAD	C4X-C10-N1	-2.66	118.06	124.59
6	K	301	FAD	C4-C4X-N5	2.65	121.88	118.21
6	K	301	FAD	C5A-N7A-C8A	2.57	107.50	103.45
6	B	301	FAD	C4A-N9A-C8A	2.56	108.43	105.74
6	E	301	FAD	C4-C4X-N5	2.54	121.71	118.21
6	E	301	FAD	C4X-C10-N1	-2.53	118.38	124.59
6	H	301	FAD	C4A-N9A-C8A	2.53	108.39	105.74
6	H	301	FAD	C5A-N7A-C8A	2.52	107.41	103.45
6	H	301	FAD	C4X-C10-N1	-2.47	118.52	124.59
6	K	301	FAD	C4X-C10-N1	-2.47	118.53	124.59
6	E	301	FAD	C5A-N7A-C8A	2.47	107.33	103.45
6	B	301	FAD	C4-C4X-N5	2.43	121.56	118.21
6	B	301	FAD	C5A-N7A-C8A	2.42	107.25	103.45
6	H	301	FAD	C3B-C2B-C1B	2.36	105.94	101.46
6	H	301	FAD	O2-C2-N1	-2.35	117.90	121.80
6	H	301	FAD	C4X-C10-N10	2.29	119.75	116.48
6	K	301	FAD	C6A-C5A-N7A	2.28	136.48	132.09
6	K	301	FAD	O4-C4-C4X	-2.25	120.59	126.53
6	E	301	FAD	O4-C4-C4X	-2.19	120.76	126.53
6	E	301	FAD	C6A-C5A-N7A	2.18	136.29	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	301	FAD	C5X-C9A-N10	2.17	119.93	117.97
6	H	301	FAD	C10-N1-C2	2.13	121.47	116.85
6	H	301	FAD	C6A-C5A-N7A	2.12	136.17	132.09
6	B	301	FAD	C10-N1-C2	2.09	121.37	116.85
6	K	301	FAD	C10-N1-C2	2.07	121.33	116.85
6	K	301	FAD	N9A-C8A-N7A	-2.07	111.00	113.94
6	K	301	FAD	C4X-C4-N3	2.07	118.51	113.25
6	E	301	FAD	N9A-C8A-N7A	-2.06	111.01	113.94
6	B	301	FAD	O4-C4-C4X	-2.06	121.11	126.53
6	E	301	FAD	C10-N1-C2	2.05	121.29	116.85
6	E	301	FAD	C4X-C4-N3	2.04	118.44	113.25
6	E	301	FAD	C4X-C10-N10	2.02	119.37	116.48
6	B	301	FAD	C4X-C10-N10	2.01	119.35	116.48
6	K	301	FAD	C3B-C2B-C1B	2.00	105.25	101.46

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	505	GOL	O1-C1-C2-C3
7	D	506	GOL	O1-C1-C2-C3
7	D	507	GOL	O1-C1-C2-C3
7	G	504	GOL	C1-C2-C3-O3
7	J	509	GOL	C1-C2-C3-O3
7	B	304	GOL	O1-C1-C2-C3
7	D	508	GOL	O1-C1-C2-C3
7	D	509	GOL	O1-C1-C2-C3
7	D	510	GOL	C1-C2-C3-O3
7	G	504	GOL	O1-C1-C2-C3
7	J	506	GOL	C1-C2-C3-O3
7	J	508	GOL	C1-C2-C3-O3
7	J	509	GOL	O1-C1-C2-C3
7	B	304	GOL	O1-C1-C2-O2
7	D	505	GOL	O1-C1-C2-O2
7	D	506	GOL	O1-C1-C2-O2
7	D	508	GOL	O1-C1-C2-O2
7	G	504	GOL	O2-C2-C3-O3
7	J	509	GOL	O2-C2-C3-O3
7	J	509	GOL	O1-C1-C2-O2
7	D	508	GOL	O2-C2-C3-O3
7	G	504	GOL	O1-C1-C2-O2
7	D	507	GOL	O1-C1-C2-O2

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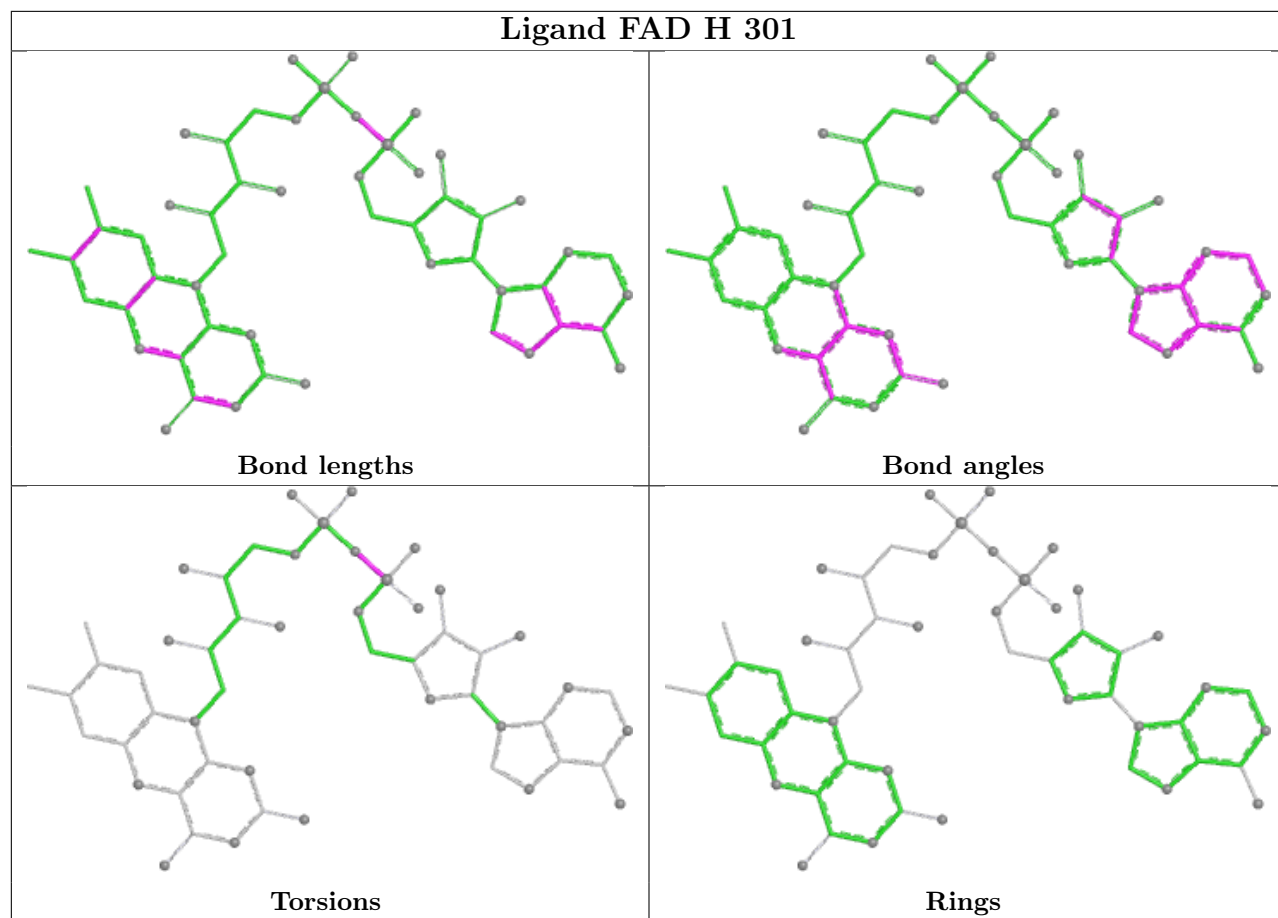
Mol	Chain	Res	Type	Atoms
7	D	510	GOL	O2-C2-C3-O3
7	D	509	GOL	O1-C1-C2-O2
7	D	509	GOL	C1-C2-C3-O3
7	G	503	GOL	C1-C2-C3-O3
6	H	301	FAD	P-O3P-PA-O2A
6	K	301	FAD	P-O3P-PA-O2A
6	B	301	FAD	P-O3P-PA-O2A
6	K	301	FAD	P-O3P-PA-O1A
7	J	506	GOL	O2-C2-C3-O3
7	J	508	GOL	O1-C1-C2-O2
6	H	301	FAD	P-O3P-PA-O1A

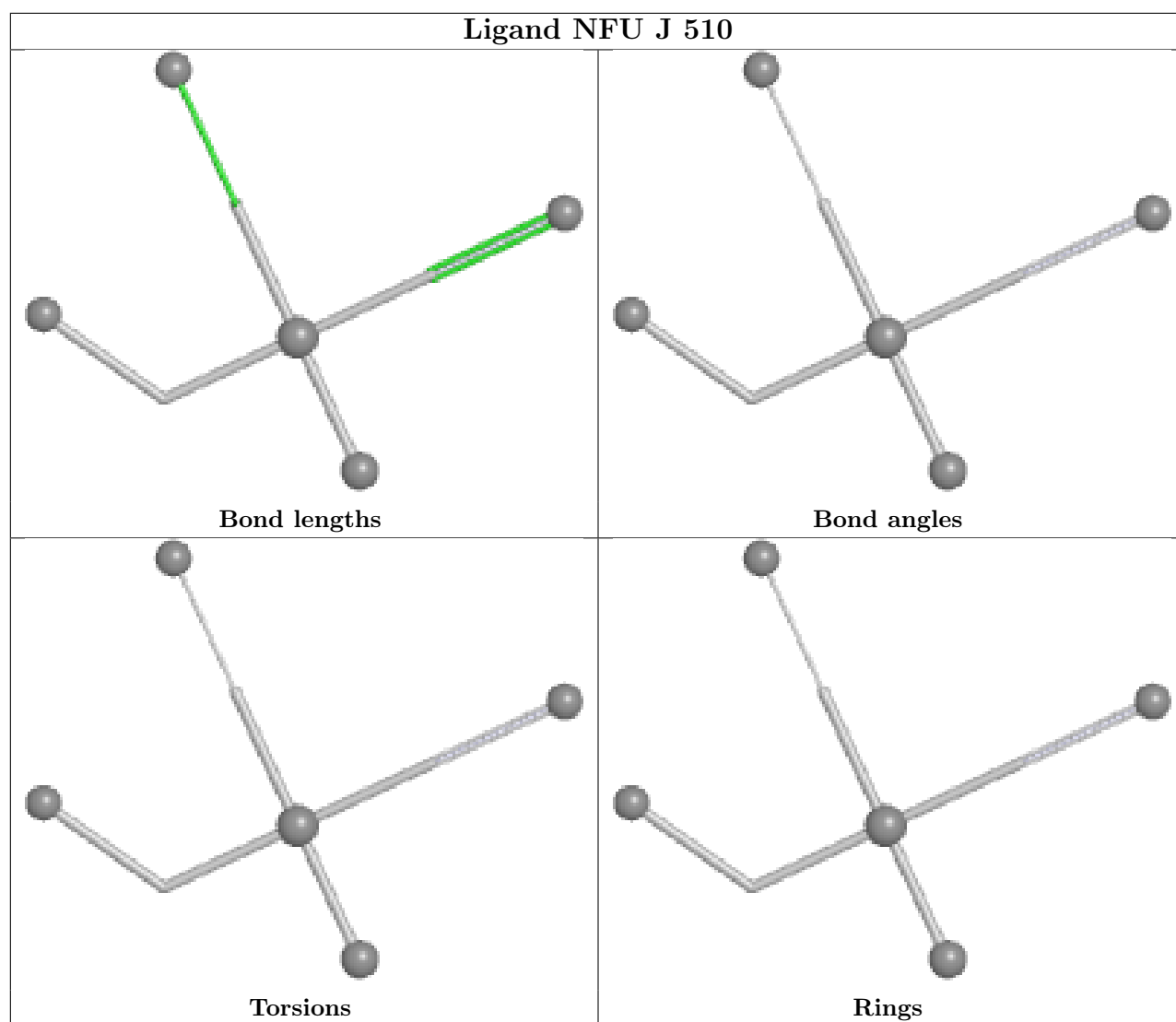
There are no ring outliers.

13 monomers are involved in 20 short contacts:

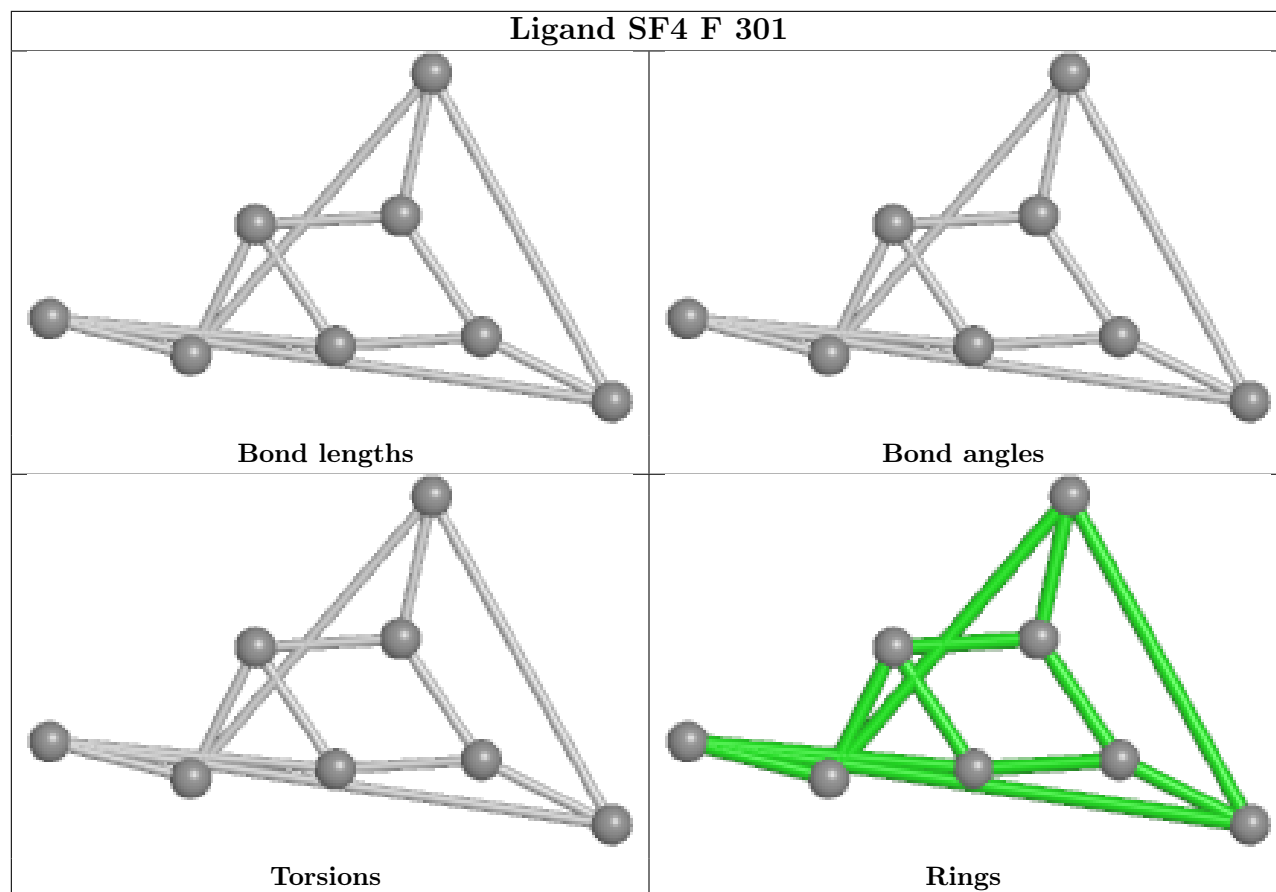
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	301	FAD	2	0
5	J	510	NFU	1	0
7	D	506	GOL	1	0
5	A	503	NFU	1	0
5	D	511	NFU	2	0
6	K	301	FAD	1	0
8	E	305	SF4	1	0
8	H	303	SF4	1	0
8	B	305	SF4	1	0
6	B	301	FAD	1	0
7	D	509	GOL	1	0
8	K	303	SF4	1	0
6	E	301	FAD	6	0

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

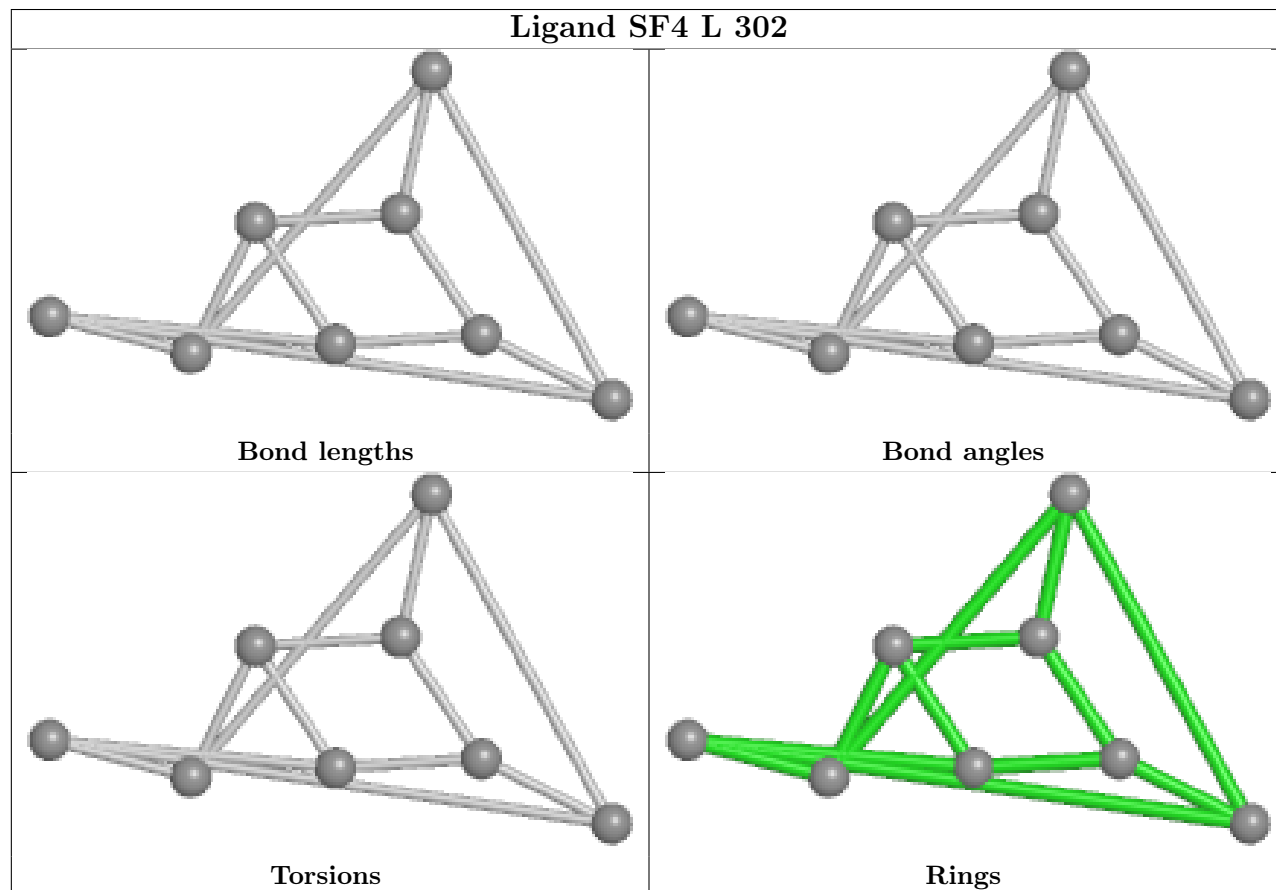


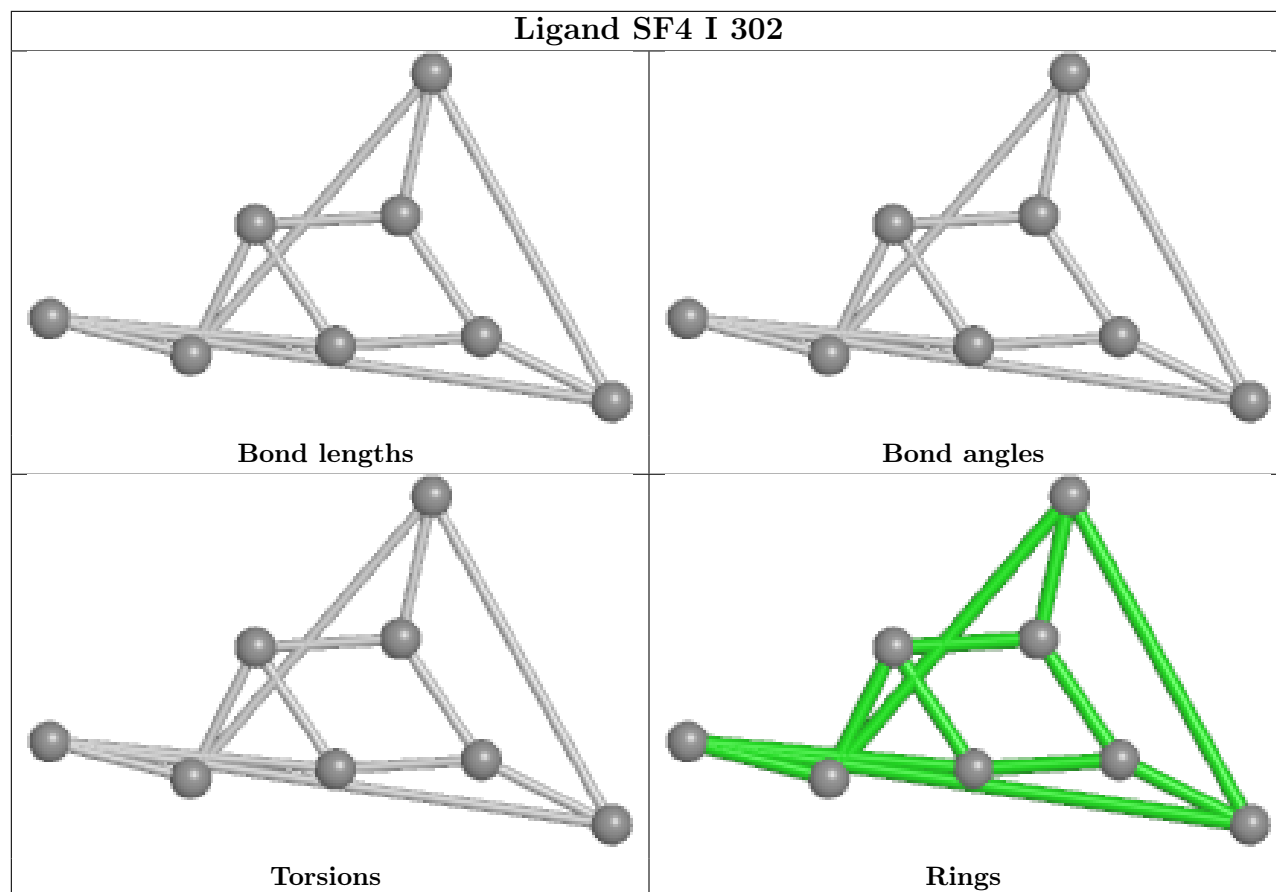


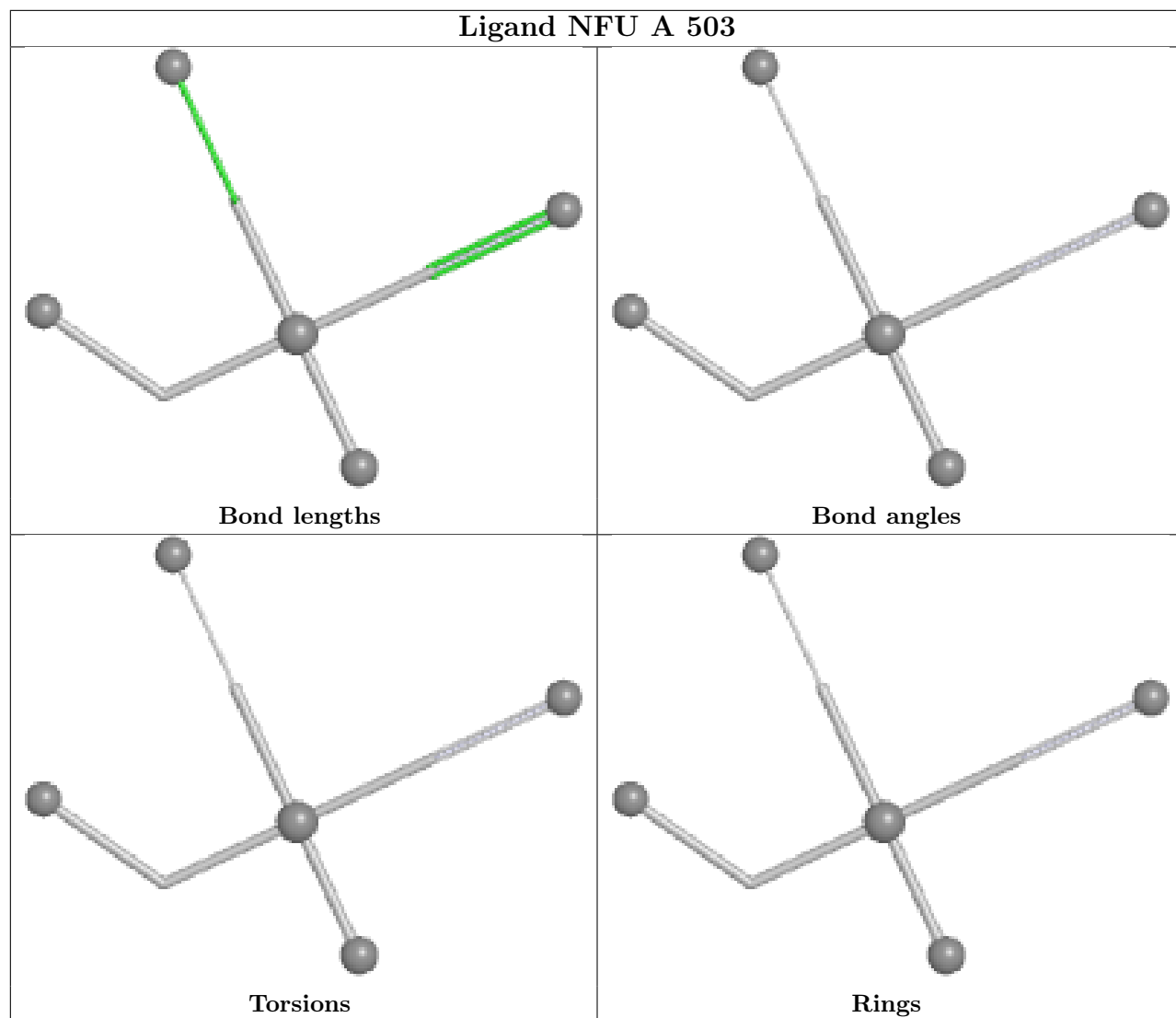
Ligand SF4 F 301

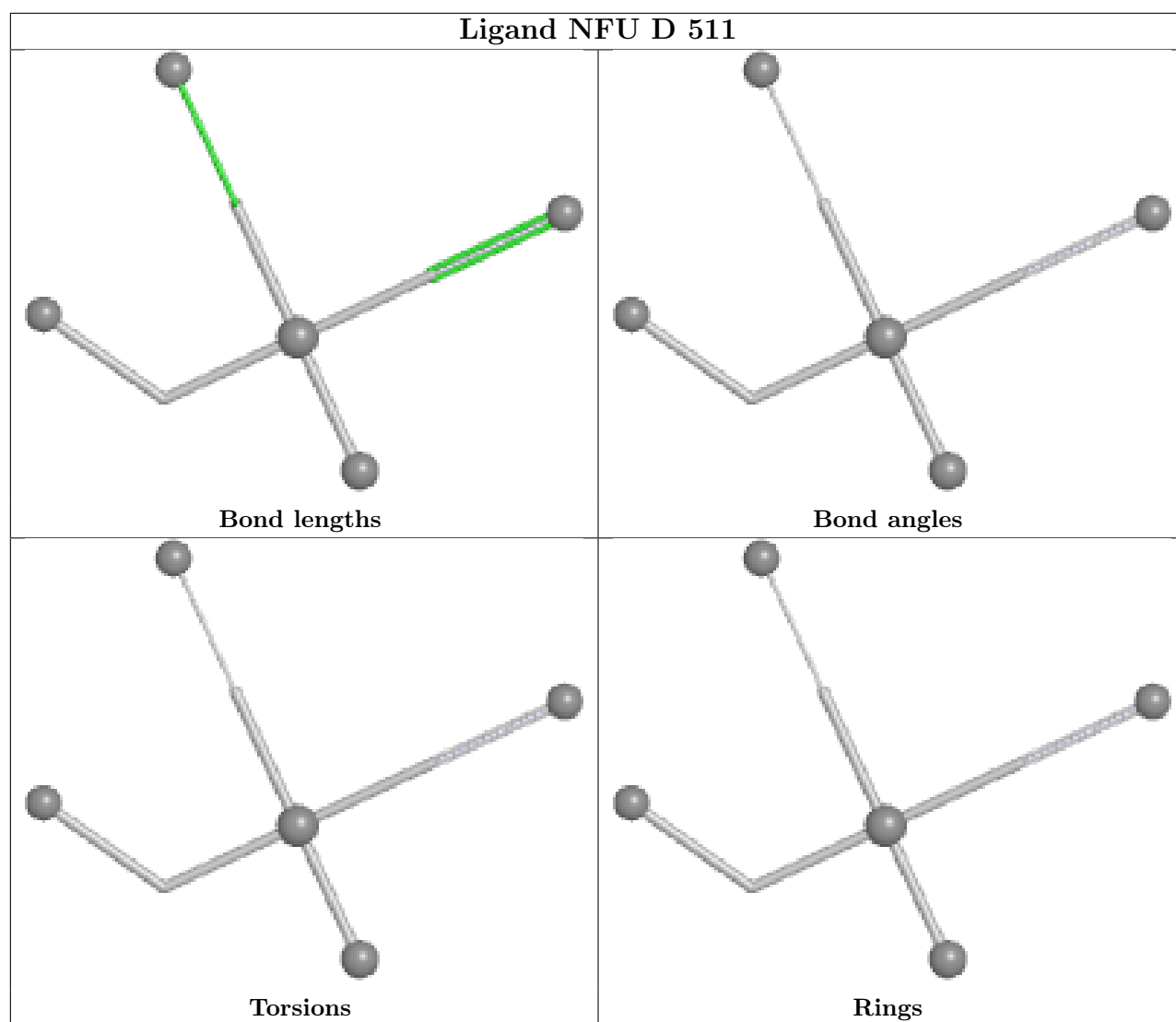


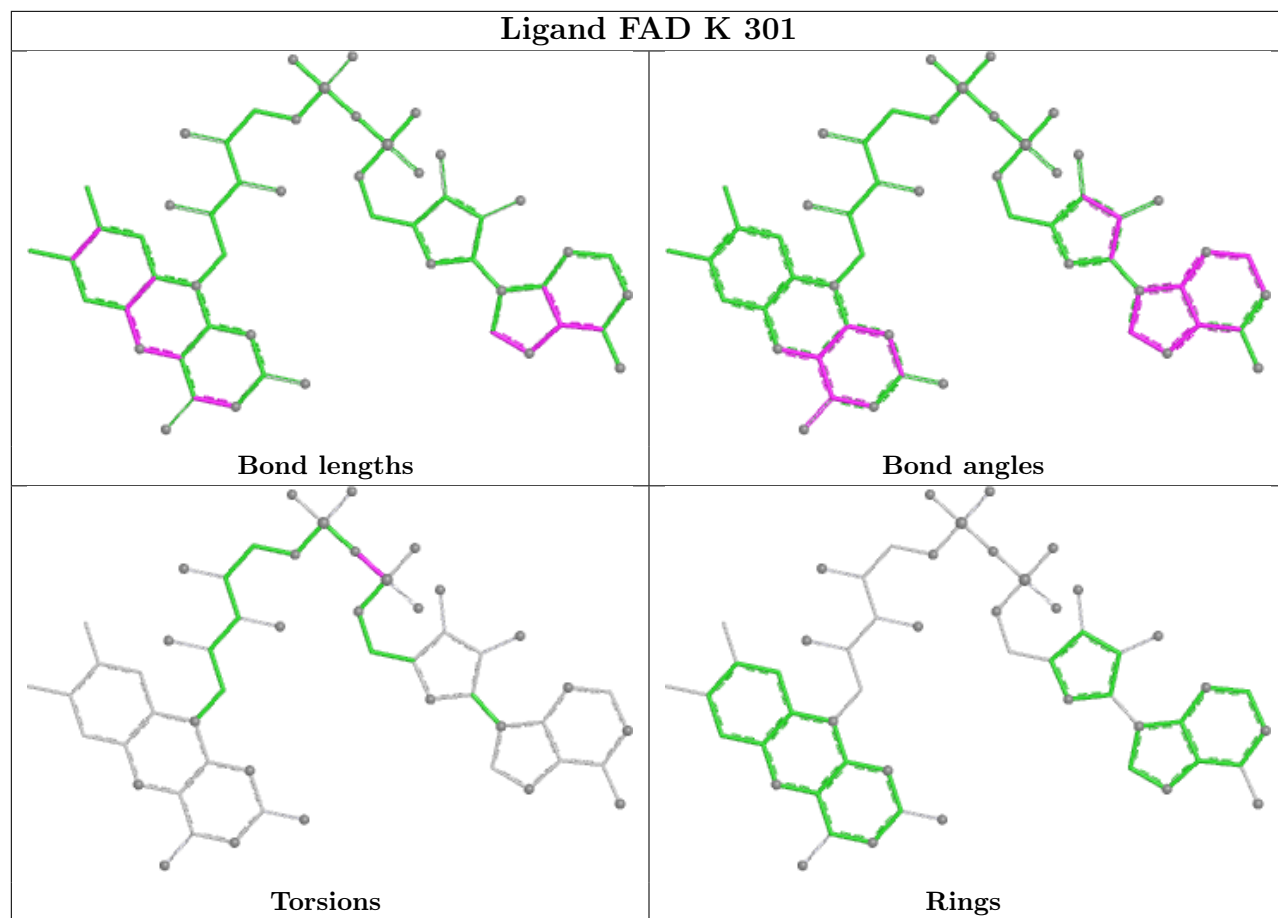
Ligand SF4 L 302

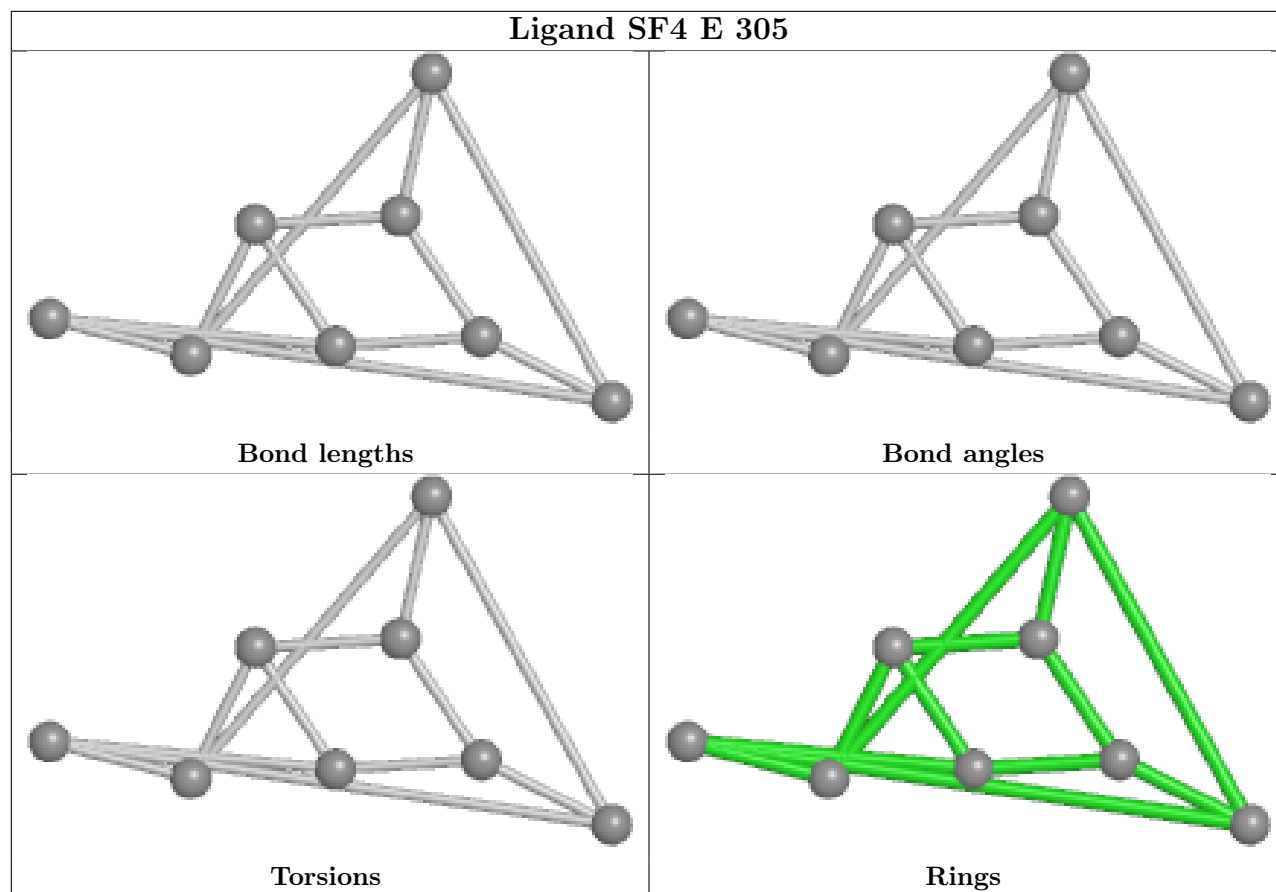


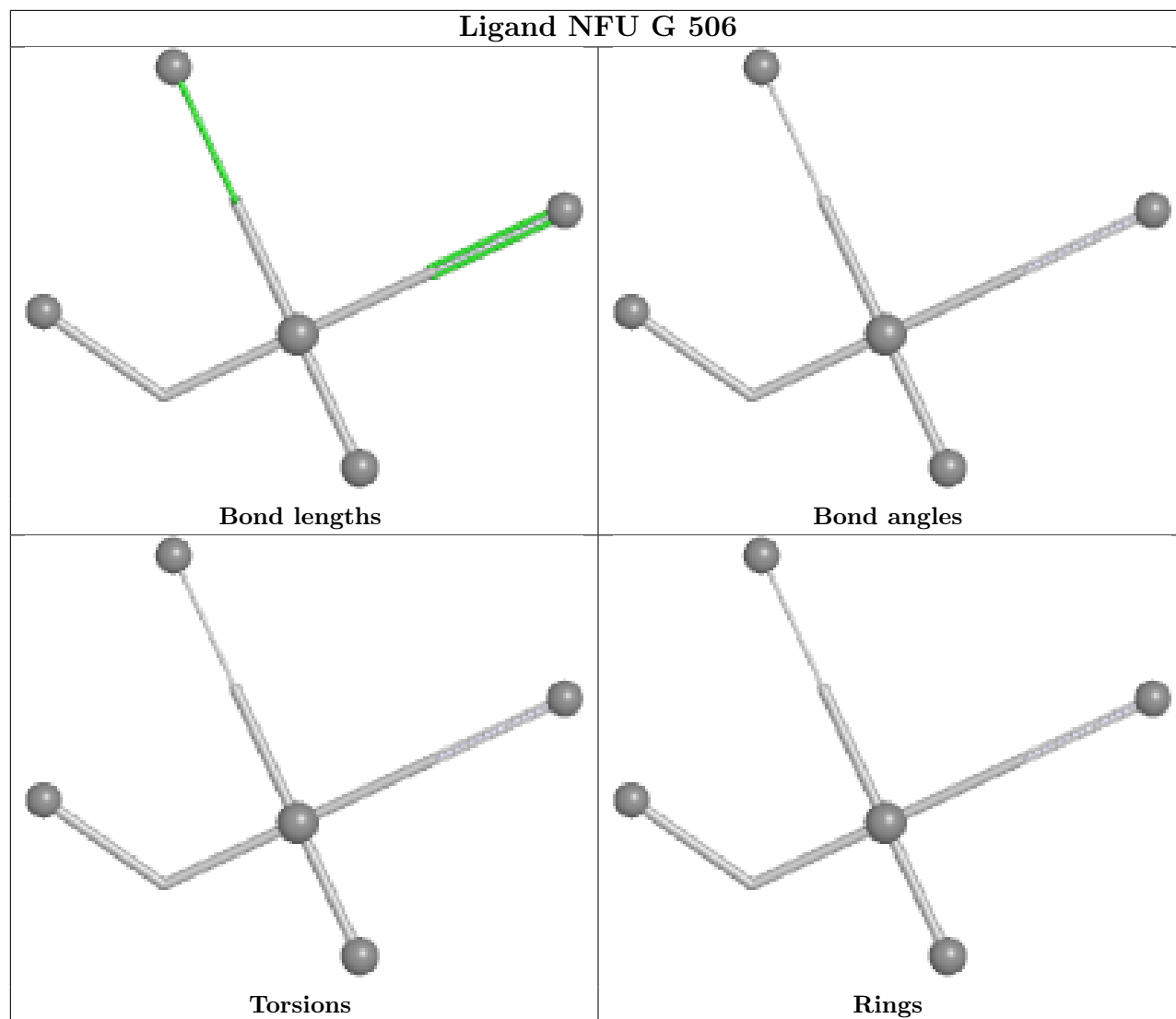




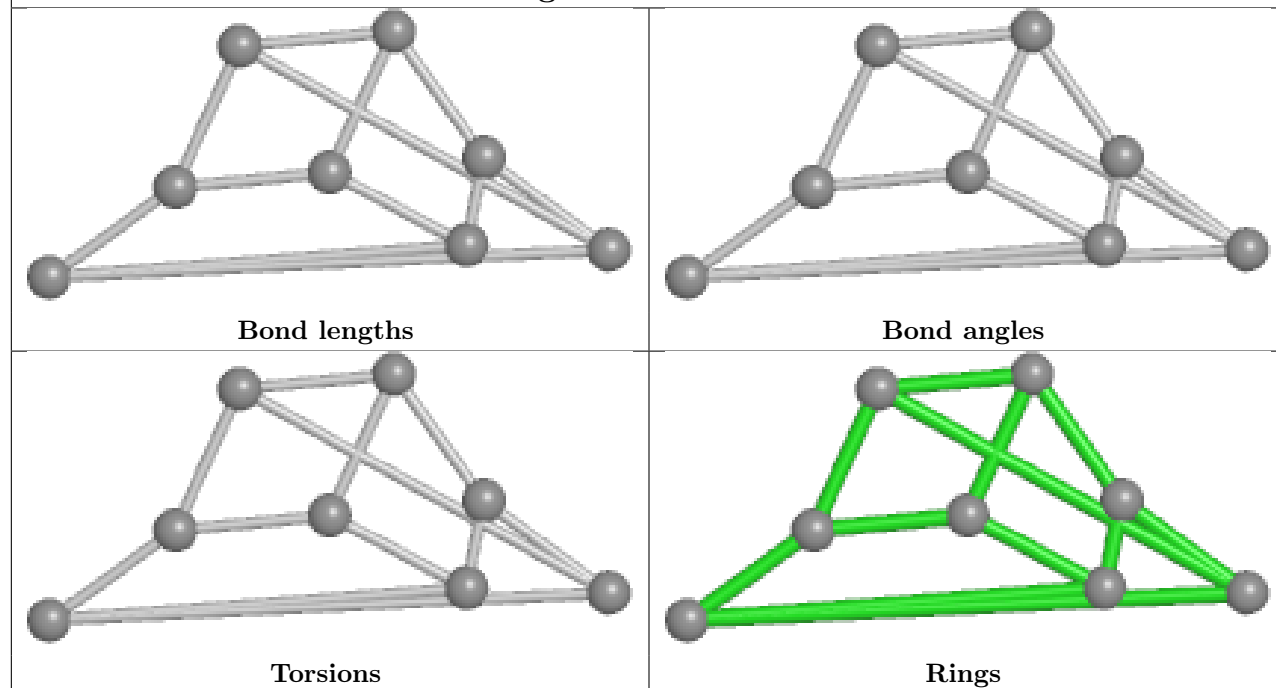




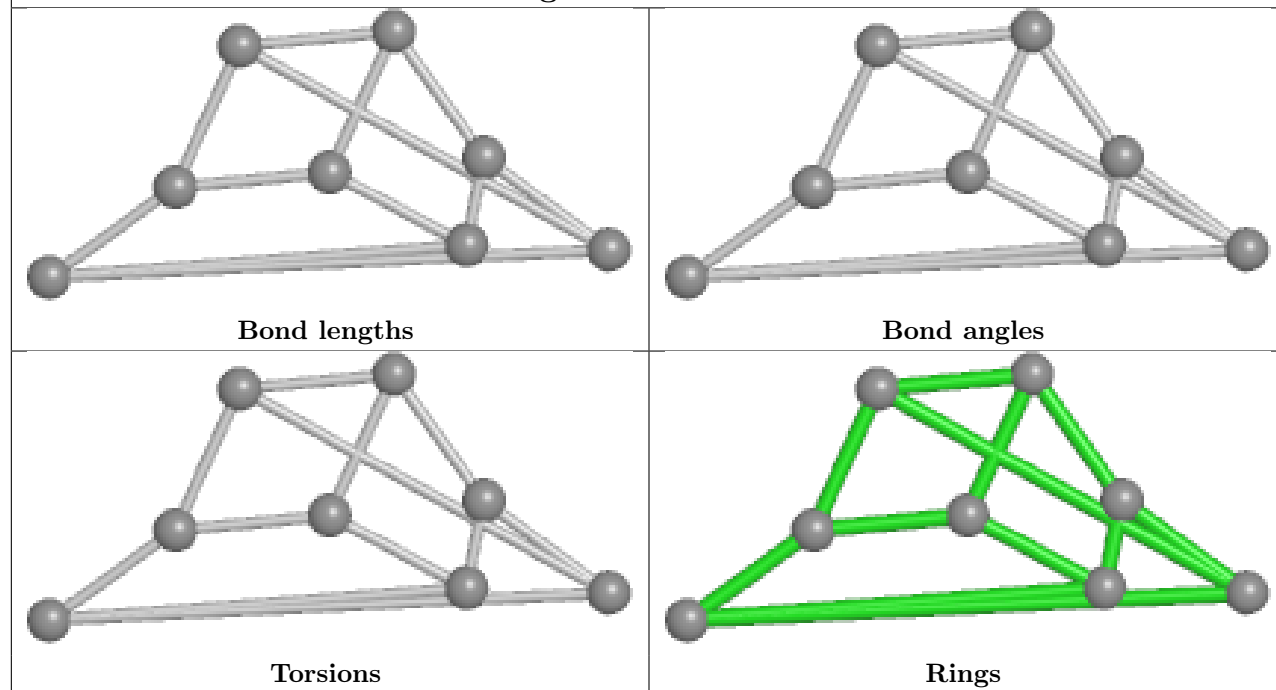




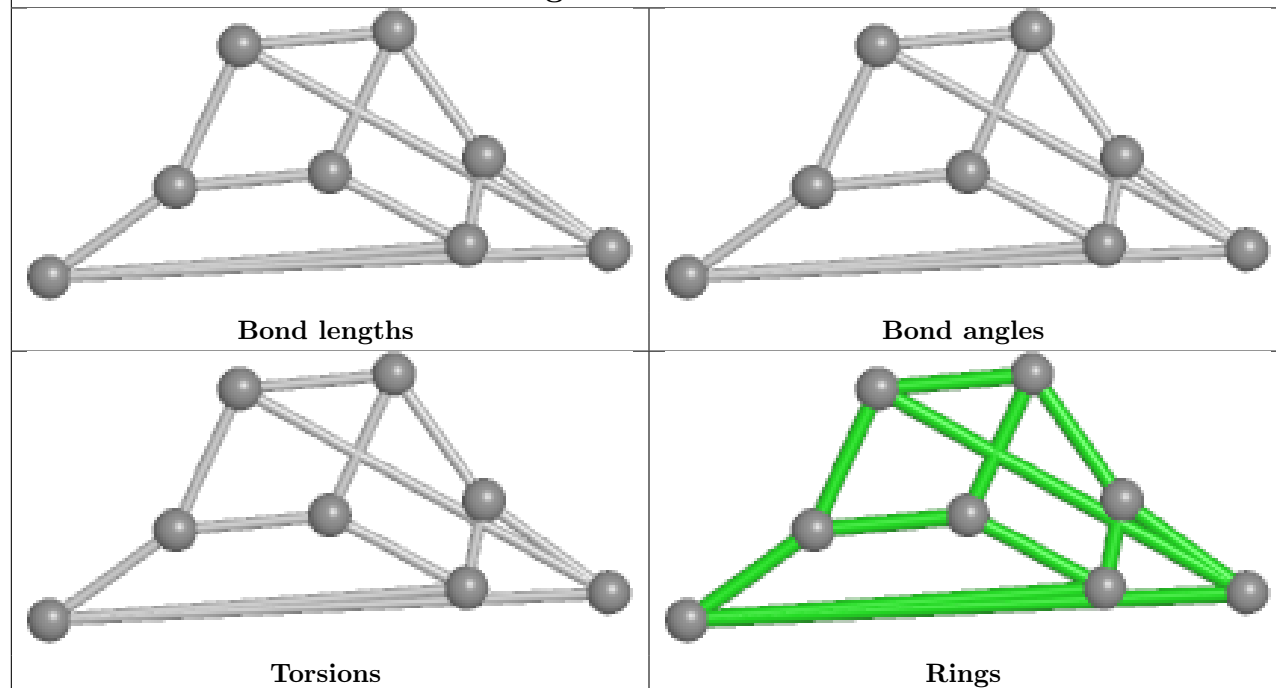
Ligand SF4 H 303



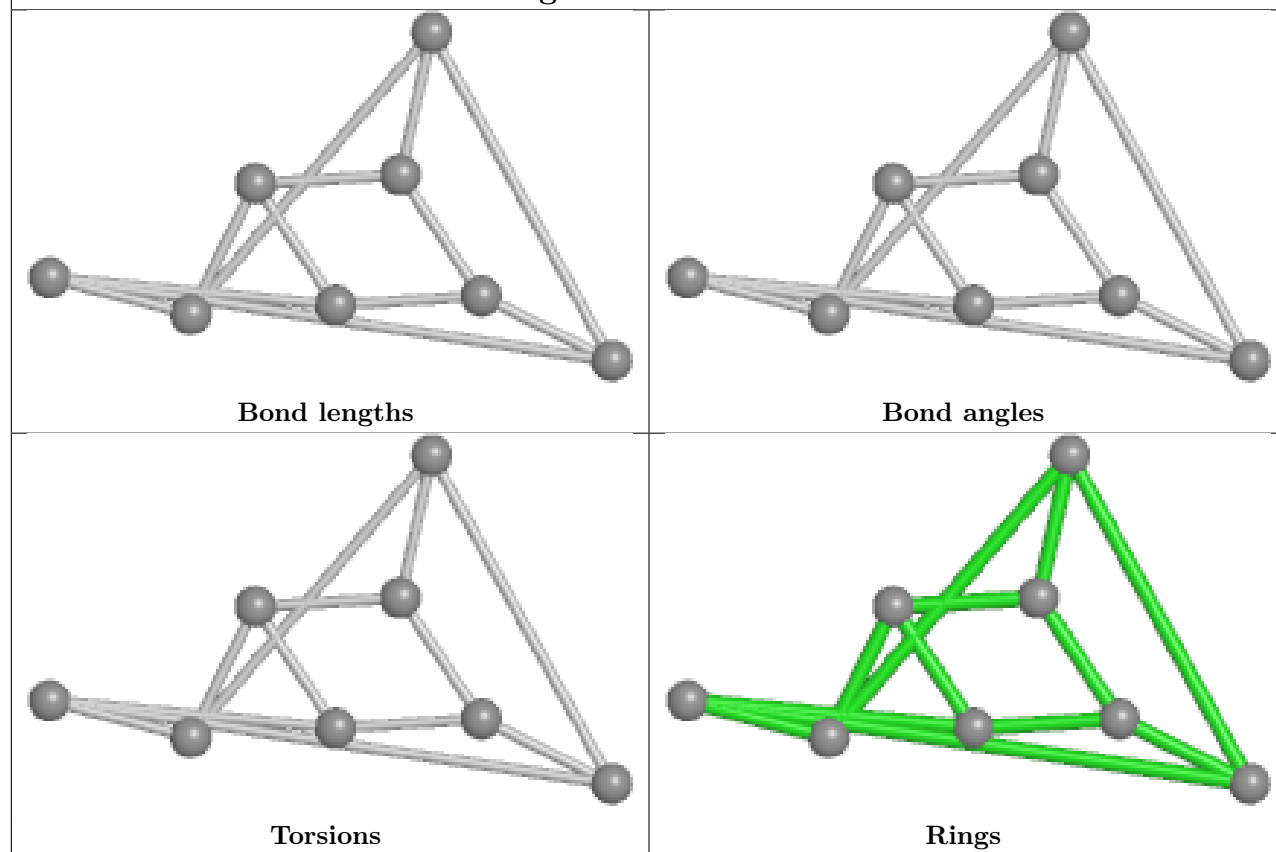
Ligand SF4 B 305

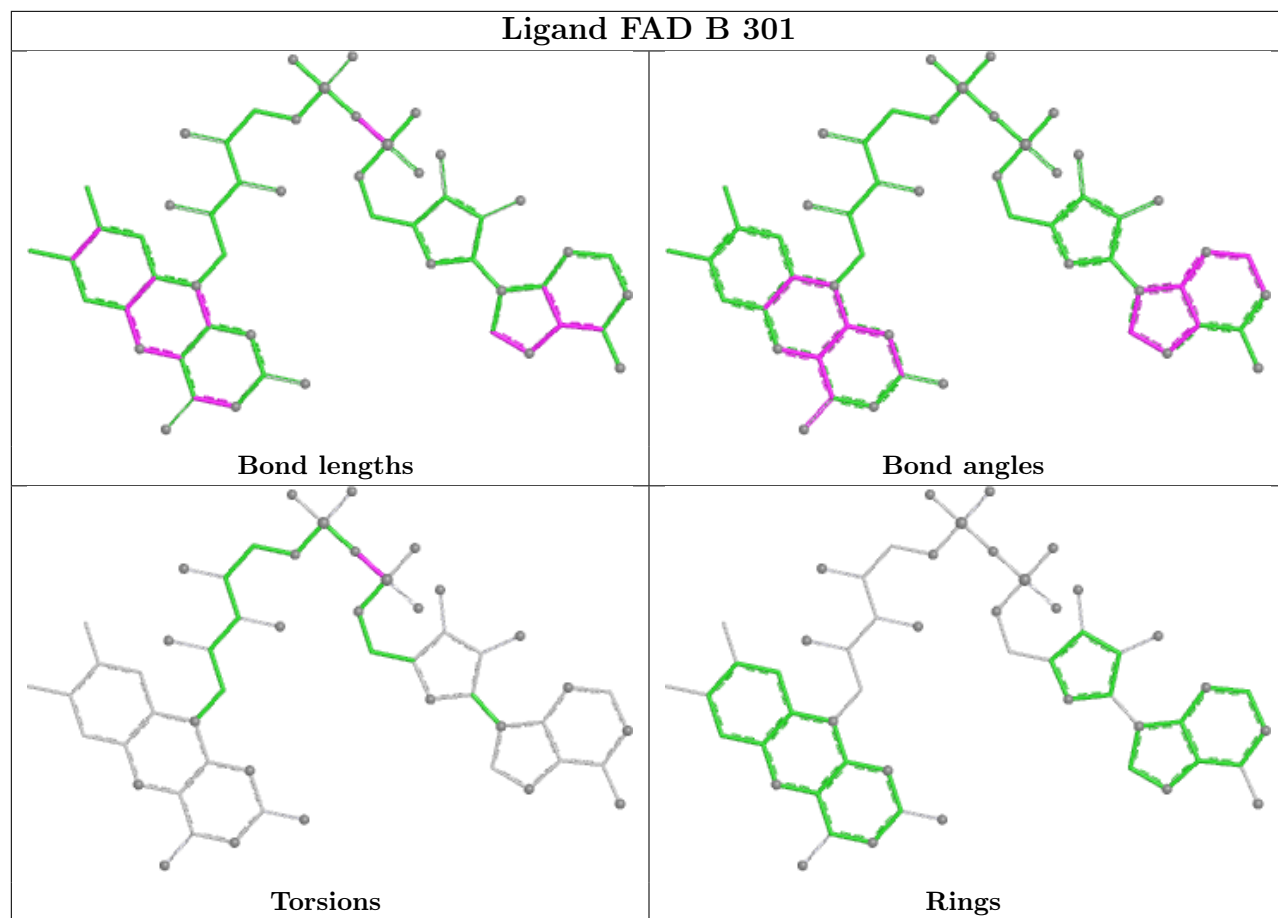


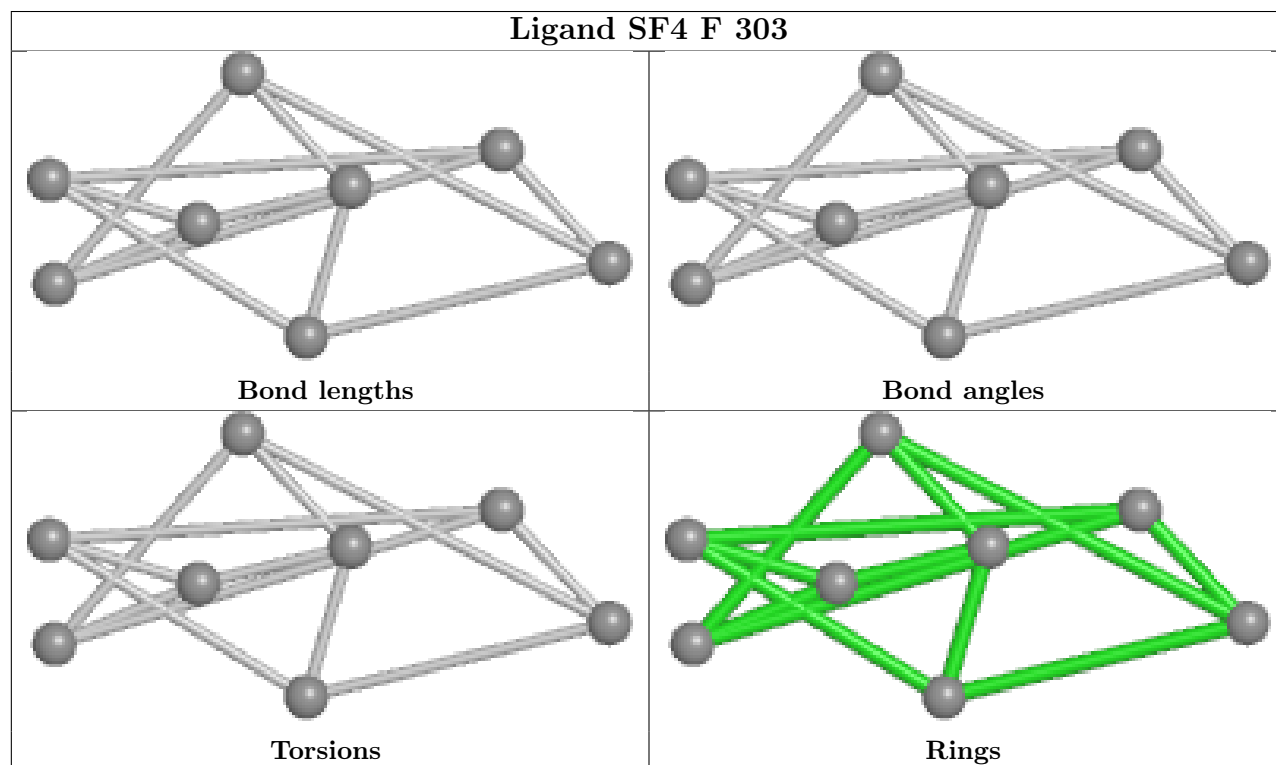
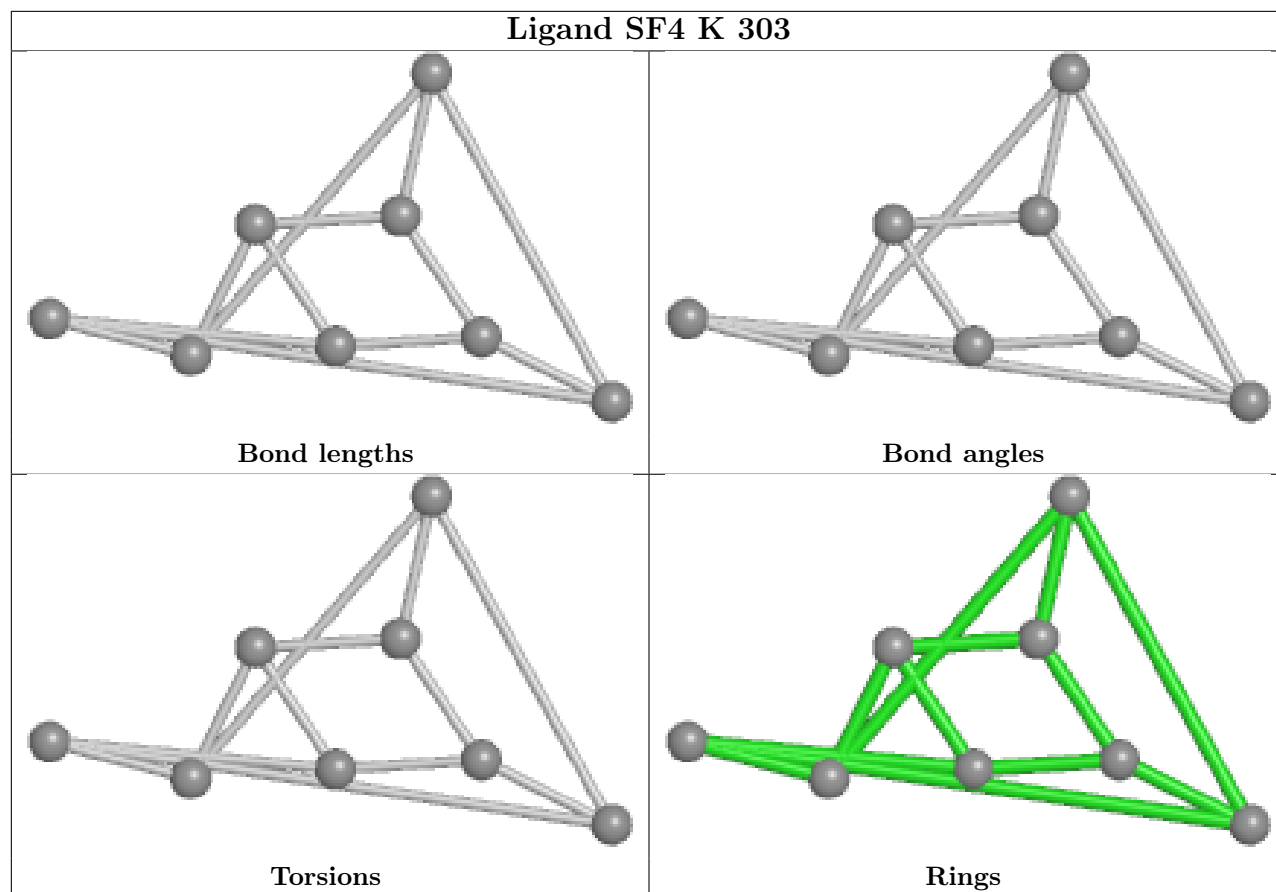
Ligand SF4 I 303



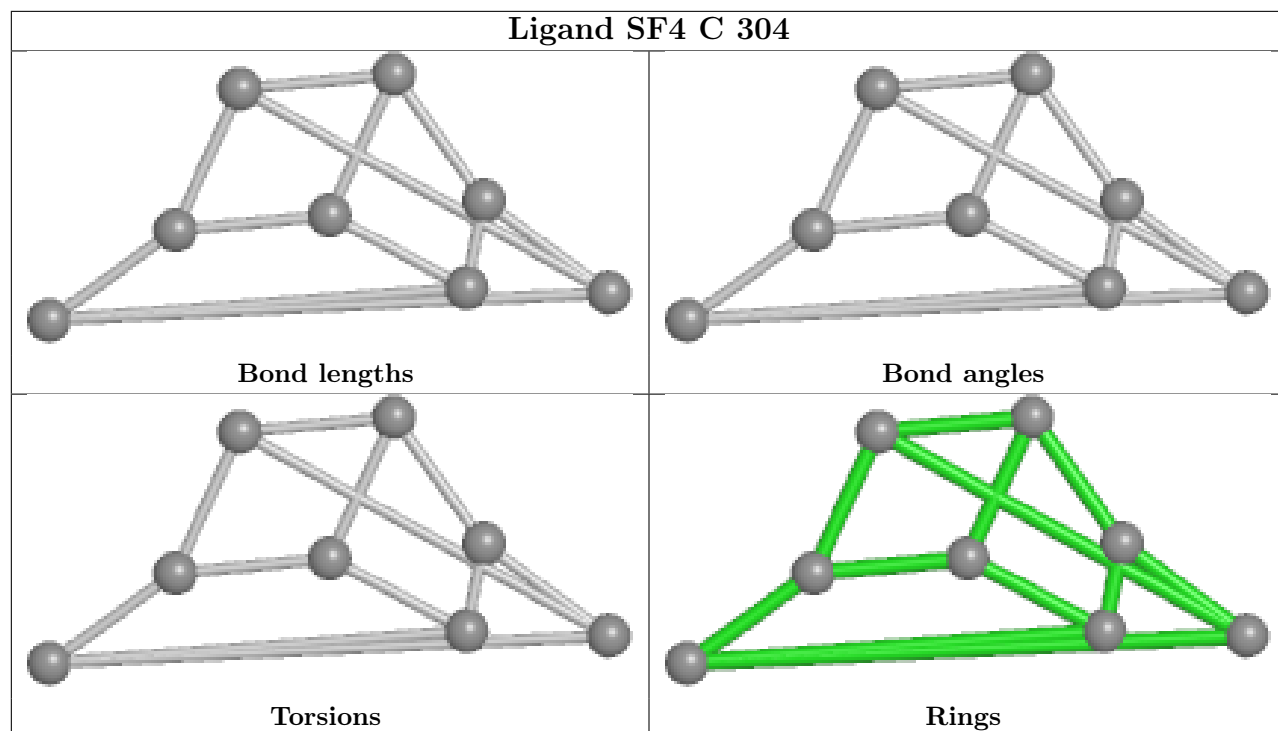
Ligand SF4 C 303



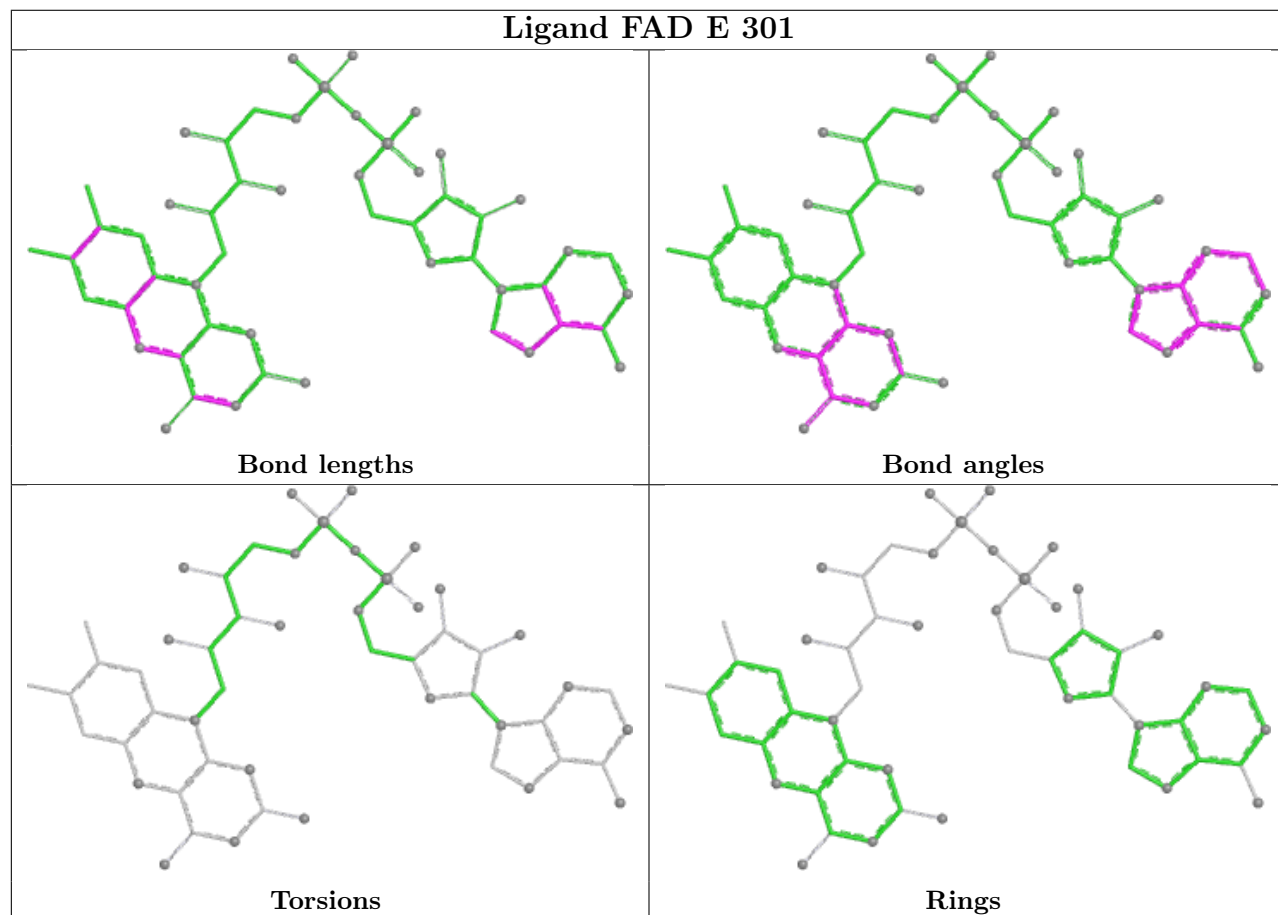


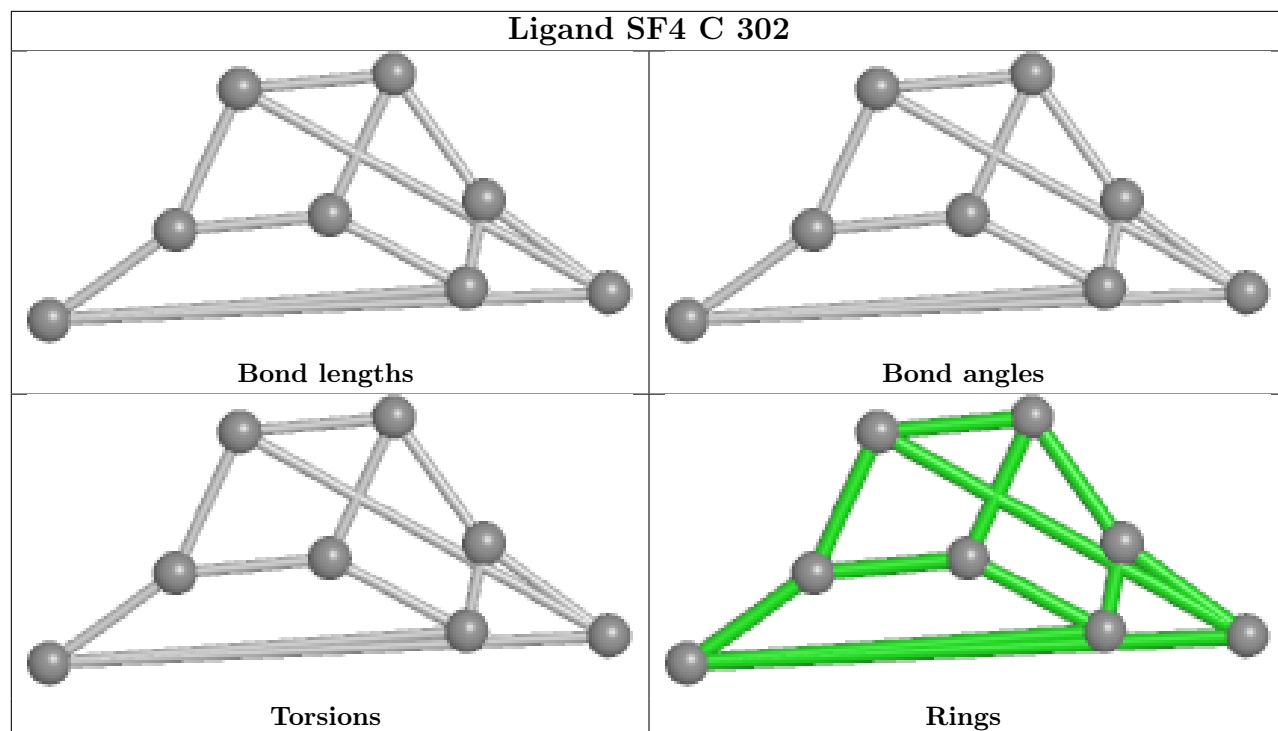


Ligand SF4 C 304

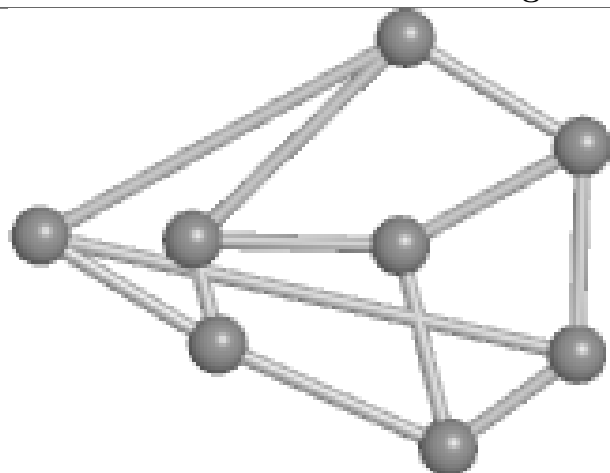


Ligand FAD E 301

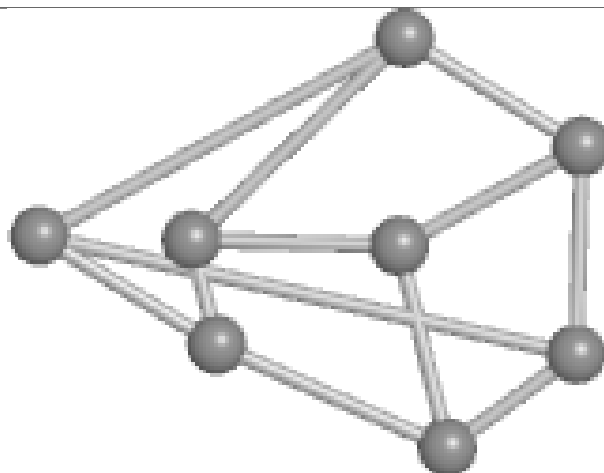




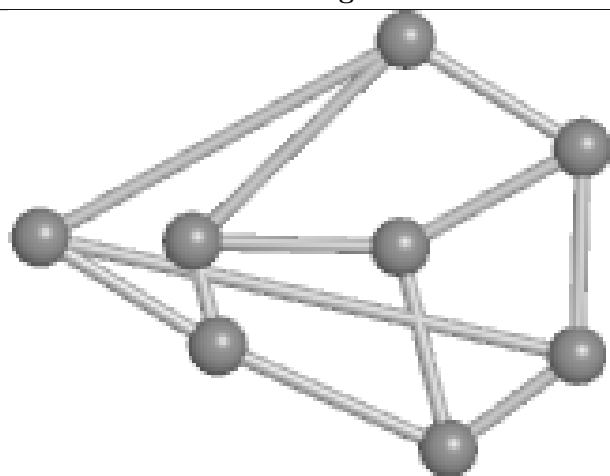
Ligand SF4 L 303



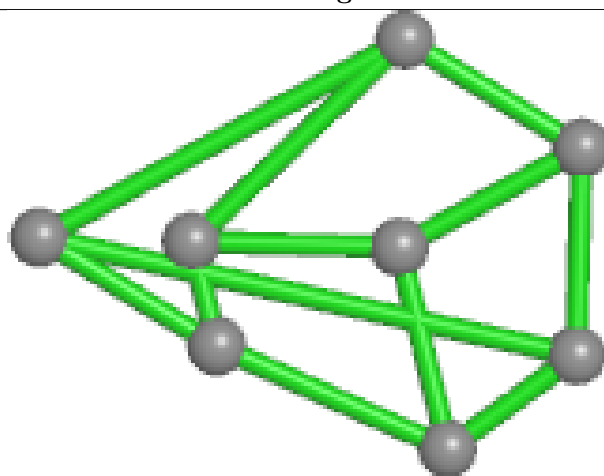
Bond lengths



Bond angles

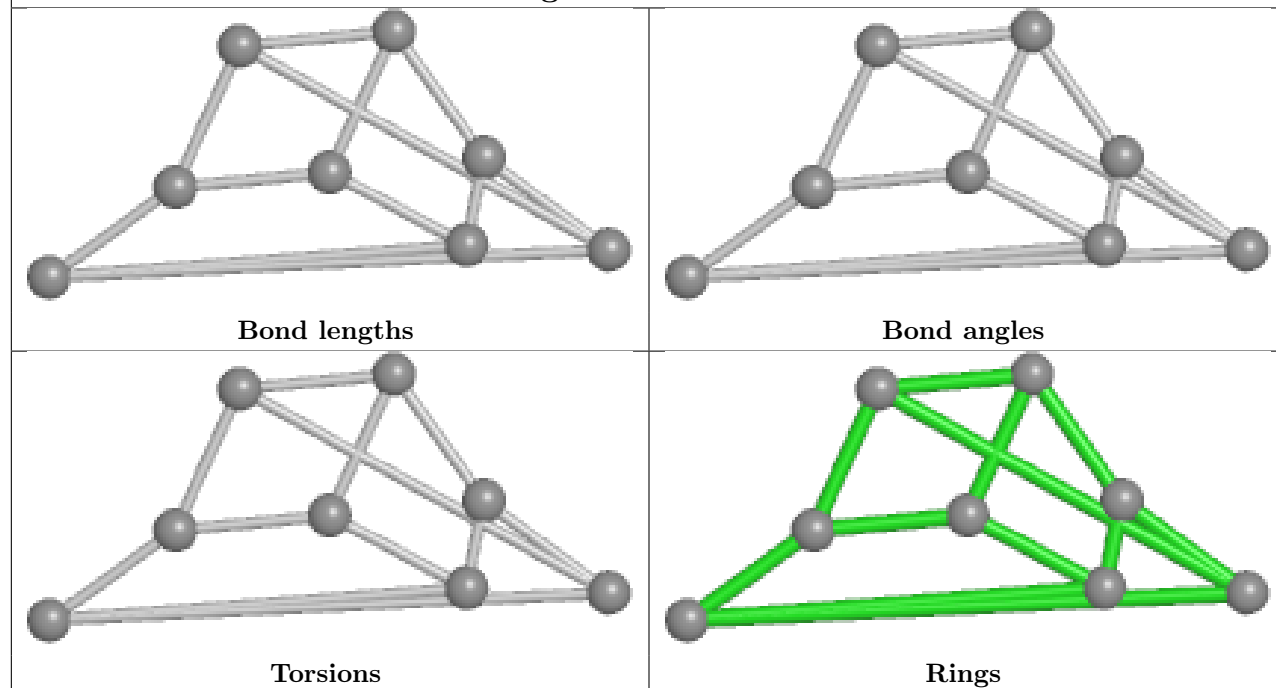


Torsions

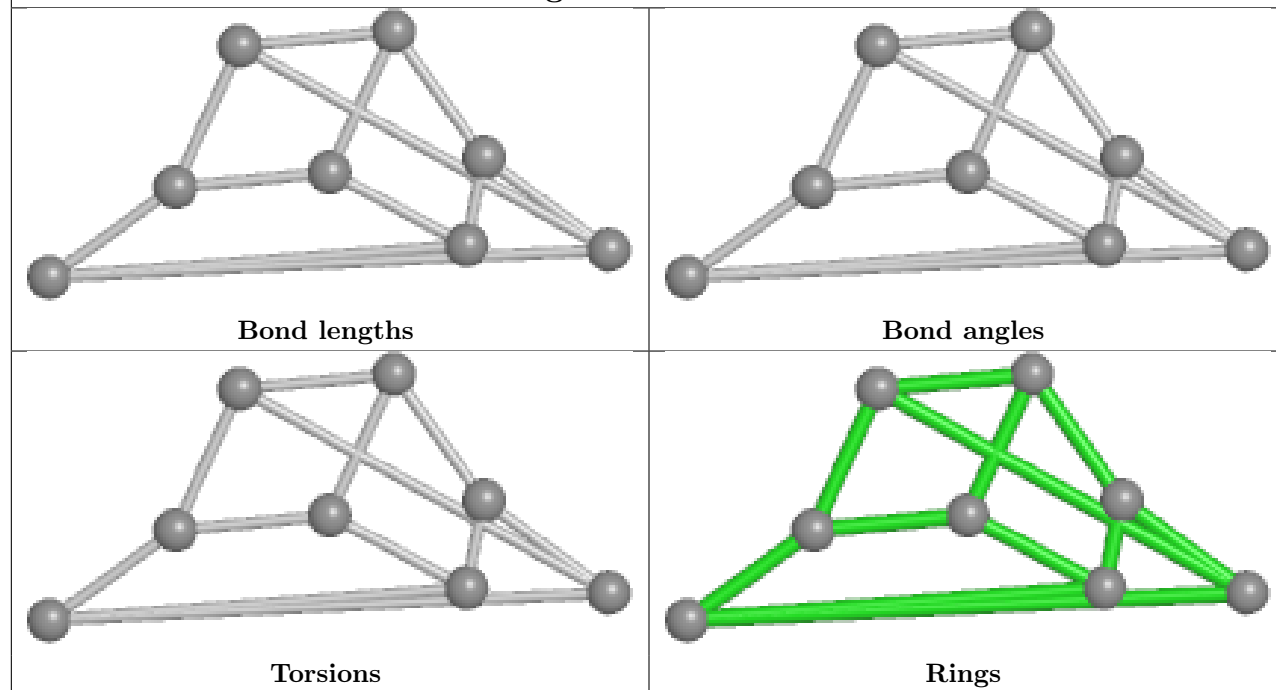


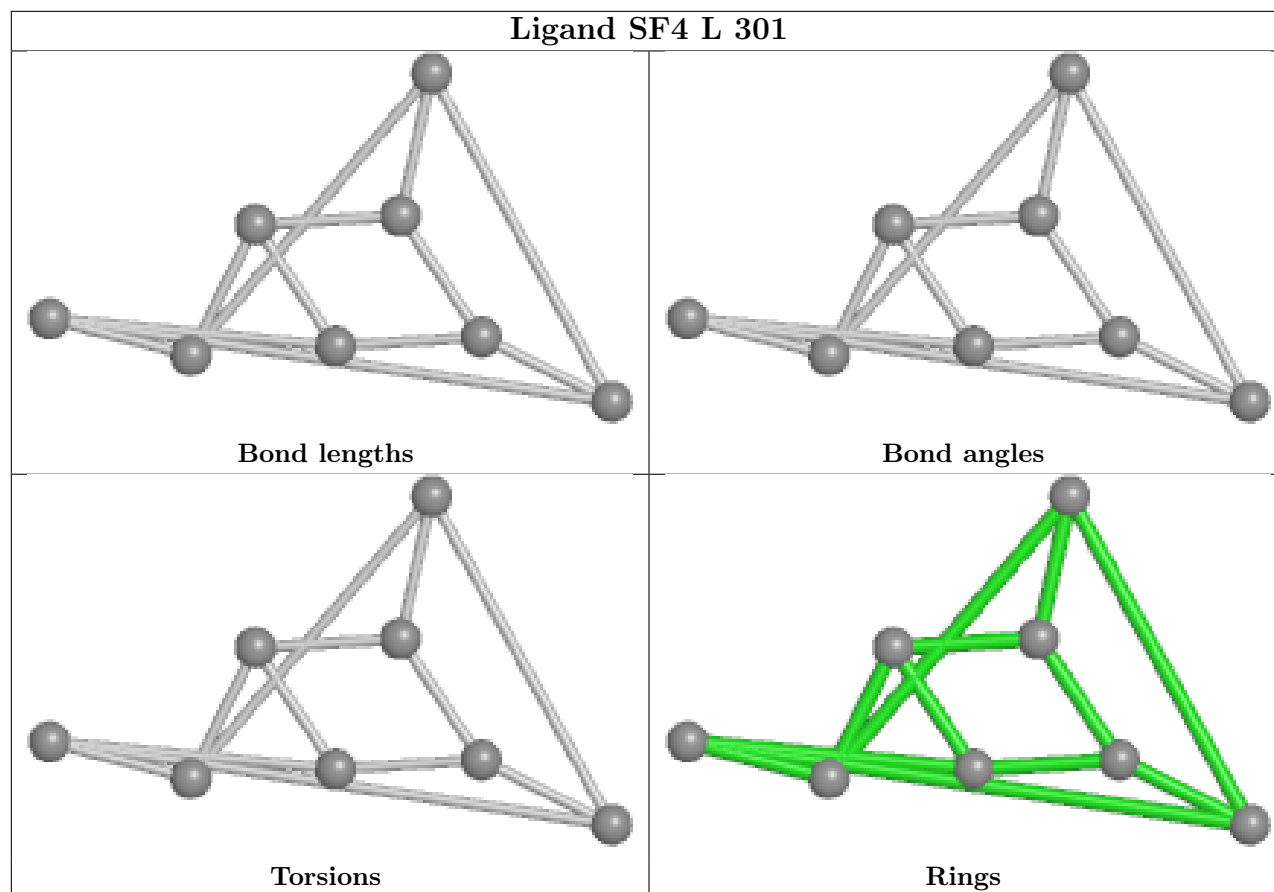
Rings

Ligand SF4 F 302



Ligand SF4 I 301





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%)	-0.17	0 100 100	65, 83, 116, 152	0
1	D	392/410 (95%)	-0.54	0 100 100	50, 66, 92, 111	0
1	G	392/410 (95%)	-0.59	2 (0%) 87 85	47, 63, 88, 125	0
1	J	392/410 (95%)	-0.55	1 (0%) 90 89	48, 65, 96, 135	0
2	B	282/282 (100%)	-0.15	0 100 100	65, 87, 115, 135	0
2	E	282/282 (100%)	-0.03	1 (0%) 88 87	68, 96, 121, 158	0
2	H	282/282 (100%)	-0.30	0 100 100	59, 82, 106, 133	0
2	K	282/282 (100%)	-0.34	0 100 100	59, 81, 110, 137	0
3	C	240/241 (99%)	0.17	10 (4%) 40 32	70, 94, 138, 163	0
3	F	240/241 (99%)	0.05	9 (3%) 44 35	66, 84, 124, 164	0
3	I	240/241 (99%)	-0.14	9 (3%) 44 35	58, 77, 122, 148	1 (0%)
3	L	240/241 (99%)	-0.15	5 (2%) 63 55	55, 79, 124, 153	1 (0%)
All	All	3656/3732 (97%)	-0.26	37 (1%) 79 74	47, 78, 115, 164	2 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	115	GLN	5.9
3	F	27	LEU	5.9
3	F	116	MET	4.4
3	I	115	GLN	4.2
3	F	115	GLN	3.8
3	L	115	GLN	3.7
3	C	27	LEU	3.3
3	F	117	SER	3.3
3	I	27	LEU	3.2
3	F	139	GLY	3.1
1	G	2	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
3	L	117	SER	3.0
3	I	116	MET	2.6
3	L	27	LEU	2.6
3	I	30	LEU	2.5
3	L	116	MET	2.4
2	E	1	MET	2.4
3	I	182	ASN	2.4
3	I	25	GLN	2.4
3	I	2	VAL	2.3
3	I	26	LEU	2.3
3	C	240	ILE	2.2
3	C	116	MET	2.2
3	C	114	GLY	2.2
3	C	26	LEU	2.2
3	L	139	GLY	2.1
3	F	30	LEU	2.1
3	C	117	SER	2.1
1	G	3	LYS	2.1
3	C	235	LYS	2.1
3	C	40	THR	2.1
3	F	26	LEU	2.1
3	F	241	GLU	2.1
3	I	117	SER	2.0
3	C	215	LYS	2.0
1	J	2	GLY	2.0
3	F	29	ILE	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($\text{\AA}^2$)	Q<0.9
7	GOL	G	503	6/6	0.39	0.19	100,117,133,138	0
4	SO4	B	303	5/5	0.48	0.11	139,139,179,193	0
4	SO4	J	504	5/5	0.53	0.13	122,123,142,159	0
4	SO4	E	303	5/5	0.56	0.10	149,168,179,191	0
4	SO4	J	502	5/5	0.59	0.11	131,143,178,180	0
7	GOL	J	509	6/6	0.59	0.21	92,109,113,117	0
7	GOL	D	504	6/6	0.65	0.26	89,98,105,110	0
4	SO4	K	302	5/5	0.68	0.07	149,152,176,182	0
4	SO4	E	302	5/5	0.68	0.12	125,132,148,151	0
4	SO4	E	304	5/5	0.69	0.07	144,162,167,176	0
4	SO4	A	501	5/5	0.71	0.13	118,134,161,168	0
4	SO4	J	505	5/5	0.71	0.15	132,133,153,165	0
7	GOL	B	304	6/6	0.72	0.16	85,98,102,108	0
4	SO4	B	302	5/5	0.72	0.07	136,139,156,163	0
4	SO4	D	503	5/5	0.73	0.08	131,133,169,175	0
7	GOL	D	505	6/6	0.73	0.21	84,101,105,107	0
7	GOL	D	508	6/6	0.75	0.21	94,109,111,116	0
7	GOL	D	510	6/6	0.75	0.13	103,106,121,125	0
7	GOL	D	509	6/6	0.76	0.17	102,104,107,114	0
7	GOL	D	506	6/6	0.76	0.17	78,93,101,111	0
7	GOL	G	504	6/6	0.77	0.23	86,88,104,106	0
4	SO4	H	302	5/5	0.78	0.06	126,139,150,151	0
4	SO4	D	502	5/5	0.80	0.15	101,104,137,137	0
4	SO4	C	301	5/5	0.82	0.10	122,128,144,162	0
7	GOL	J	508	6/6	0.82	0.12	97,110,114,116	0
4	SO4	J	501	5/5	0.82	0.15	94,106,119,122	0
4	SO4	A	502	5/5	0.85	0.19	98,111,130,133	0
7	GOL	D	507	6/6	0.86	0.22	95,102,117,132	0
7	GOL	J	506	6/6	0.86	0.15	78,90,100,103	0
7	GOL	G	505	6/6	0.87	0.15	77,90,95,101	0
7	GOL	J	507	6/6	0.87	0.15	86,92,97,102	0
4	SO4	G	502	5/5	0.88	0.16	103,118,123,136	0
4	SO4	D	501	5/5	0.90	0.20	88,93,111,116	0
4	SO4	G	501	5/5	0.90	0.17	98,98,124,128	0
4	SO4	J	503	5/5	0.90	0.15	76,88,114,126	0
5	NFU	A	503	8/8	0.92	0.17	65,77,104,171	0
6	FAD	K	301	53/53	0.95	0.11	49,78,91,100	0
6	FAD	E	301	53/53	0.95	0.11	58,89,104,110	0
6	FAD	B	301	53/53	0.97	0.08	55,78,89,97	0
6	FAD	H	301	53/53	0.97	0.08	58,77,89,92	0
5	NFU	G	506	8/8	0.98	0.09	49,60,79,84	0
5	NFU	J	510	8/8	0.98	0.12	52,61,81,83	0
5	NFU	D	511	8/8	0.98	0.11	48,63,74,78	0

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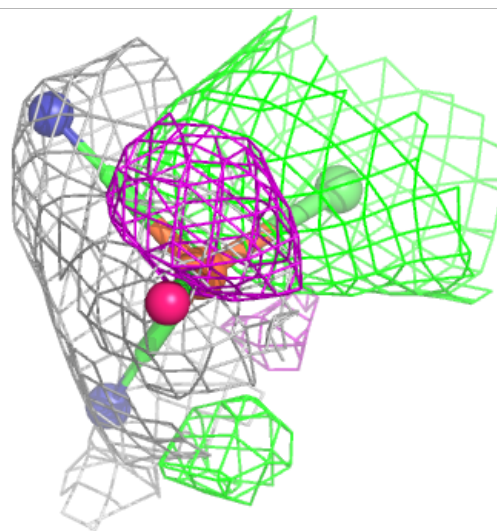
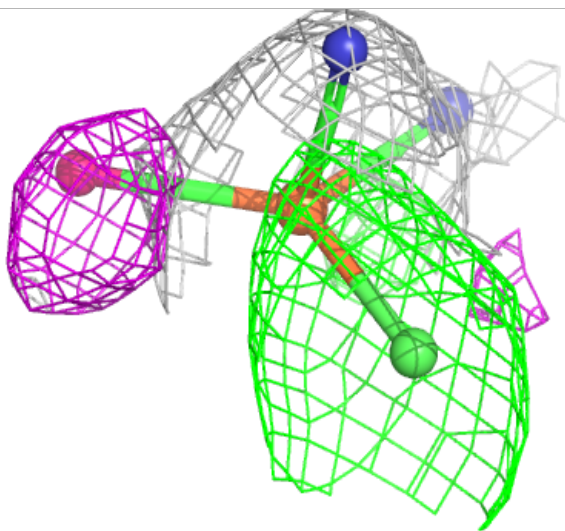
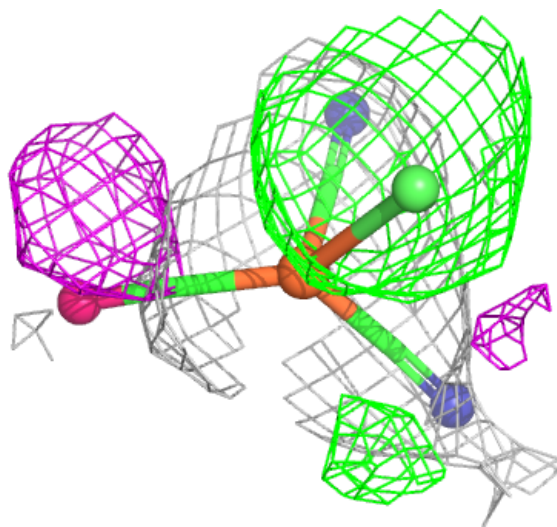
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SF4	B	305	8/8	0.99	0.04	70,77,79,89	0
8	SF4	C	302	8/8	0.99	0.04	66,78,84,93	0
8	SF4	C	304	8/8	0.99	0.03	61,67,71,71	0
8	SF4	E	305	8/8	0.99	0.04	79,85,92,92	0
8	SF4	F	301	8/8	0.99	0.04	61,64,68,68	0
8	SF4	F	302	8/8	0.99	0.03	61,64,68,72	0
8	SF4	F	303	8/8	0.99	0.04	70,73,81,82	0
8	SF4	H	303	8/8	0.99	0.04	55,66,71,73	0
8	SF4	I	301	8/8	0.99	0.04	58,60,65,65	0
8	SF4	I	302	8/8	0.99	0.03	55,59,60,61	0
8	SF4	I	303	8/8	0.99	0.04	56,62,65,66	0
8	SF4	K	303	8/8	0.99	0.05	59,68,74,83	0
8	SF4	L	301	8/8	0.99	0.03	54,59,61,62	0
8	SF4	L	302	8/8	0.99	0.03	51,59,60,64	0
8	SF4	L	303	8/8	0.99	0.03	53,57,59,59	0
8	SF4	C	303	8/8	1.00	0.03	62,69,72,73	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.

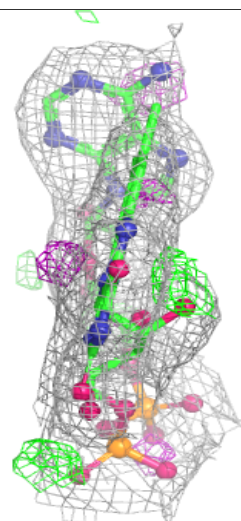
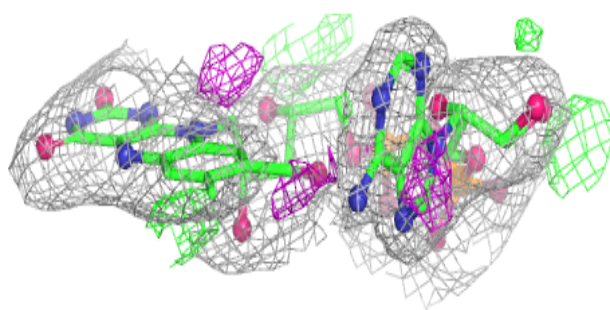
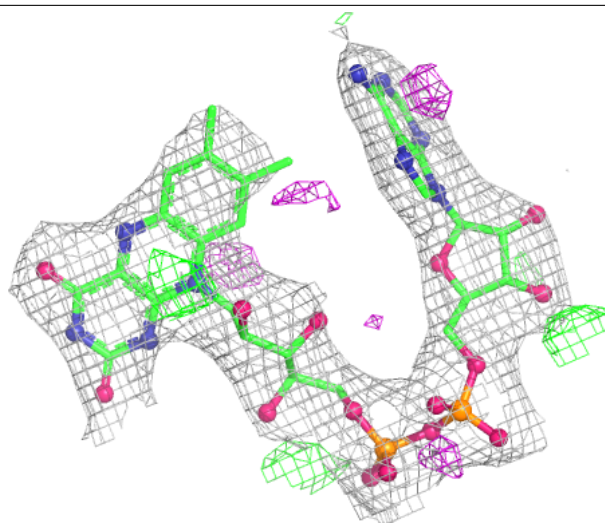
Electron density around NFU A 503:

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



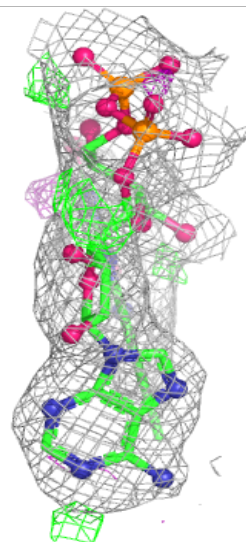
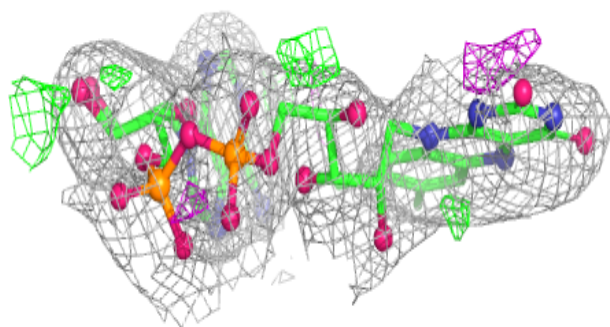
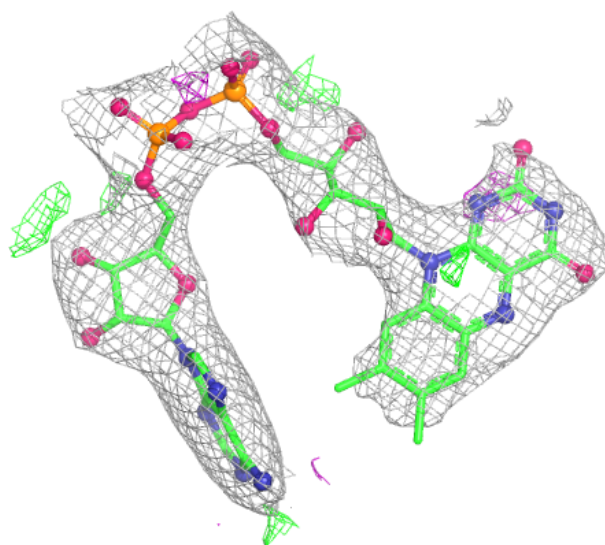
Electron density around FAD K 301:

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



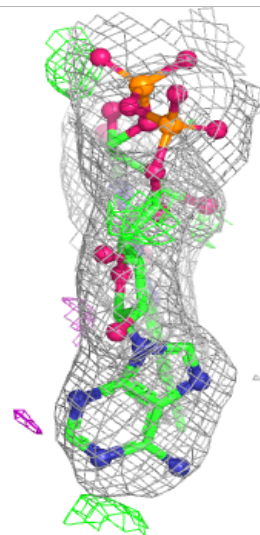
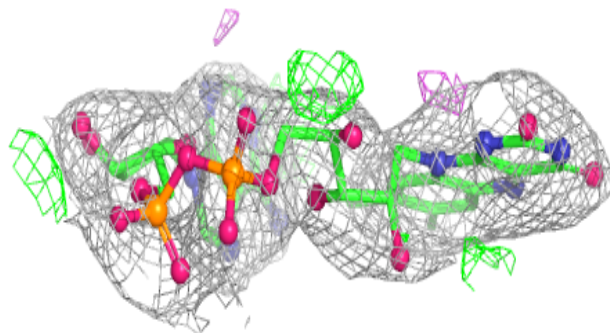
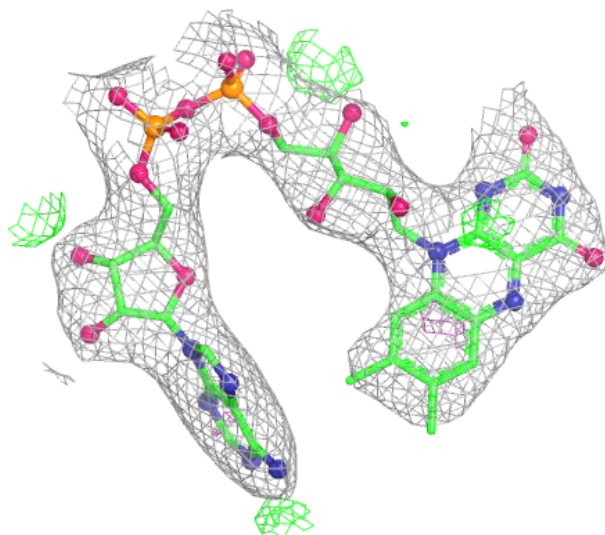
Electron density around FAD E 301:

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



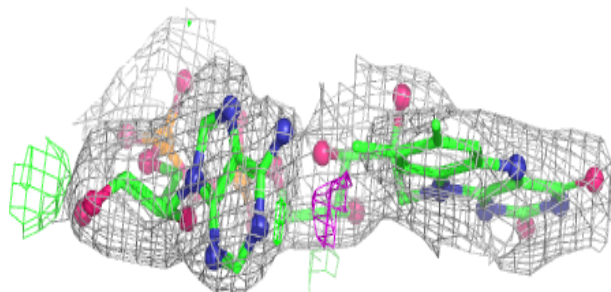
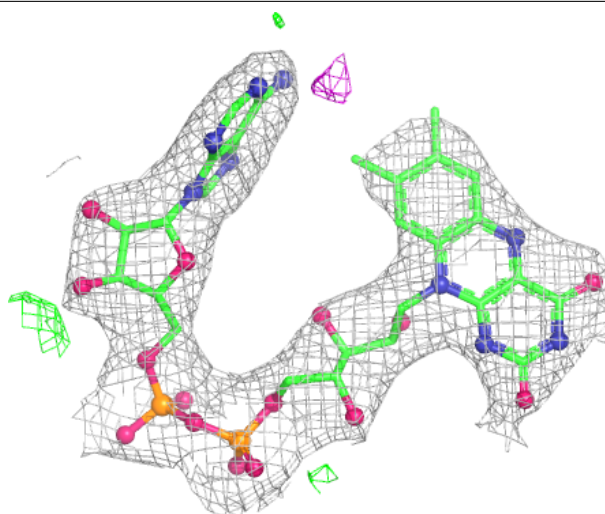
Electron density around FAD B 301:

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



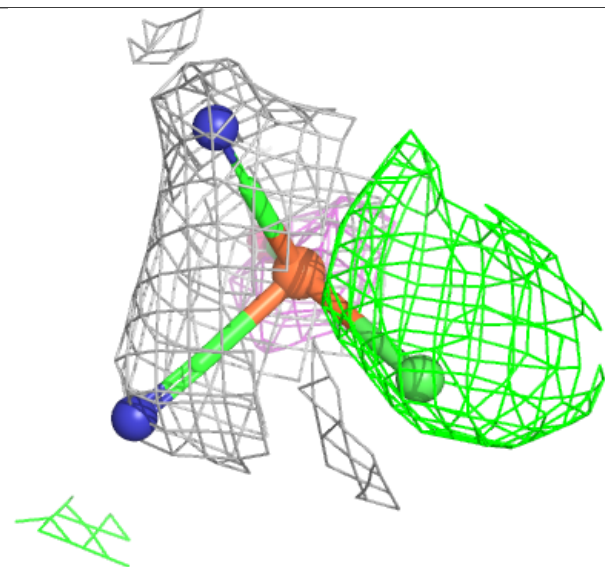
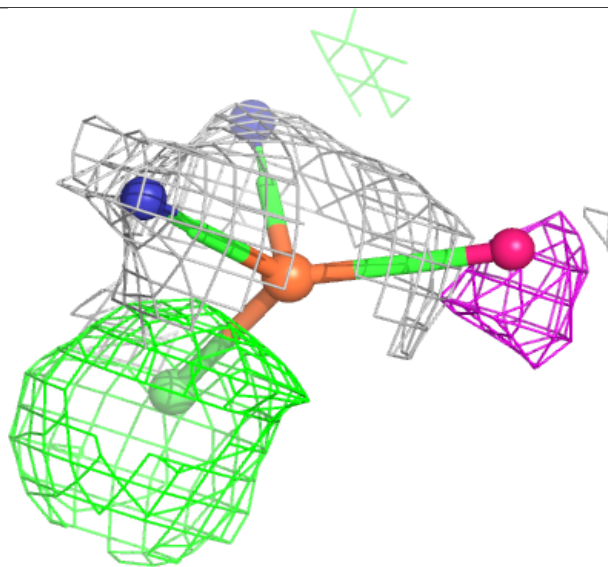
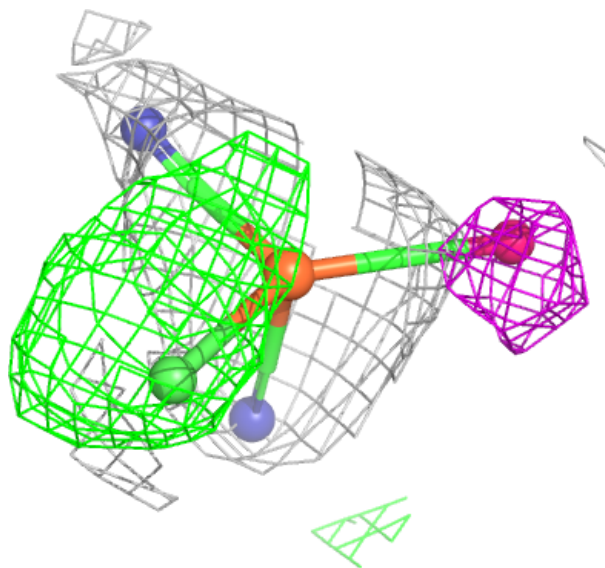
Electron density around FAD H 301:

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



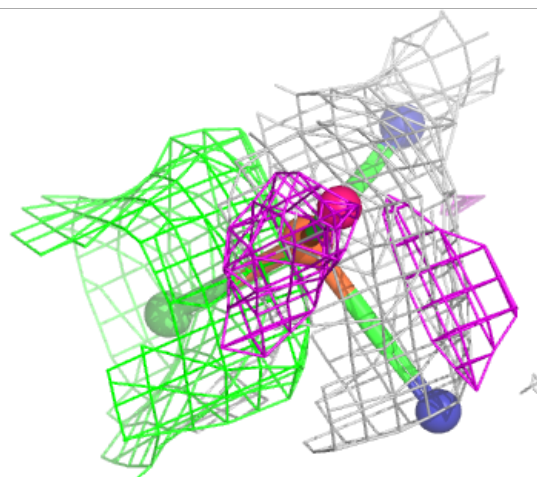
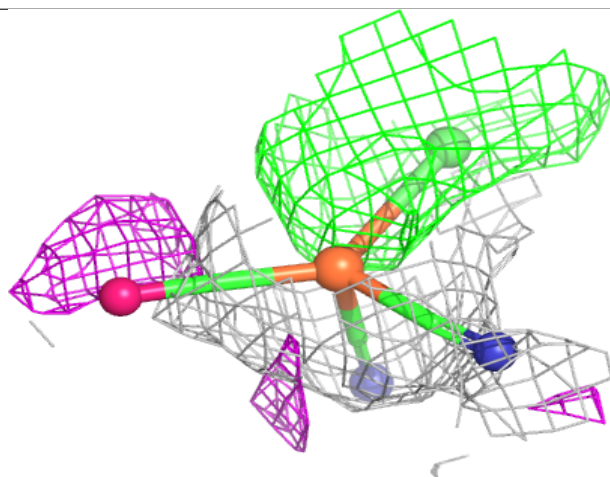
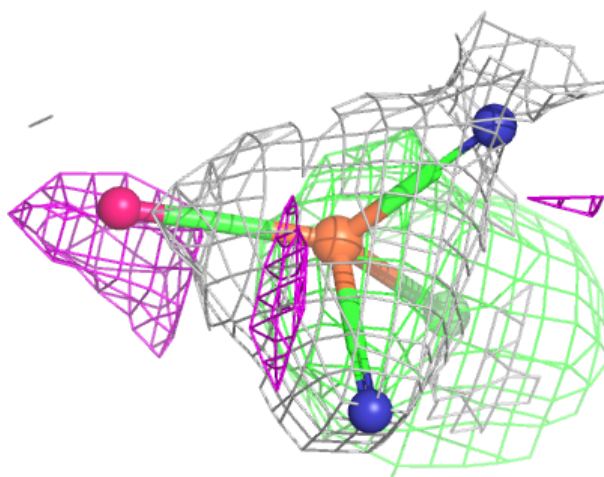
Electron density around NFU G 506:

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



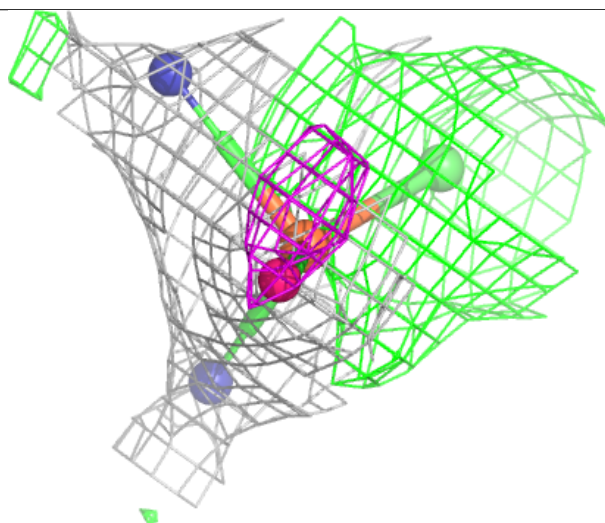
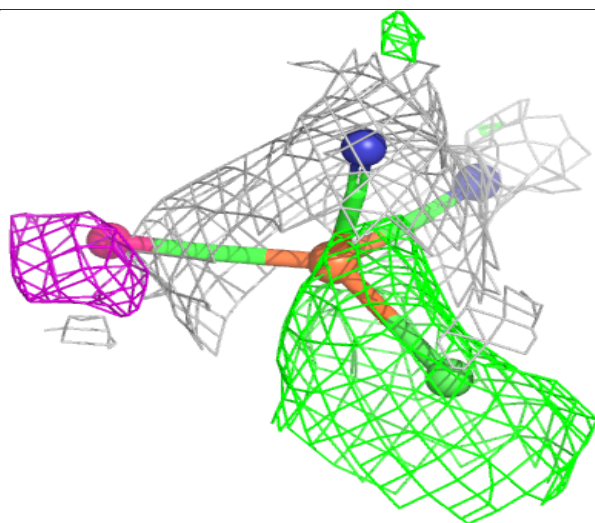
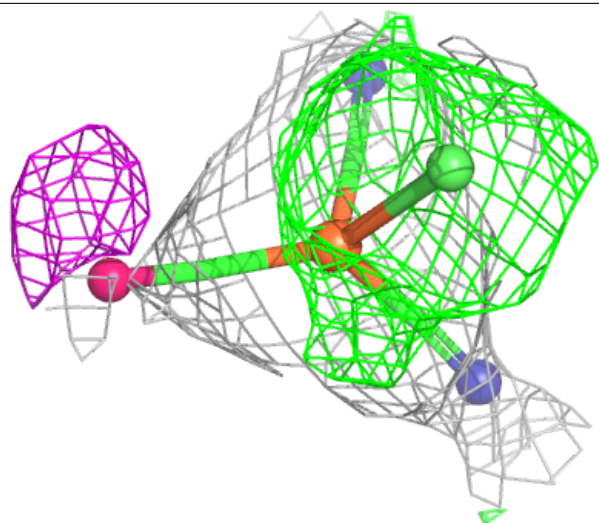
Electron density around NFU J 510:

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



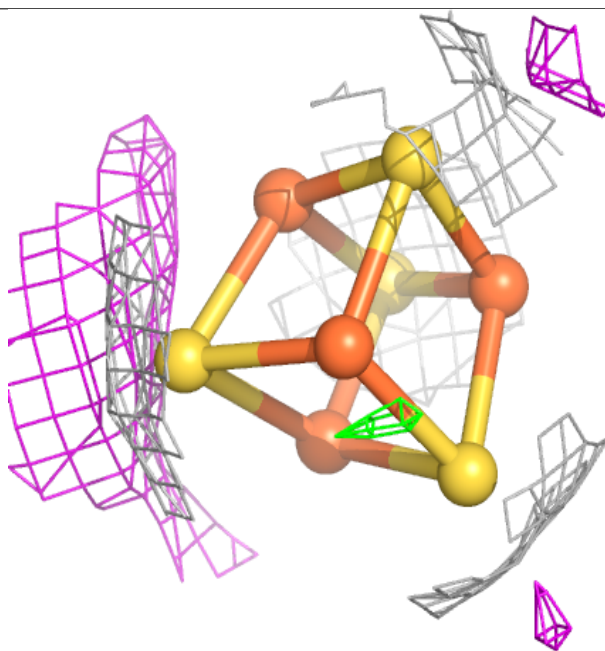
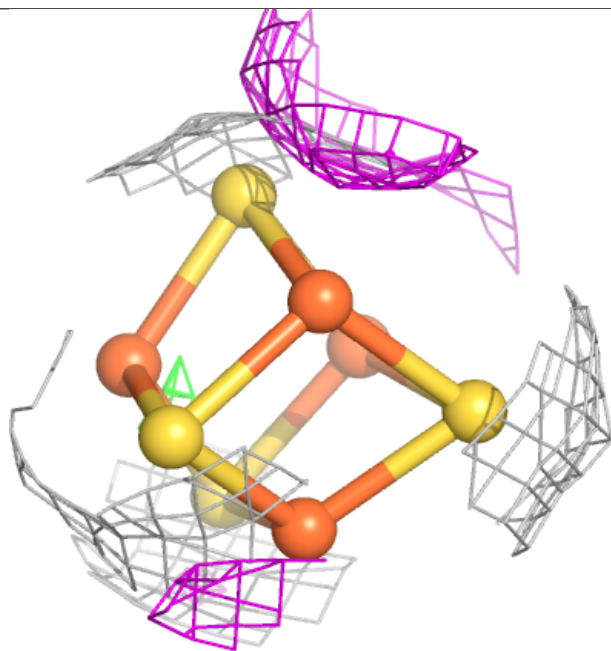
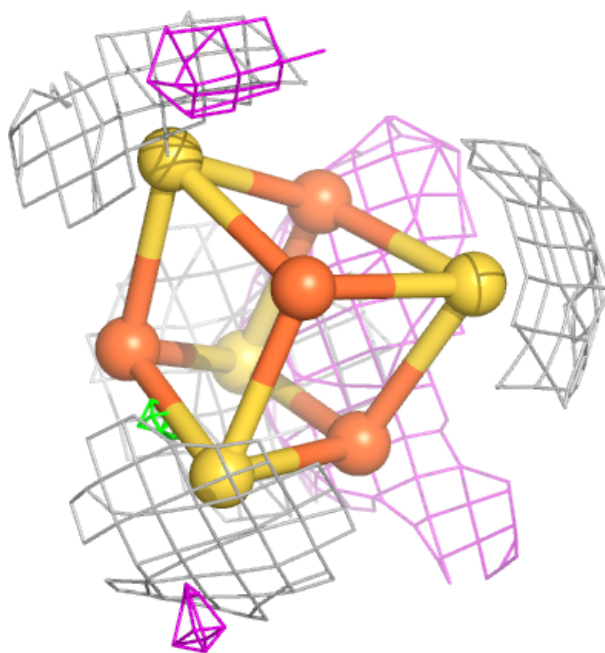
Electron density around NFU D 511:

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



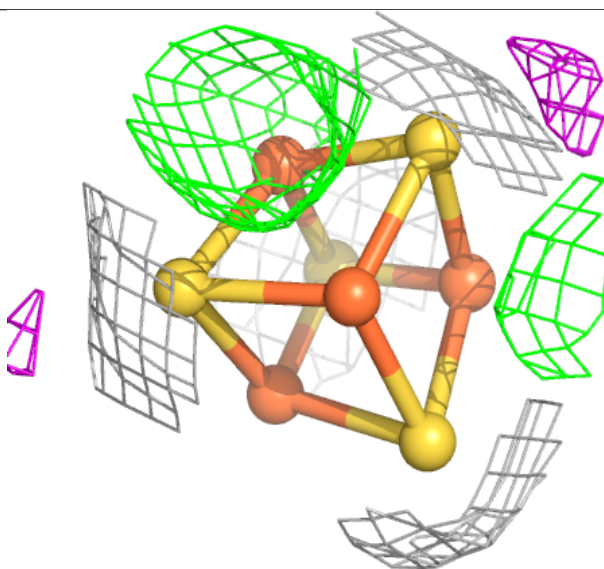
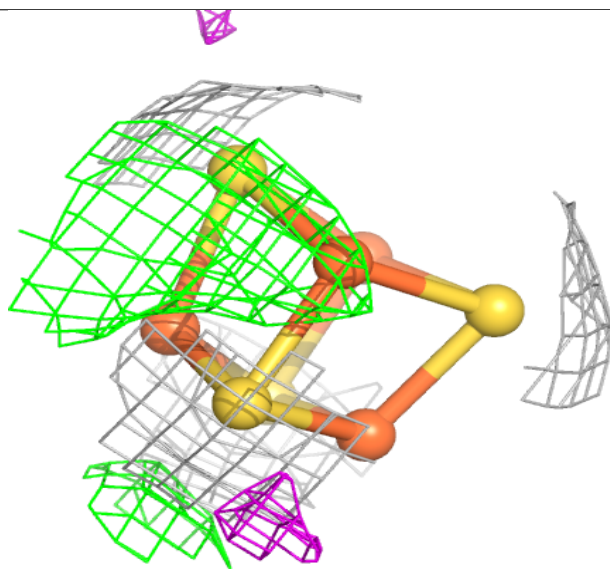
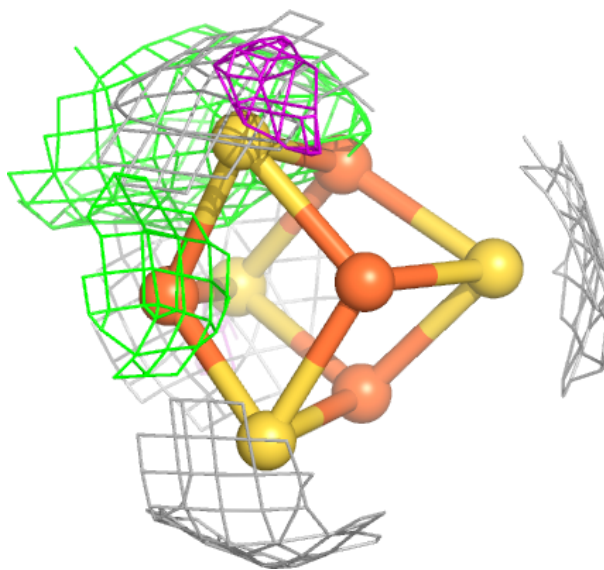
Electron density around SF4 B 305:

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



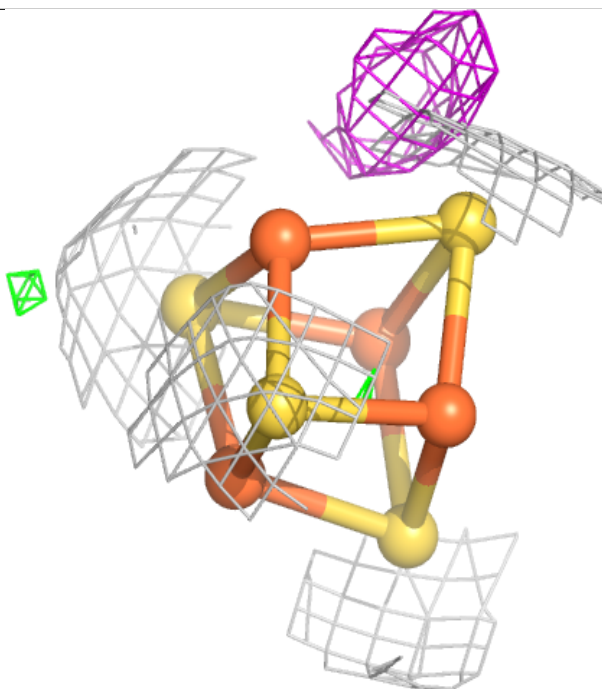
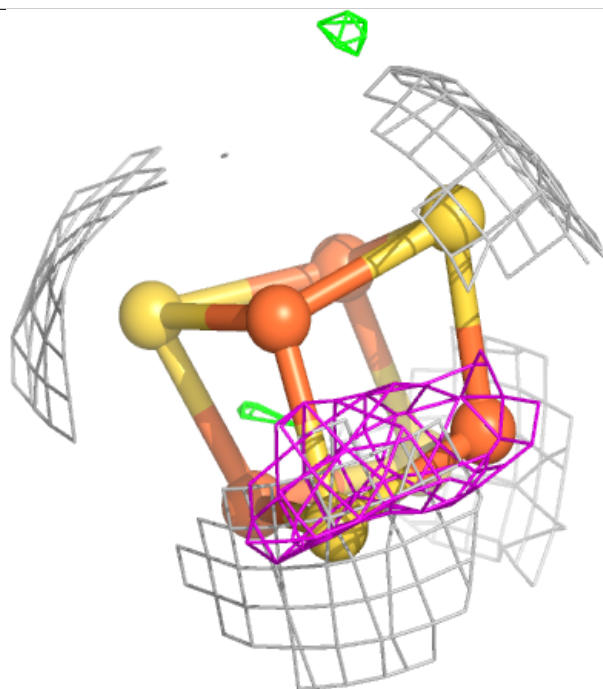
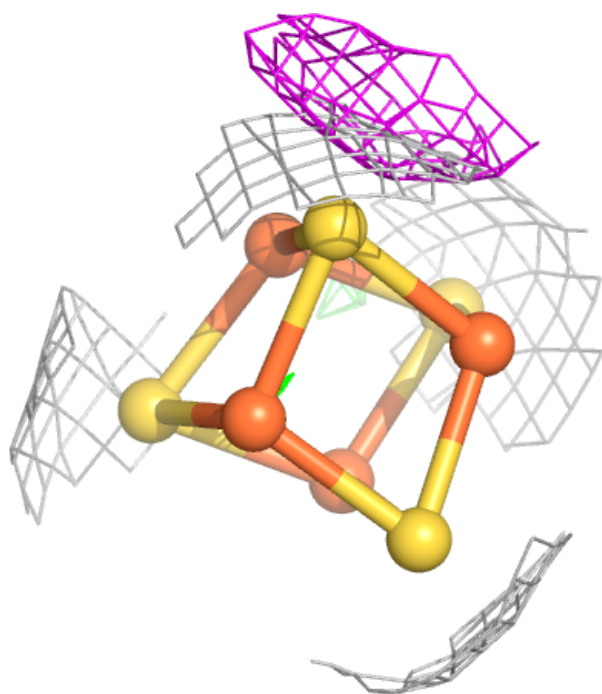
Electron density around SF4 C 302:

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



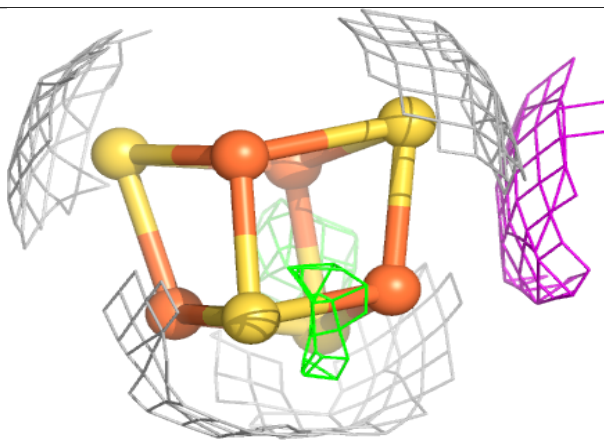
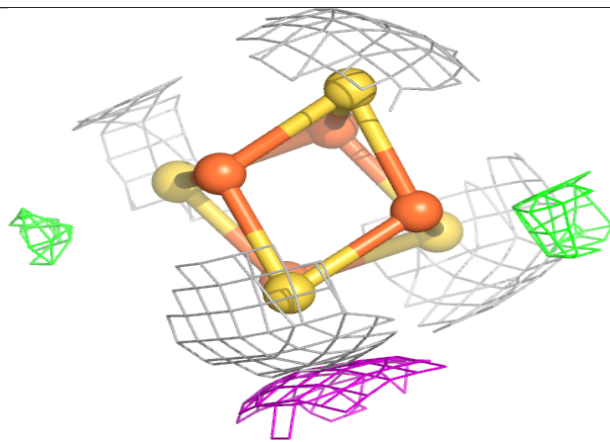
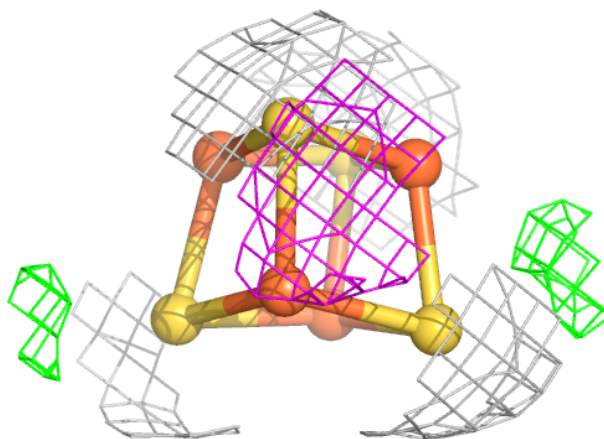
Electron density around SF4 C 304:

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



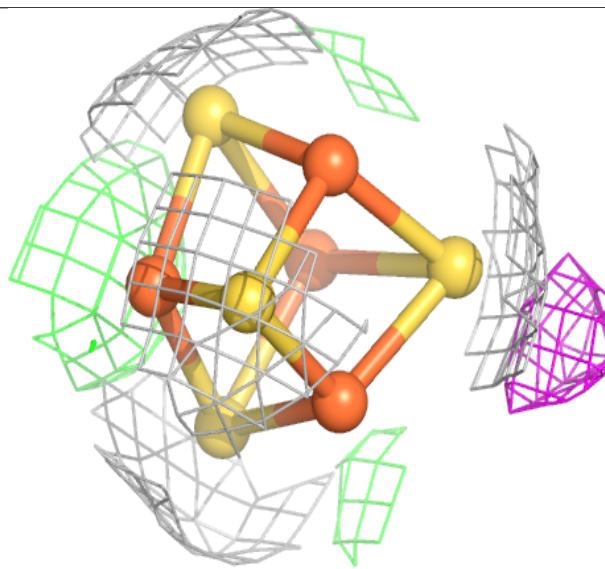
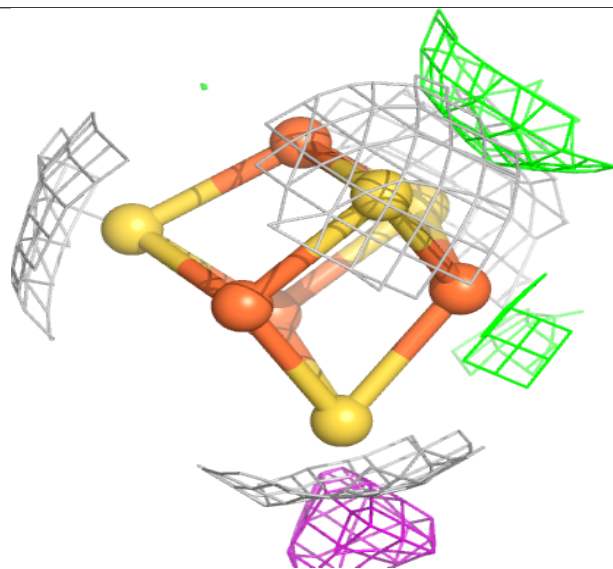
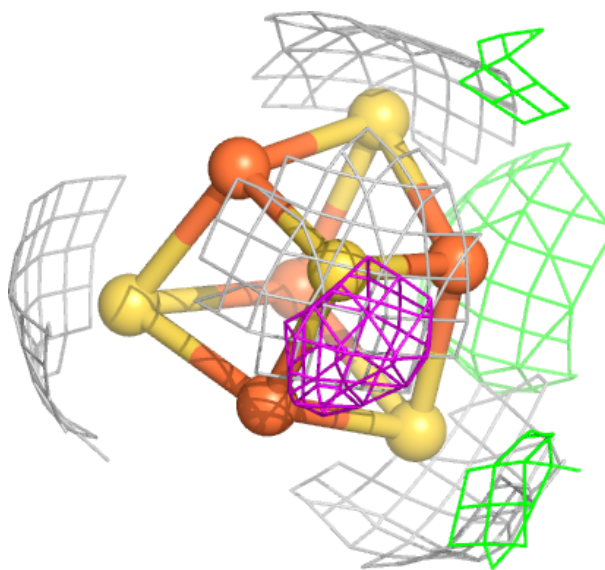
Electron density around SF4 E 305:

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



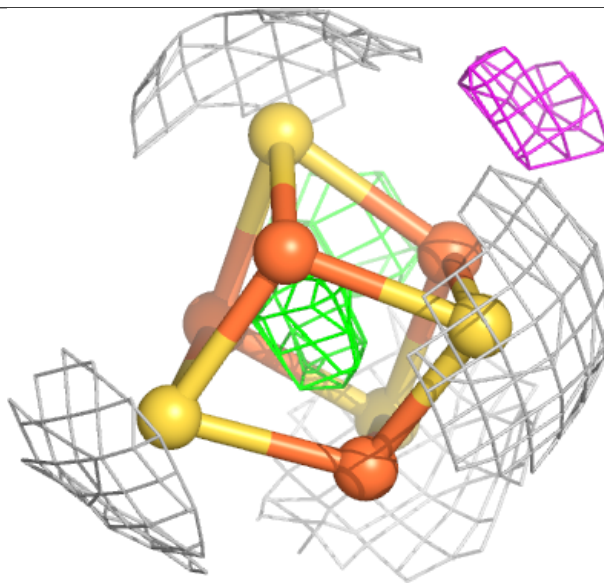
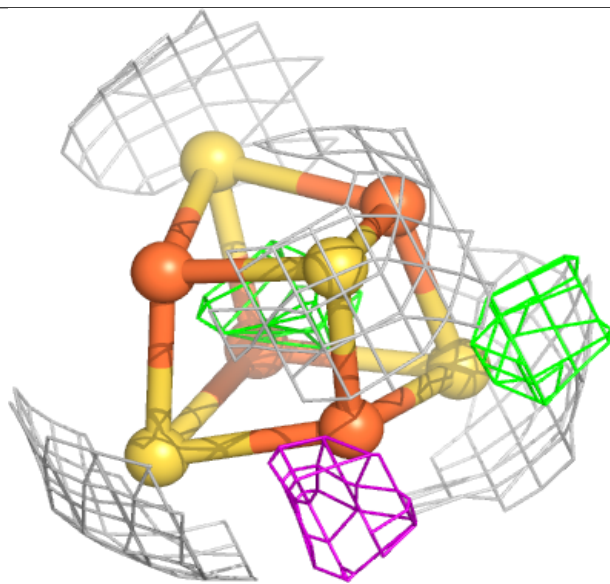
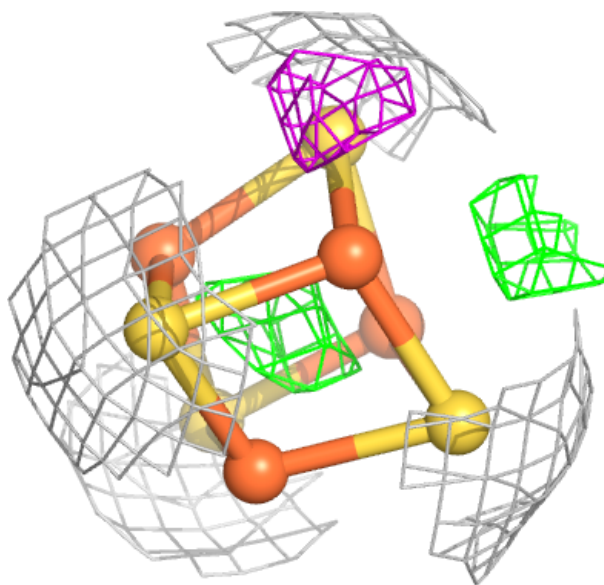
Electron density around SF4 F 301:

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



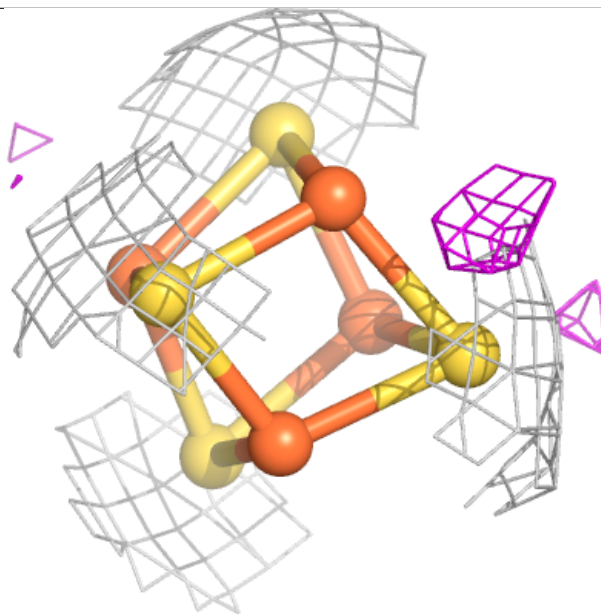
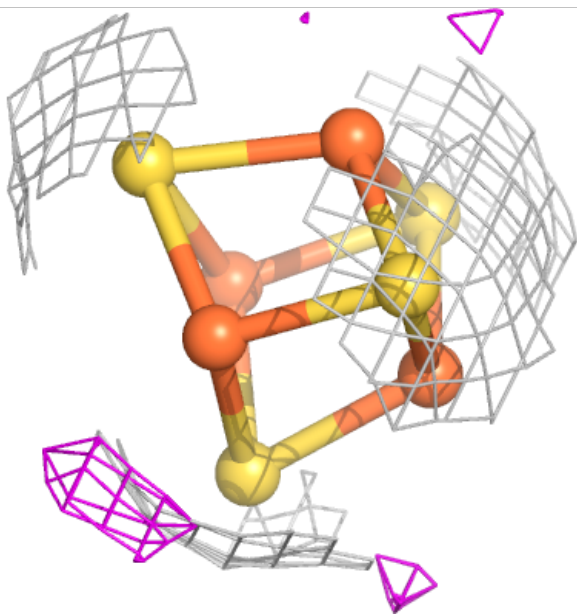
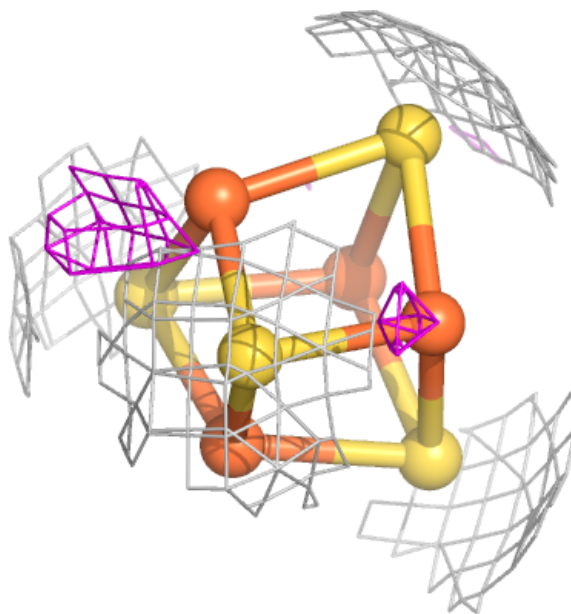
Electron density around SF4 F 302:

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



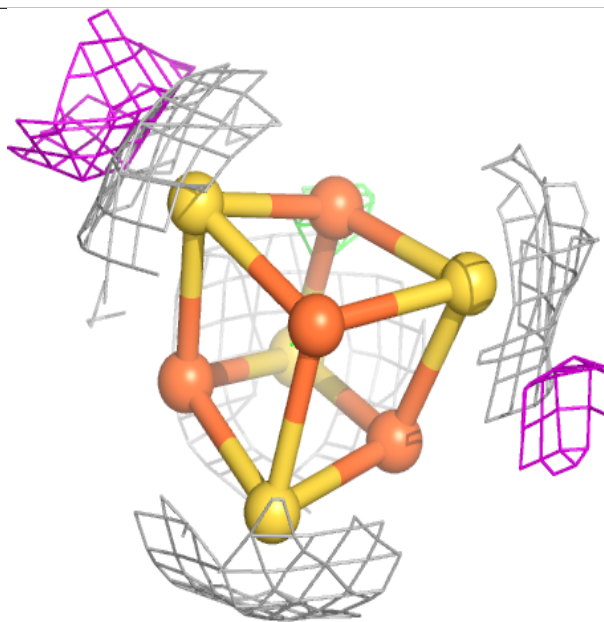
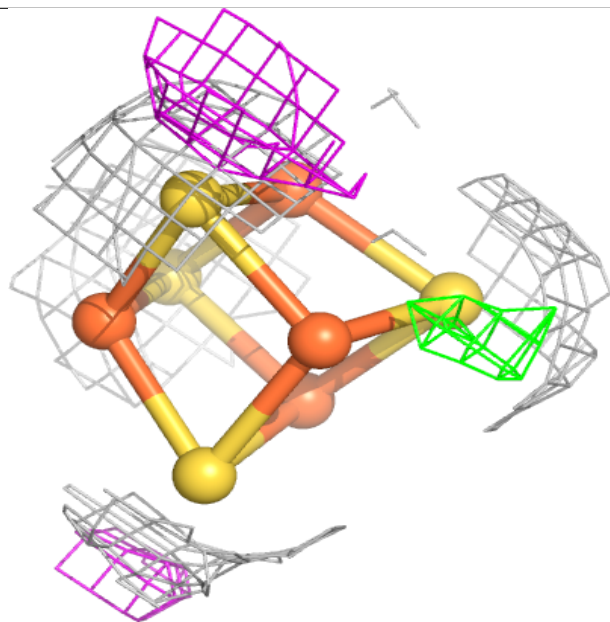
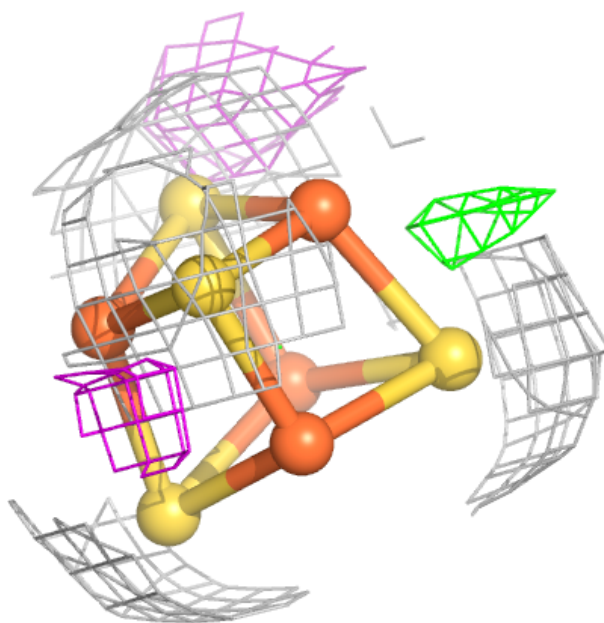
Electron density around SF4 F 303:

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



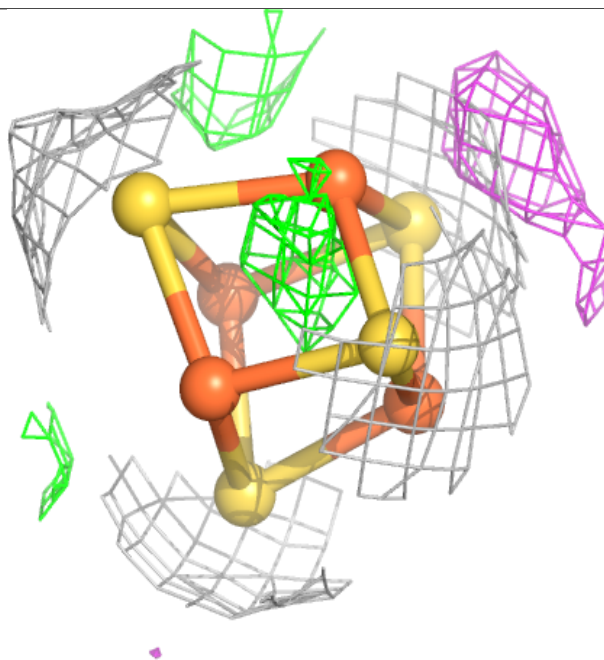
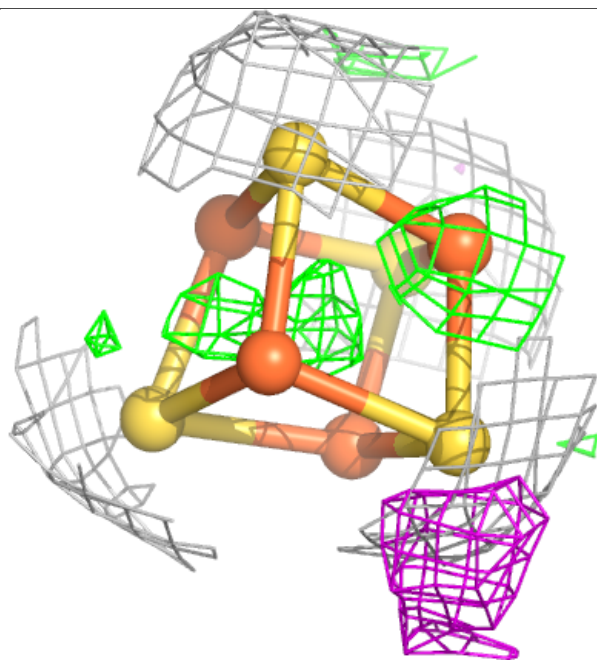
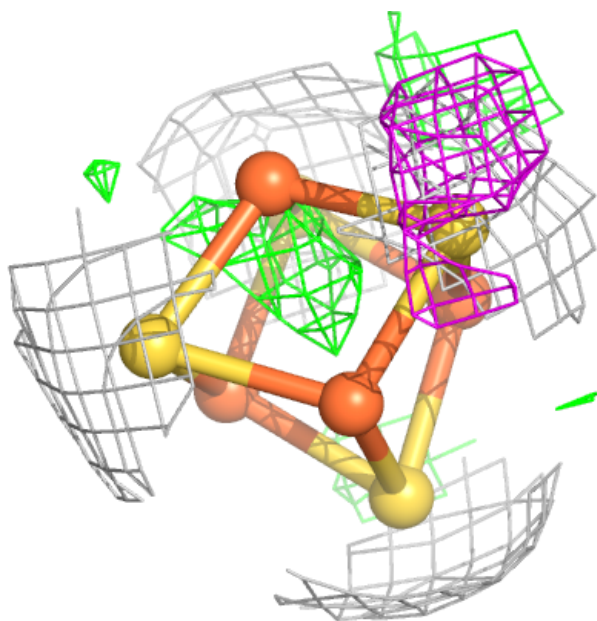
Electron density around SF4 H 303:

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



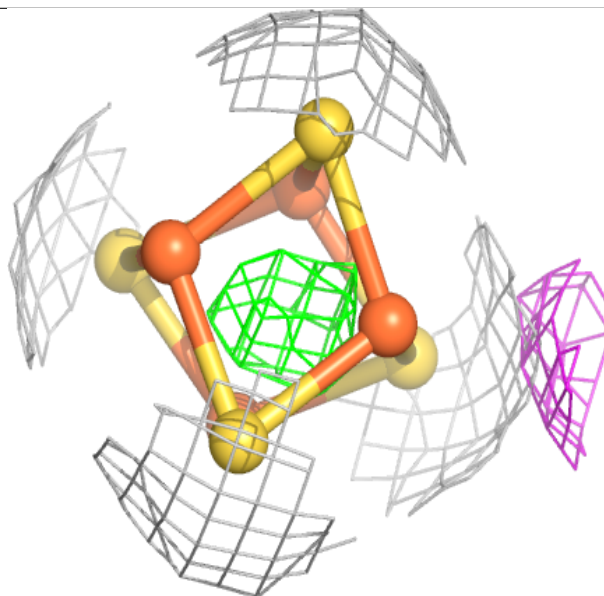
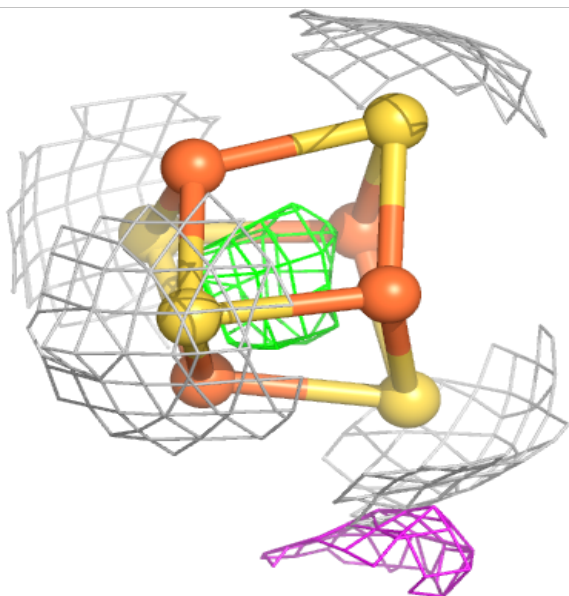
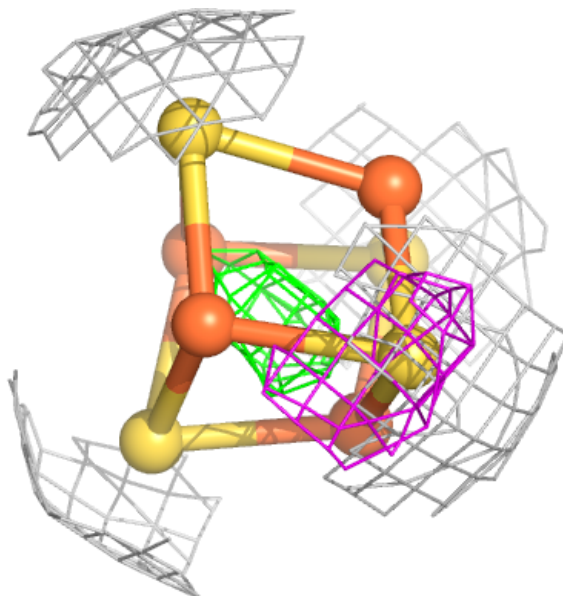
Electron density around SF4 I 301:

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



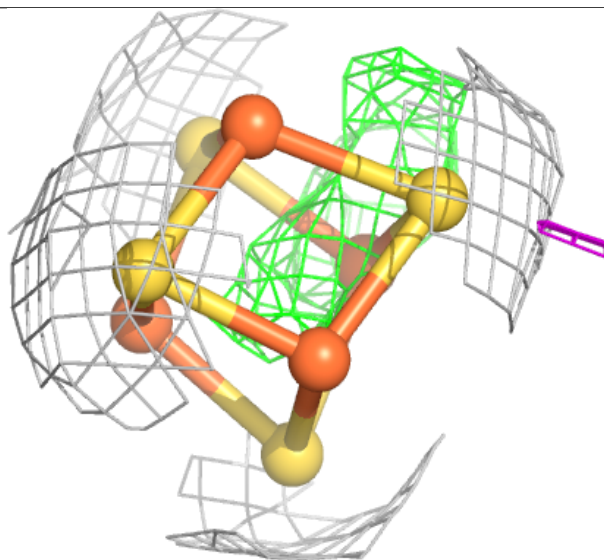
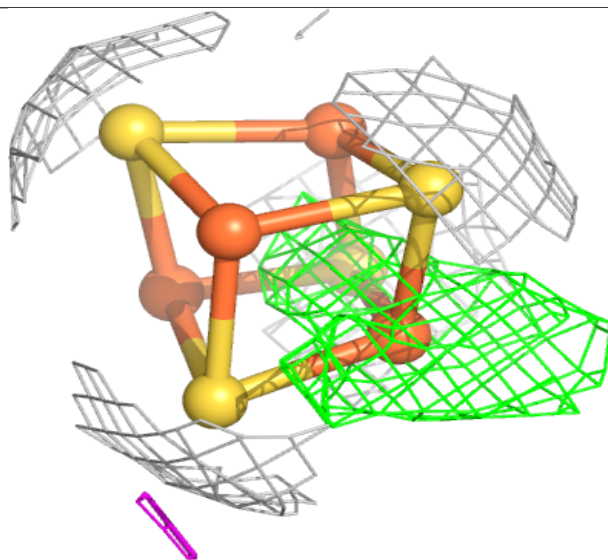
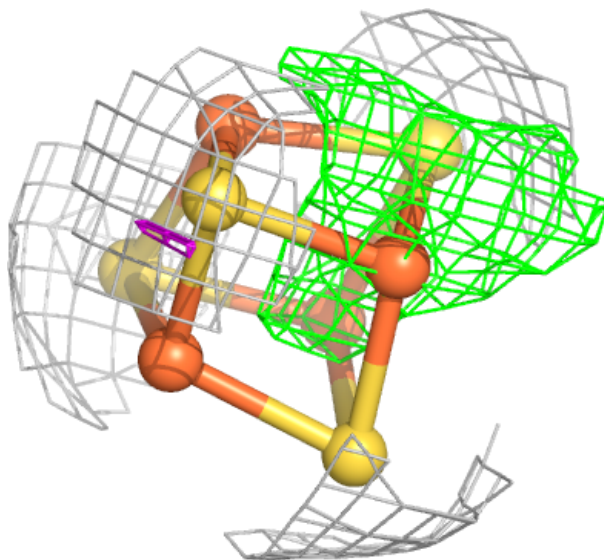
Electron density around SF4 I 302:

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



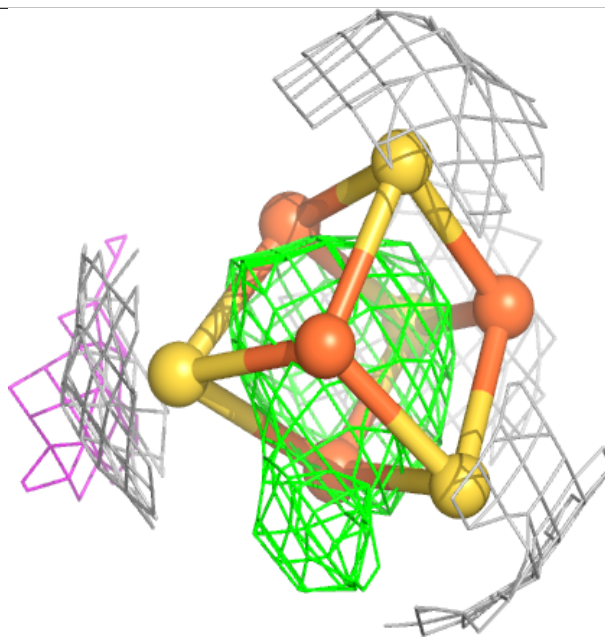
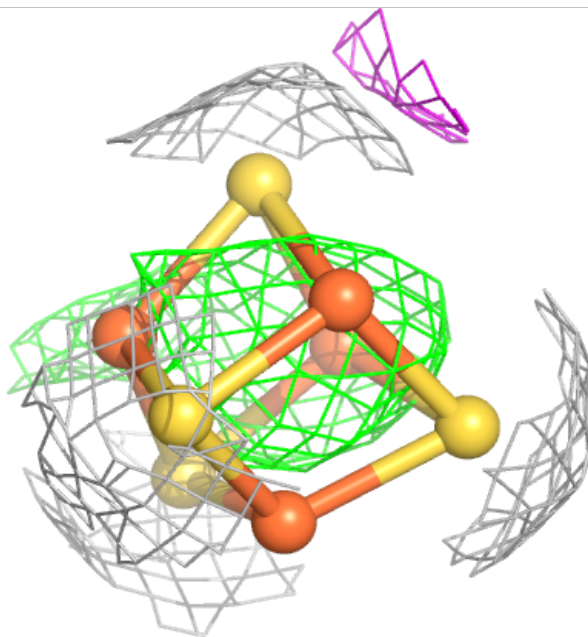
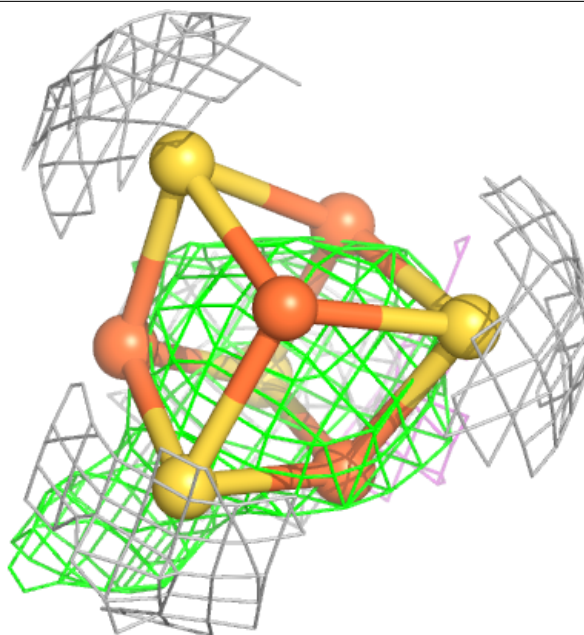
Electron density around SF4 I 303:

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



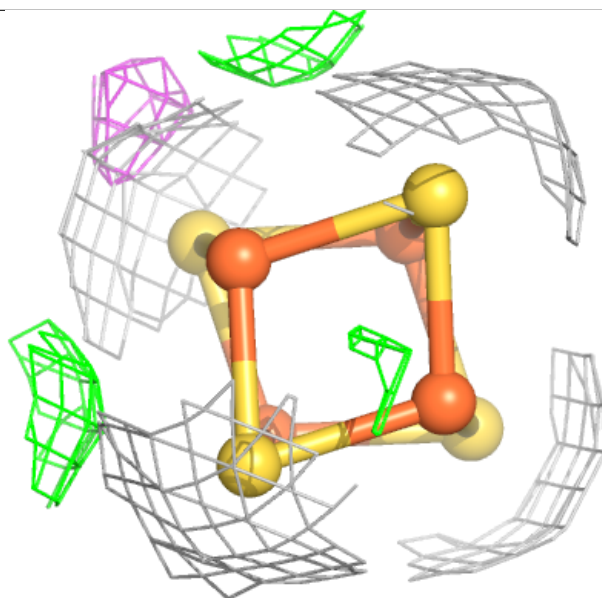
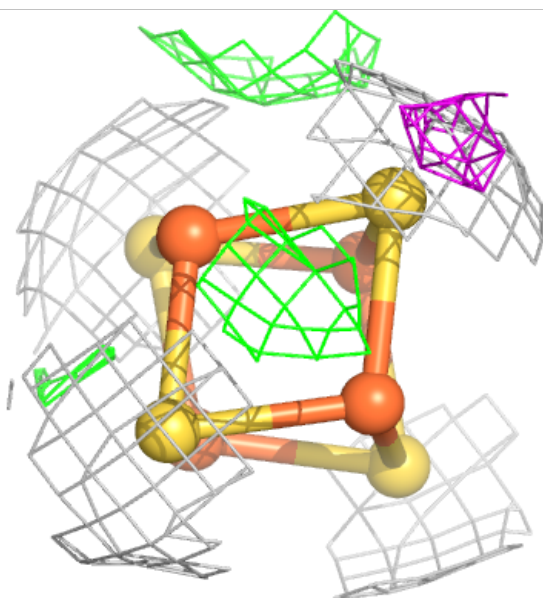
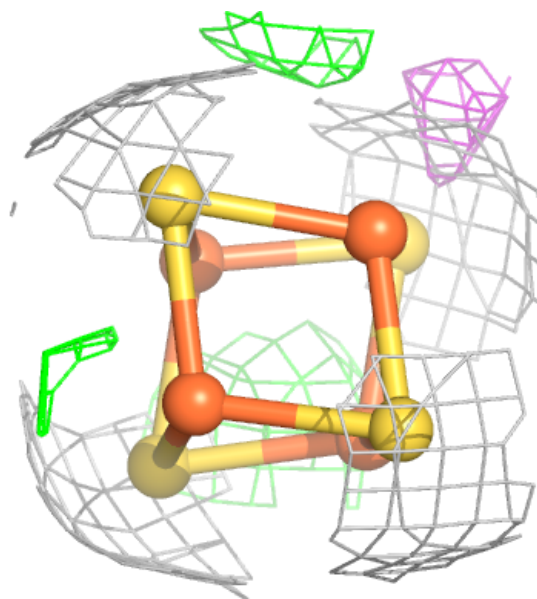
Electron density around SF4 K 303:

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



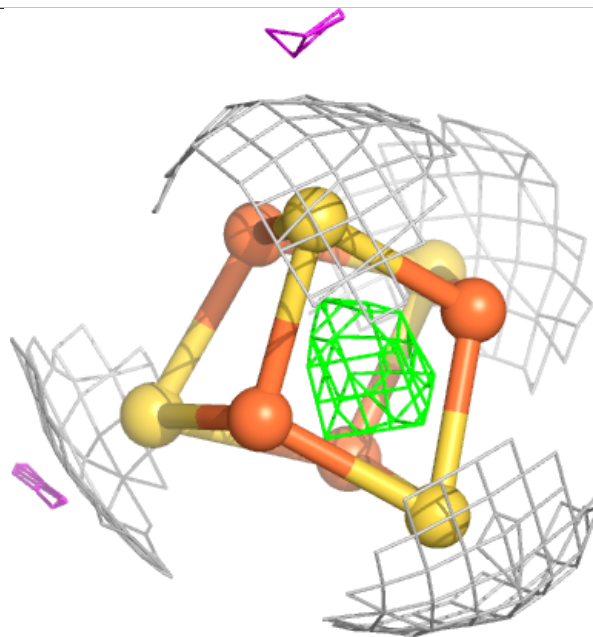
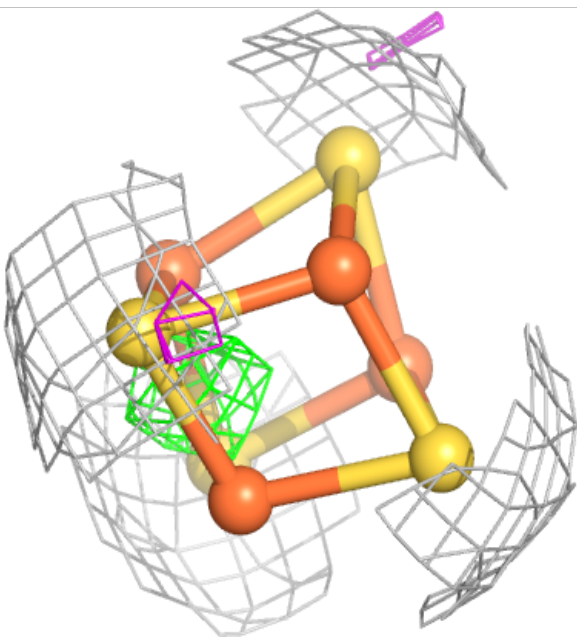
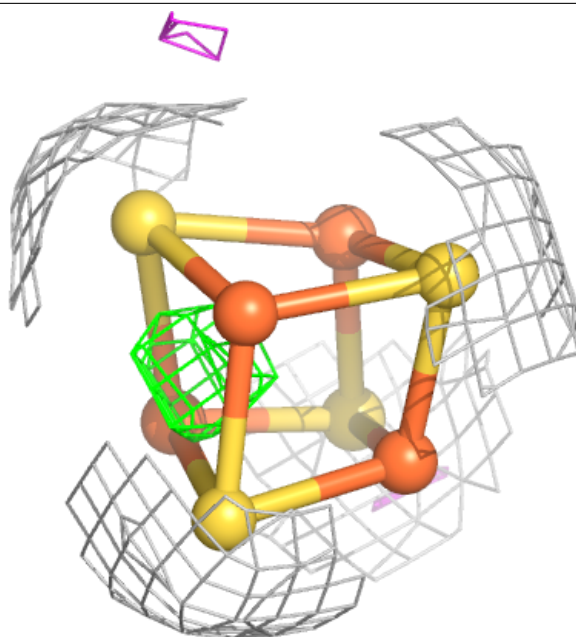
Electron density around SF4 L 301:

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



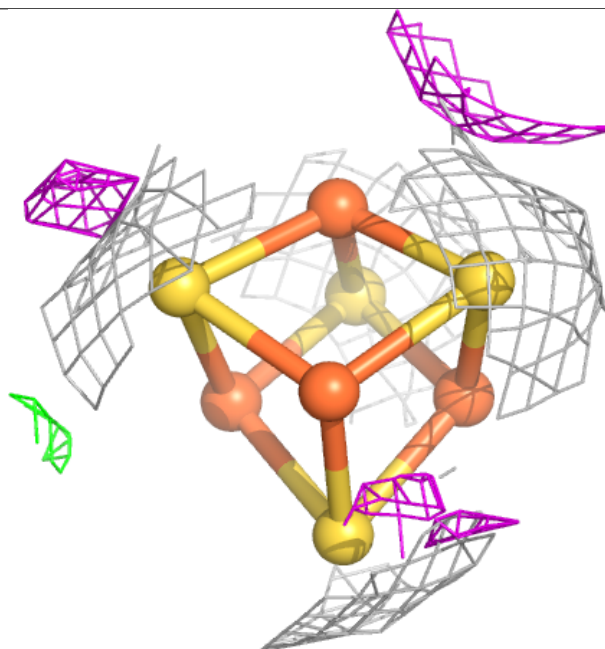
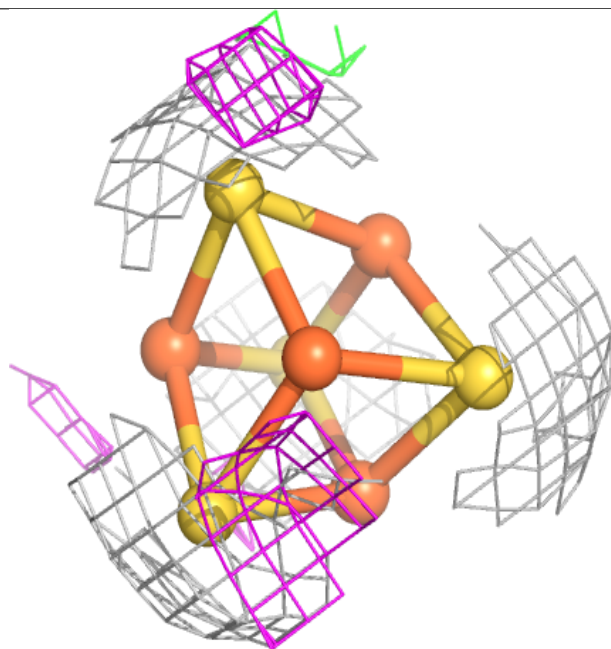
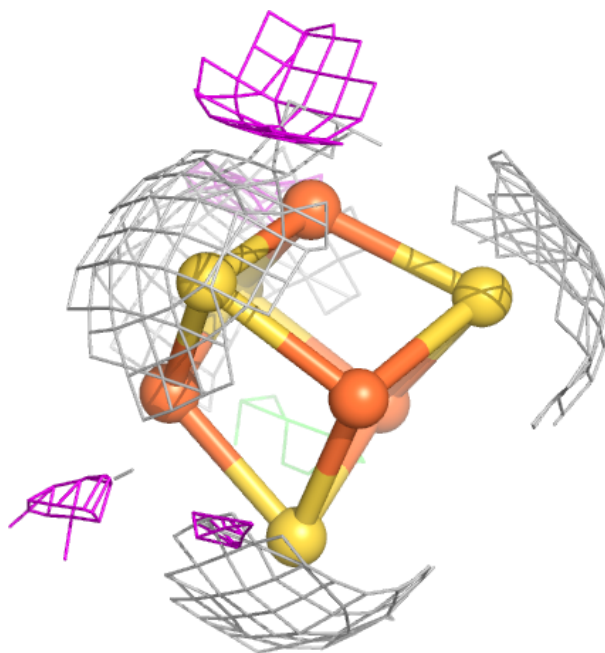
Electron density around SF4 L 302:

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



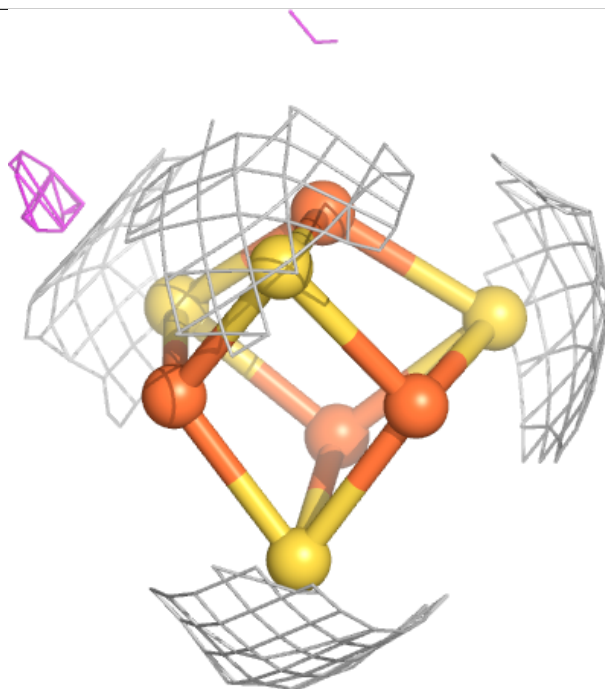
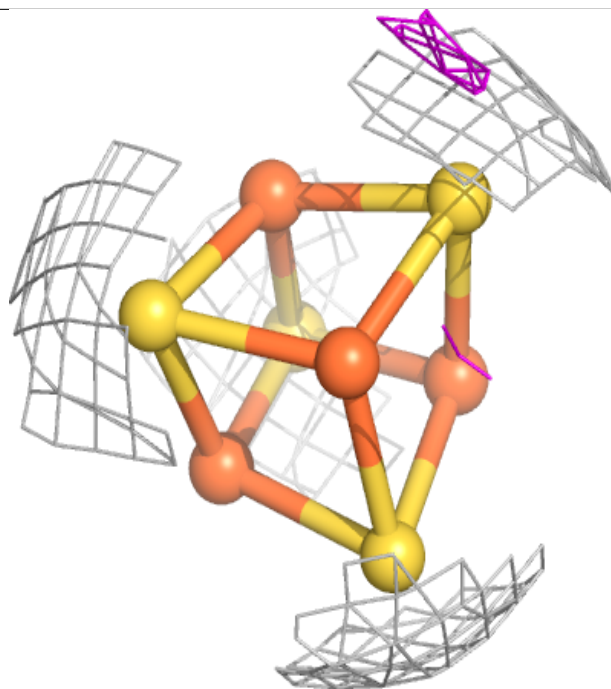
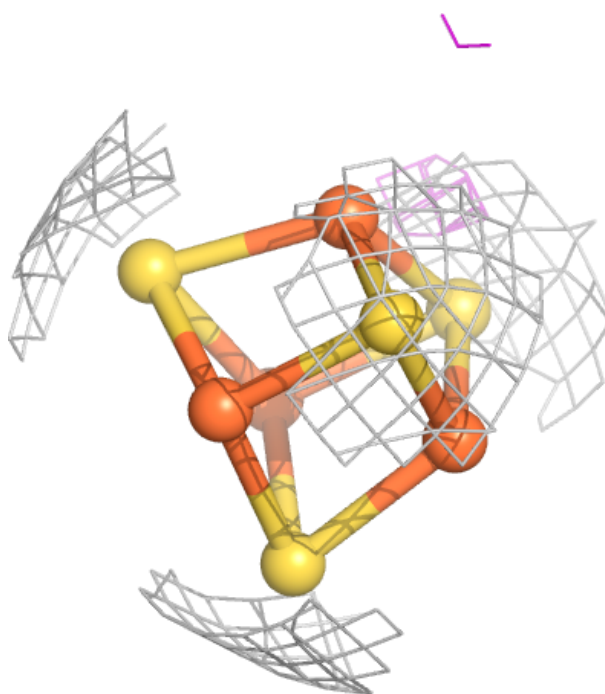
Electron density around SF4 L 303:

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



Electron density around SF4 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.