



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:39 PM UTC

PDB ID : 8RJA / pdb_00008rja
Title : Crystal structure of the F420-reducing formylmethanofuran dehydrogenase complex from the ethanotroph Candidatus Ethanoperedens thermophilum
Authors : Lemaire, O.N.; Wagner, T.
Deposited on : 2023-12-20
Resolution : 1.97 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

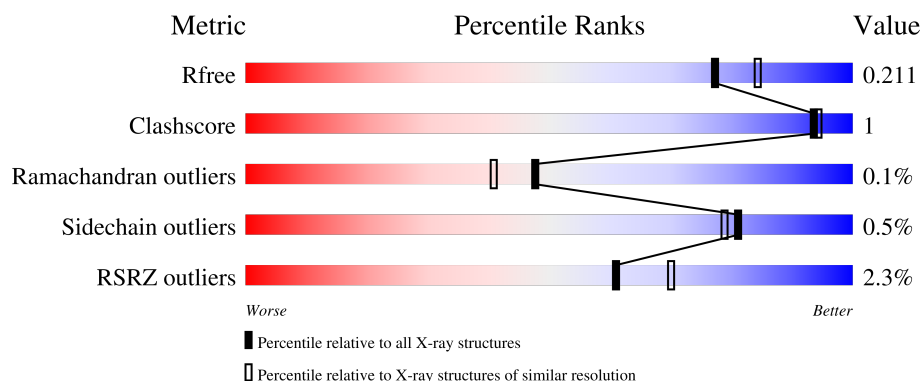
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	567	95% 5%
1	G	567	95% 5%
2	B	430	94% 6%
2	H	430	93% 7%
3	C	253	98% .

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Mol	Chain	Length	Quality of chain
3	I	253	% 98% .
4	D	126	2% 94% . . .
4	J	126	% 97% . .
5	E	359	4% 96% . .
5	K	359	11% 94% . .
6	F	85	6% 91% 9%
6	L	85	6% 91% . 8%

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 30528 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 Formylmethanofuran dehydrogenase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	566	Total	C	N	O	S	0	0	0
			4390	2784	761	823	22			
1	G	566	Total	C	N	O	S	0	1	0
			4396	2788	761	825	22			

- Molecule 2 is a protein called Formylmethanofuran dehydrogenase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	429	Total	C	N	O	S	0	0	0
			3282	2060	575	623	24			
2	H	429	Total	C	N	O	S	0	1	0
			3293	2066	579	624	24			

- Molecule 3 is a protein called formylmethanofuran dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	253	Total	C	N	O	S	0	0	0
			1888	1172	326	378	12			
3	I	253	Total	C	N	O	S	0	0	0
			1888	1172	326	378	12			

- Molecule 4 is a protein called Formylmethanofuran dehydrogenase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	124	Total	C	N	O	S	0	0	0
			927	582	159	179	7			
4	J	125	Total	C	N	O	S	0	0	0
			936	587	160	182	7			

- Molecule 5 is a protein called Coenzyme F420 hydrogenase/dehydrogenase, beta subunit C terminus.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	351	Total	C	N	O	S	0	0	0
			2763	1735	470	539	19			
5	K	351	Total	C	N	O	S	0	0	0
			2763	1735	470	539	19			

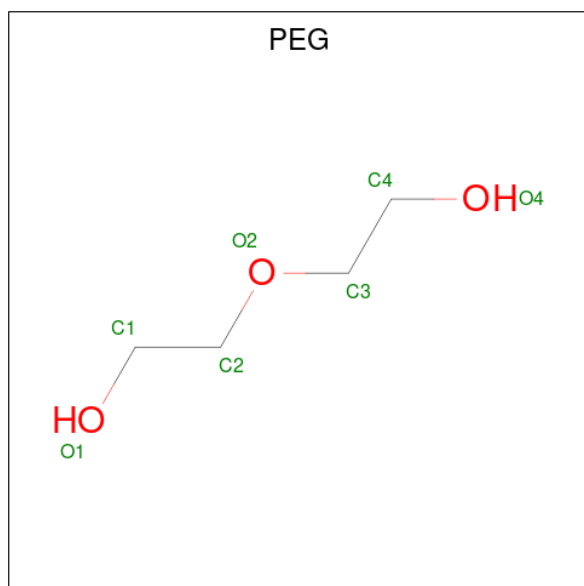
- Molecule 6 is a protein called NAD(P)H-quinone oxidoreductase subunit I, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	77	Total	C	N	O	S	0	0	0
			566	349	89	119	9			
6	L	78	Total	C	N	O	S	0	0	0
			573	354	90	120	9			

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Zn	0	0
			2	2		
7	G	2	Total	Zn	0	0
			2	2		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



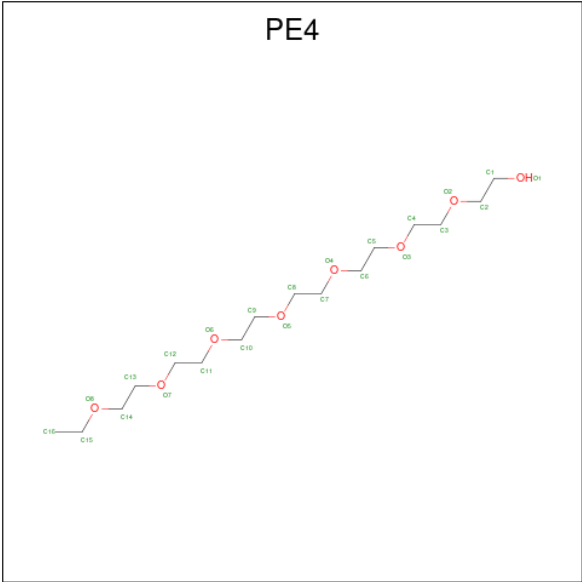
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	E	1	Total	C	O	0	0
			6	3	3		
9	H	1	Total	C	O	0	0
			6	3	3		
9	H	1	Total	C	O	0	0
			6	3	3		
9	H	1	Total	C	O	0	0
			6	3	3		
9	I	1	Total	C	O	0	0
			6	3	3		
9	I	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



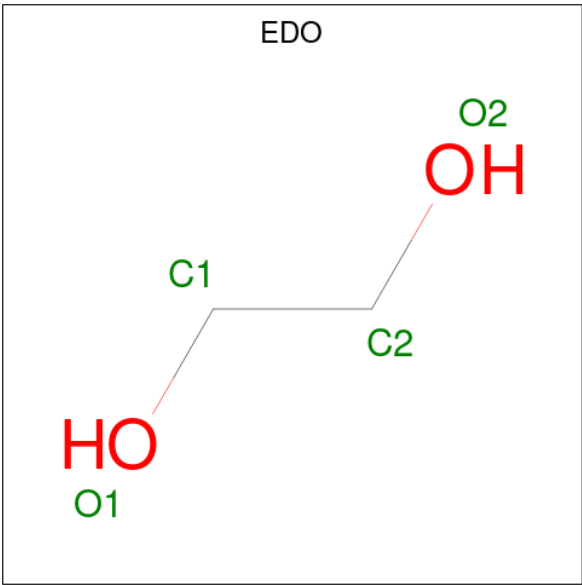
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		
10	H	1	Total	C	O	0	0
			4	2	2		
10	I	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 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
11	A	1	Total	C	O	0	0
			11	7	4		
11	B	1	Total	C	O	0	0
			7	4	3		
11	I	1	Total	C	O	0	0
			10	6	4		

- Molecule 12 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			4	2	2		

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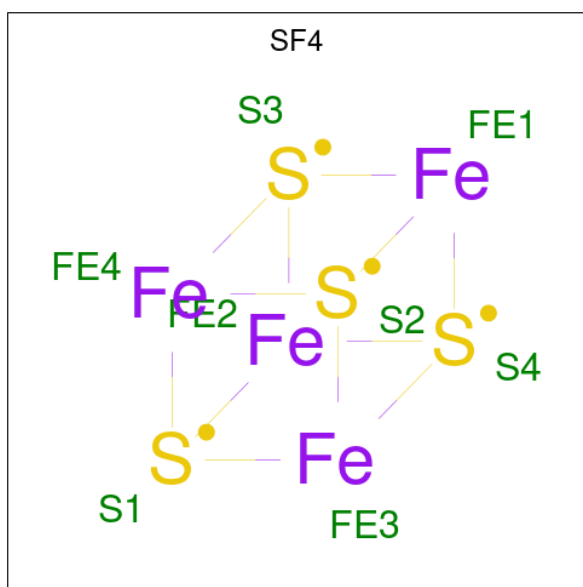
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total 4	C 2	O 2	0	0
12	B	1	Total 4	C 2	O 2	0	0
12	E	1	Total 4	C 2	O 2	0	0
12	E	1	Total 4	C 2	O 2	0	0
12	E	1	Total 4	C 2	O 2	0	0
12	E	1	Total 4	C 2	O 2	0	0
12	G	1	Total 4	C 2	O 2	0	0
12	G	1	Total 4	C 2	O 2	0	0
12	G	1	Total 4	C 2	O 2	0	0
12	G	1	Total 4	C 2	O 2	0	0
12	H	1	Total 4	C 2	O 2	0	0
12	K	1	Total 4	C 2	O 2	0	0
12	K	1	Total 4	C 2	O 2	0	0

- Molecule 13 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total 1	Cl 1	0	0
13	C	1	Total 1	Cl 1	0	0
13	F	1	Total 1	Cl 1	0	0
13	L	1	Total 1	Cl 1	0	0

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).

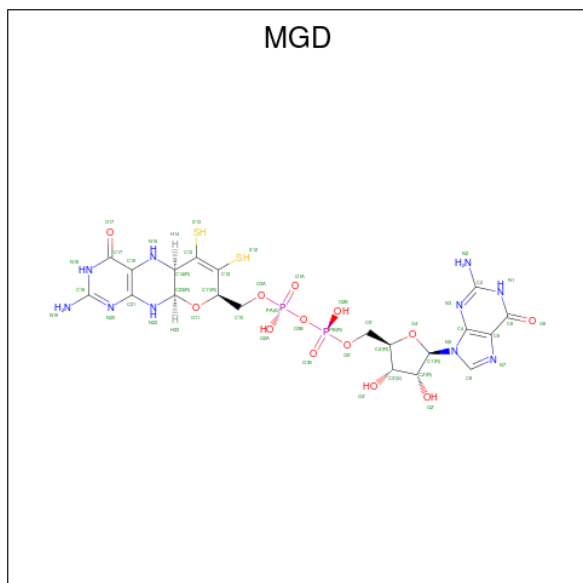


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	B	1	Total	Fe	S	0	0
			8	4	4		
14	E	1	Total	Fe	S	0	0
			8	4	4		
14	E	1	Total	Fe	S	0	0
			8	4	4		
14	E	1	Total	Fe	S	0	0
			8	4	4		
14	F	1	Total	Fe	S	0	0
			8	4	4		
14	F	1	Total	Fe	S	0	0
			8	4	4		
14	H	1	Total	Fe	S	0	0
			8	4	4		
14	K	1	Total	Fe	S	0	0
			8	4	4		
14	K	1	Total	Fe	S	0	0
			8	4	4		
14	K	1	Total	Fe	S	0	0
			8	4	4		
14	L	1	Total	Fe	S	0	0
			8	4	4		
14	L	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 15 is TUNGSTEN ION (CCD ID: W) (formula: W) (labeled as "Ligand of Interest" by depositor).

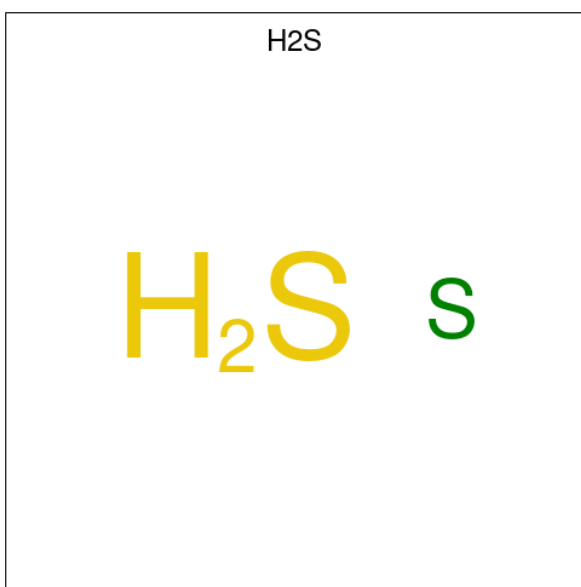
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total W 1 1	0	0
15	H	1	Total W 1 1	0	0

- Molecule 16 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).



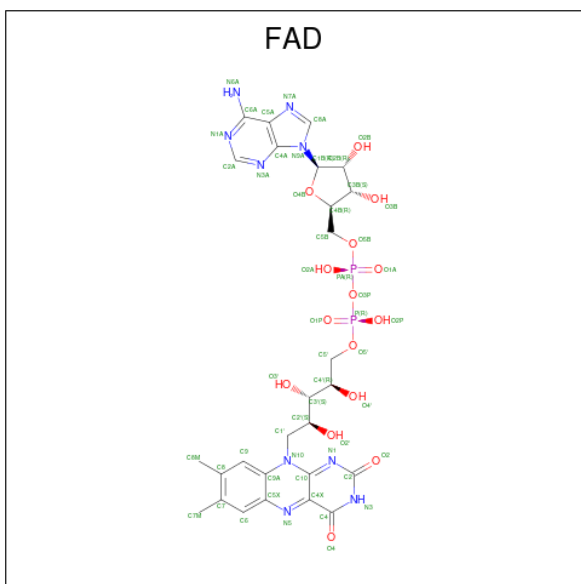
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
16	B	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
16	B	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
16	H	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
16	H	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 17 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H_2S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	B	1	Total S 1 1	0	0
17	H	1	Total S 1 1	0	0

- Molecule 18 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
18	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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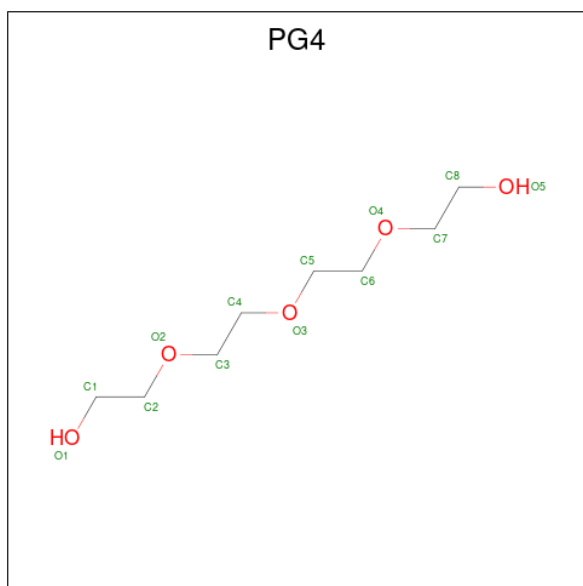
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 19 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	E	1	Total	Na	0	0
			1	1		
19	G	1	Total	Na	0	0
			1	1		
19	H	1	Total	Na	0	0
			1	1		
19	K	1	Total	Na	0	0
			1	1		

- Molecule 20 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	I	1	Total	C	O	0	0
			10	6	4		

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	416	Total	O	0	0
			416	416		

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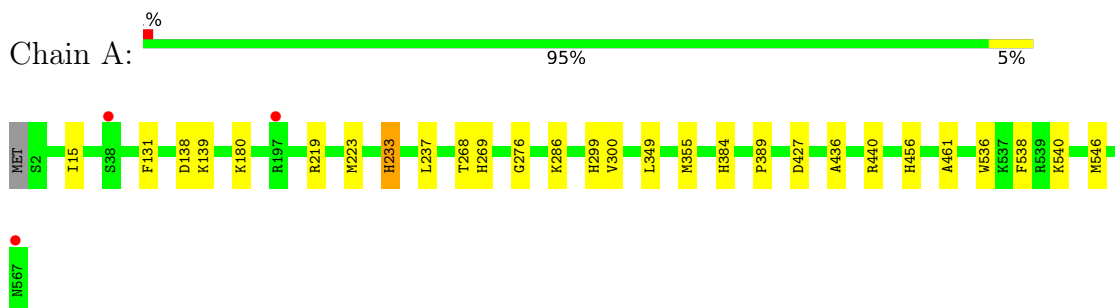
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	278	Total 278	O 278	0	0
21	C	146	Total 146	O 146	0	0
21	D	68	Total 68	O 68	0	0
21	E	195	Total 195	O 195	0	0
21	F	62	Total 62	O 62	0	0
21	G	415	Total 415	O 415	0	0
21	H	255	Total 255	O 255	0	1
21	I	211	Total 211	O 211	0	0
21	J	86	Total 86	O 86	0	0
21	K	102	Total 102	O 102	0	0
21	L	48	Total 48	O 48	0	0

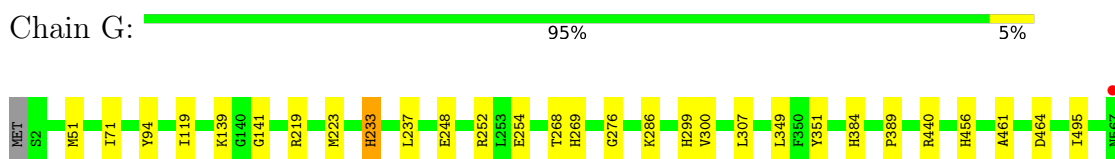
3 Residue-property plots [i](#)

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

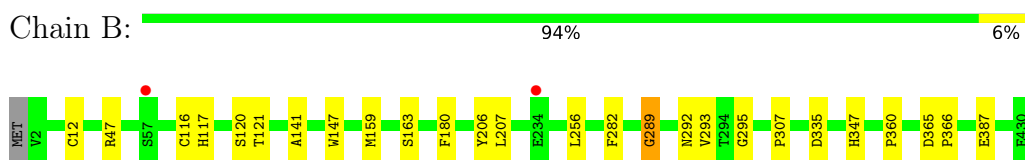
- Molecule 1: Formylmethanofuran dehydrogenase subunit A



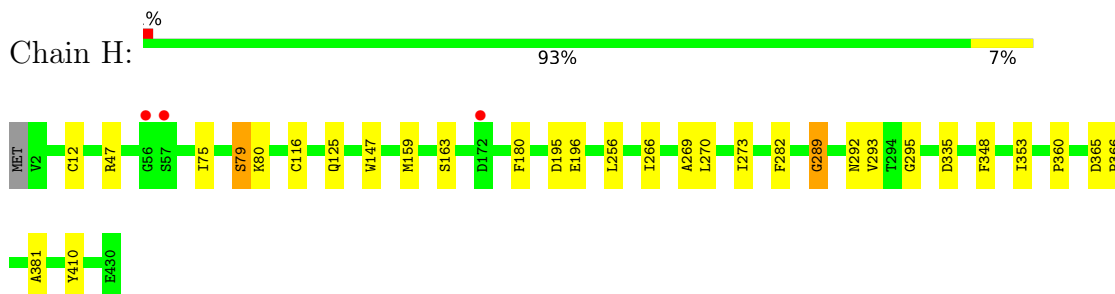
- Molecule 1: Formylmethanofuran dehydrogenase subunit A



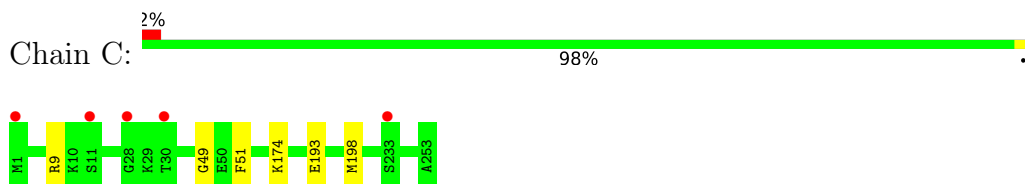
- Molecule 2: Formylmethanofuran dehydrogenase subunit B



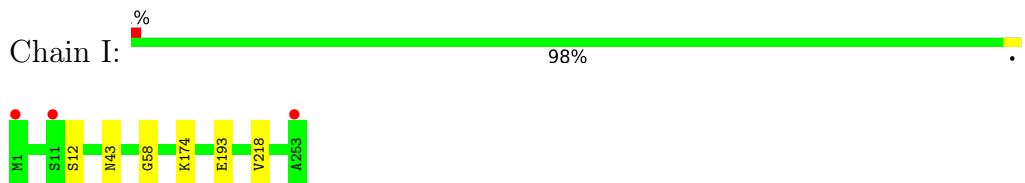
- Molecule 2: Formylmethanofuran dehydrogenase subunit B



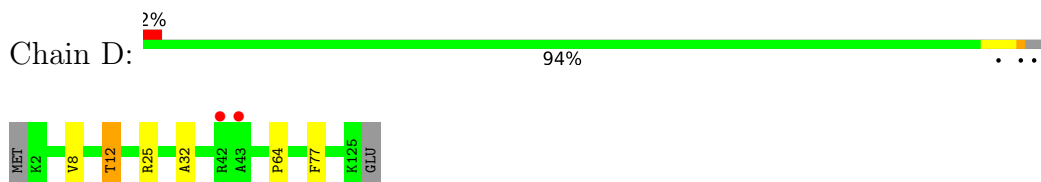
- Molecule 3: formylmethanofuran dehydrogenase



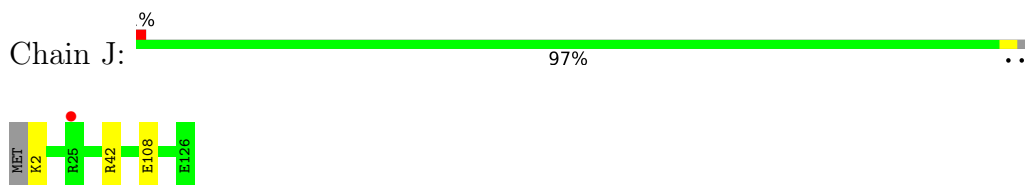
- Molecule 3: formylmethanofuran dehydrogenase



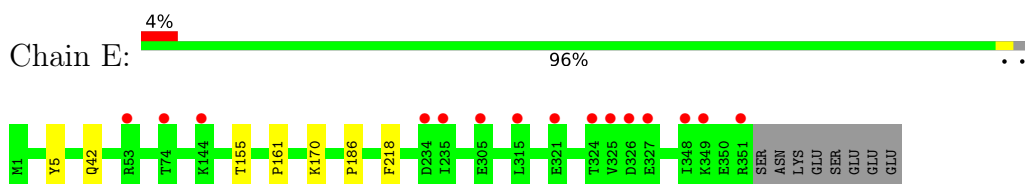
- Molecule 4: Formylmethanofuran dehydrogenase subunit D



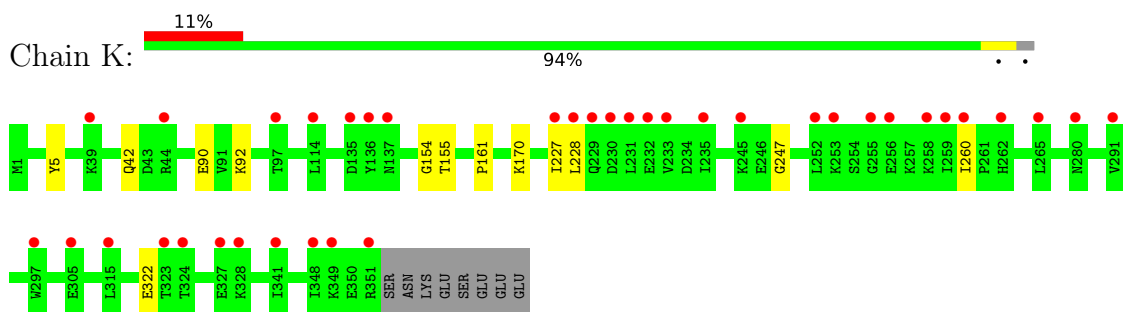
- Molecule 4: Formylmethanofuran dehydrogenase subunit D



- Molecule 5: Coenzyme F420 hydrogenase/dehydrogenase, beta subunit C terminus

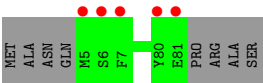


- Molecule 5: Coenzyme F420 hydrogenase/dehydrogenase, beta subunit C terminus

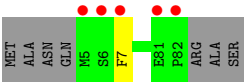
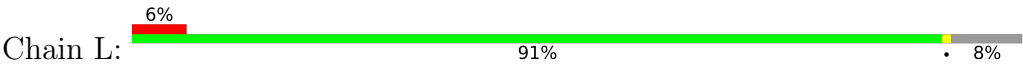


- Molecule 6: NAD(P)H-quinone oxidoreductase subunit I, chloroplastic





● Molecule 6: NAD(P)H-quinone oxidoreductase subunit I, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.63Å 135.64Å 149.90Å 90.00° 90.49° 90.00°	Depositor
Resolution (Å)	57.38 – 1.97 57.38 – 1.97	Depositor EDS
% Data completeness (in resolution range)	55.7 (57.38-1.97) 55.7 (57.38-1.97)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.97Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.176 , 0.210 0.176 , 0.211	Depositor DCC
R_{free} test set	8351 reflections (3.33%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30528	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, H2S, PE4, FAD, GOL, NA, EDO, MGD, ZN, KCX, ACT, PG4, PEG, W, SF4

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	0.61	0/4477	0.94	3/6068 (0.0%)
1	G	0.60	0/4486	0.94	0/6080
2	B	0.61	0/3336	0.91	2/4515 (0.0%)
2	H	0.61	0/3347	0.92	1/4529 (0.0%)
3	C	0.57	0/1912	0.82	0/2568
3	I	0.58	0/1912	0.83	1/2568 (0.0%)
4	D	0.57	0/945	0.82	0/1283
4	J	0.55	0/954	0.82	0/1295
5	E	0.58	0/2806	0.84	1/3788 (0.0%)
5	K	0.59	0/2806	0.86	1/3788 (0.0%)
6	F	0.53	0/573	0.76	0/776
6	L	0.55	0/581	0.72	0/788
All	All	0.59	0/28135	0.89	9/38046 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	180	PHE	CA-CB-CG	7.00	120.80	113.80
2	B	180	PHE	CA-CB-CG	6.77	120.57	113.80
5	E	218	PHE	CA-CB-CG	6.50	120.30	113.80
1	A	131	PHE	CA-CB-CG	6.42	120.22	113.80
1	A	427	ASP	CA-CB-CG	5.65	118.25	112.60

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	4390	0	4335	13	0
1	G	4396	0	4341	16	0
2	B	3282	0	3306	14	0
2	H	3293	0	3318	17	0
3	C	1888	0	1887	5	0
3	I	1888	0	1887	4	0
4	D	927	0	927	3	0
4	J	936	0	933	1	0
5	E	2763	0	2769	4	0
5	K	2763	0	2769	8	0
6	F	566	0	532	0	0
6	L	573	0	539	1	0
7	A	2	0	0	0	0
7	G	2	0	0	0	0
8	A	7	0	10	0	0
9	A	18	0	24	0	0
9	E	6	0	8	0	0
9	H	18	0	24	0	0
9	I	12	0	16	0	0
10	A	8	0	6	1	0
10	B	4	0	3	0	0
10	H	4	0	3	0	0
10	I	4	0	3	0	0
11	A	11	0	13	0	0
11	B	7	0	9	0	0
11	I	10	0	12	0	0
12	A	8	0	12	0	0
12	B	4	0	6	0	0
12	E	16	0	24	0	0
12	G	16	0	24	0	0
12	H	4	0	6	0	0
12	K	8	0	12	0	0
13	A	1	0	0	0	0
13	C	1	0	0	0	0
13	F	1	0	0	0	0
13	L	1	0	0	0	0
14	B	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	E	24	0	0	1	0
14	F	16	0	0	0	0
14	H	8	0	0	0	0
14	K	24	0	0	0	0
14	L	16	0	0	0	0
15	B	1	0	0	0	0
15	H	1	0	0	0	0
16	B	94	0	45	3	0
16	H	94	0	44	2	0
17	B	1	0	0	1	0
17	H	1	0	0	1	0
18	E	53	0	31	1	0
18	K	53	0	31	1	0
19	E	1	0	0	0	0
19	G	1	0	0	0	0
19	H	1	0	0	0	0
19	K	1	0	0	0	0
20	I	10	0	13	0	0
21	A	416	0	0	0	0
21	B	278	0	0	0	0
21	C	146	0	0	0	0
21	D	68	0	0	1	0
21	E	195	0	0	1	0
21	F	62	0	0	0	0
21	G	415	0	0	0	0
21	H	255	0	0	0	0
21	I	211	0	0	1	0
21	J	86	0	0	0	0
21	K	102	0	0	0	0
21	L	48	0	0	0	0
All	All	30528	0	27922	80	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 1.

The worst 5 of 80 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:B:116:CYS:HB2	16:B:504:MGD:S13	2.31	0.69
2:H:116:CYS:HB2	16:H:504:MGD:S13	2.32	0.69
2:B:293:VAL:HG21	17:B:505:H2S:S	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:155:THR:HG23	18:K:1103:FAD:HM82	1.93	0.51
5:E:155:THR:HG23	18:E:1103:FAD:HM82	1.93	0.49

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	563/567 (99%)	551 (98%)	12 (2%)	0	100	100
1	G	564/567 (100%)	553 (98%)	11 (2%)	0	100	100
2	B	427/430 (99%)	410 (96%)	16 (4%)	1 (0%)	43	35
2	H	428/430 (100%)	409 (96%)	18 (4%)	1 (0%)	43	35
3	C	251/253 (99%)	241 (96%)	10 (4%)	0	100	100
3	I	251/253 (99%)	242 (96%)	9 (4%)	0	100	100
4	D	122/126 (97%)	120 (98%)	2 (2%)	0	100	100
4	J	123/126 (98%)	121 (98%)	2 (2%)	0	100	100
5	E	349/359 (97%)	338 (97%)	10 (3%)	1 (0%)	36	27
5	K	349/359 (97%)	335 (96%)	13 (4%)	1 (0%)	36	27
6	F	75/85 (88%)	75 (100%)	0	0	100	100
6	L	76/85 (89%)	76 (100%)	0	0	100	100
All	All	3578/3640 (98%)	3471 (97%)	103 (3%)	4 (0%)	48	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	289	GLY
5	E	161	PRO

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Mol	Chain	Res	Type
2	H	289	GLY
5	K	161	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	458/459 (100%)	455 (99%)	3 (1%)	76	73
1	G	459/459 (100%)	456 (99%)	3 (1%)	76	73
2	B	355/356 (100%)	353 (99%)	2 (1%)	78	76
2	H	356/356 (100%)	353 (99%)	3 (1%)	73	71
3	C	198/198 (100%)	198 (100%)	0	100	100
3	I	198/198 (100%)	198 (100%)	0	100	100
4	D	103/105 (98%)	101 (98%)	2 (2%)	50	44
4	J	104/105 (99%)	103 (99%)	1 (1%)	68	65
5	E	307/315 (98%)	307 (100%)	0	100	100
5	K	307/315 (98%)	307 (100%)	0	100	100
6	F	64/70 (91%)	64 (100%)	0	100	100
6	L	65/70 (93%)	65 (100%)	0	100	100
All	All	2974/3006 (99%)	2960 (100%)	14 (0%)	81	79

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	139	LYS
1	G	233	HIS
4	J	42	ARG
2	H	79	SER
2	H	282	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	325	ASN
2	H	199	GLN
5	K	87	HIS
5	K	78	GLN
2	B	199	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	KCX	G	180	7,1	10,11,12	0.55	0	6,12,14	0.69	0
1	KCX	A	180	7,1	10,11,12	2.20	1 (10%)	6,12,14	1.68	1 (16%)

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
1	KCX	G	180	7,1	-	0/9/10/12	-
1	KCX	A	180	7,1	-	0/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	KCX	OQ1-CX	6.67	1.33	1.21

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	KCX	OQ1-CX-NZ	-4.06	118.75	124.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 67 ligands modelled in this entry, 14 are monoatomic and 2 are modelled with single atom - leaving 51 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
12	EDO	H	510	-	3,3,3	0.06	0	2,2,2	0.12	0
16	MGD	B	504	15	47,52,52	1.40	7 (14%)	58,81,81	1.95	14 (24%)
9	GOL	H	508	-	5,5,5	0.31	0	5,5,5	0.29	0
12	EDO	G	606	-	3,3,3	0.07	0	2,2,2	0.10	0
9	GOL	A	608	-	5,5,5	0.27	0	5,5,5	0.21	0
14	SF4	E	1101	5	0,12,12	-	-	-	-	-
16	MGD	B	503	15	47,52,52	1.46	7 (14%)	58,81,81	2.02	14 (24%)
14	SF4	L	101	6	0,12,12	-	-	-	-	-
9	GOL	A	604	-	5,5,5	0.29	0	5,5,5	0.12	0
11	PE4	A	606	-	10,10,23	0.46	0	9,9,22	0.46	0
14	SF4	F	101	6	0,12,12	-	-	-	-	-
14	SF4	E	1104	5	0,12,12	-	-	-	-	-
12	EDO	E	1107	-	3,3,3	0.07	0	2,2,2	0.07	0
12	EDO	E	1109	-	3,3,3	0.07	0	2,2,2	0.09	0
14	SF4	F	102	6	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	PE4	I	704	-	9,9,23	0.48	0	8,8,22	0.30	0
10	ACT	A	605	-	3,3,3	0.94	0	3,3,3	1.52	1 (33%)
14	SF4	H	501	2	0,12,12	-	-	-		
14	SF4	L	102	6	0,12,12	-	-	-		
12	EDO	A	610	-	3,3,3	0.06	0	2,2,2	0.14	0
12	EDO	G	607	-	3,3,3	0.06	0	2,2,2	0.10	0
12	EDO	K	1105	-	3,3,3	0.05	0	2,2,2	0.07	0
14	SF4	K	1102	5	0,12,12	-	-	-		
14	SF4	K	1101	5	0,12,12	-	-	-		
14	SF4	E	1102	5	0,12,12	-	-	-		
16	MGD	H	503	15	47,52,52	1.47	7 (14%)	58,81,81	1.97	12 (20%)
16	MGD	H	504	15	47,52,52	1.39	8 (17%)	58,81,81	1.91	13 (22%)
12	EDO	G	604	-	3,3,3	0.08	0	2,2,2	0.15	0
9	GOL	A	611	-	5,5,5	0.09	0	5,5,5	0.33	0
11	PE4	B	507	-	6,6,23	0.40	0	5,5,22	0.31	0
12	EDO	E	1108	-	3,3,3	0.05	0	2,2,2	0.10	0
8	PEG	A	603	-	6,6,6	0.23	0	5,5,5	0.35	0
18	FAD	E	1103	-	58,58,58	1.49	10 (17%)	85,89,89	1.55	15 (17%)
10	ACT	B	506	-	3,3,3	0.84	0	3,3,3	1.60	1 (33%)
10	ACT	I	705	-	3,3,3	0.78	0	3,3,3	1.71	1 (33%)
9	GOL	H	509	-	5,5,5	0.08	0	5,5,5	0.33	0
10	ACT	A	607	-	3,3,3	0.87	0	3,3,3	1.64	1 (33%)
12	EDO	A	609	-	3,3,3	0.32	0	2,2,2	0.18	0
20	PG4	I	702	-	9,9,12	0.21	0	8,8,11	0.23	0
9	GOL	I	703	-	5,5,5	0.35	0	5,5,5	0.30	0
12	EDO	K	1106	-	3,3,3	0.06	0	2,2,2	0.10	0
9	GOL	I	701	-	5,5,5	0.33	0	5,5,5	0.29	0
10	ACT	H	507	-	3,3,3	1.08	0	3,3,3	0.84	0
9	GOL	H	505	-	5,5,5	0.37	0	5,5,5	0.39	0
9	GOL	E	1105	-	5,5,5	0.25	0	5,5,5	0.13	0
14	SF4	K	1104	5	0,12,12	-	-	-		
14	SF4	B	501	2	0,12,12	-	-	-		
12	EDO	G	605	-	3,3,3	0.08	0	2,2,2	0.14	0
18	FAD	K	1103	-	58,58,58	1.45	9 (15%)	85,89,89	1.55	14 (16%)
12	EDO	E	1106	-	3,3,3	0.20	0	2,2,2	0.32	0
12	EDO	B	508	-	3,3,3	0.06	0	2,2,2	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
12	EDO	H	510	-	-	0/1/1/1	-
16	MGD	B	504	15	-	5/22/66/66	0/6/6/6
9	GOL	H	508	-	-	2/4/4/4	-
12	EDO	G	606	-	-	1/1/1/1	-
9	GOL	A	608	-	-	0/4/4/4	-
16	MGD	B	503	15	-	2/22/66/66	0/6/6/6
14	SF4	E	1101	5	-	-	0/6/5/5
14	SF4	L	101	6	-	-	0/6/5/5
9	GOL	A	604	-	-	0/4/4/4	-
11	PE4	A	606	-	-	7/8/8/21	-
14	SF4	F	101	6	-	-	0/6/5/5
14	SF4	E	1104	5	-	-	0/6/5/5
12	EDO	E	1107	-	-	0/1/1/1	-
12	EDO	E	1109	-	-	0/1/1/1	-
14	SF4	F	102	6	-	-	0/6/5/5
11	PE4	I	704	-	-	4/7/7/21	-
14	SF4	H	501	2	-	-	0/6/5/5
14	SF4	L	102	6	-	-	0/6/5/5
12	EDO	A	610	-	-	0/1/1/1	-
12	EDO	G	607	-	-	1/1/1/1	-
12	EDO	K	1105	-	-	1/1/1/1	-
14	SF4	K	1102	5	-	-	0/6/5/5
14	SF4	K	1101	5	-	-	0/6/5/5
14	SF4	E	1102	5	-	-	0/6/5/5
16	MGD	H	503	15	-	2/22/66/66	0/6/6/6
16	MGD	H	504	15	-	6/22/66/66	0/6/6/6
12	EDO	G	604	-	-	0/1/1/1	-
9	GOL	A	611	-	-	4/4/4/4	-
11	PE4	B	507	-	-	2/4/4/21	-
12	EDO	E	1108	-	-	1/1/1/1	-
8	PEG	A	603	-	-	2/4/4/4	-
18	FAD	E	1103	-	-	1/34/50/50	0/6/6/6
20	PG4	I	702	-	-	1/7/7/10	-
9	GOL	H	509	-	-	2/4/4/4	-
12	EDO	A	609	-	-	1/1/1/1	-
9	GOL	I	703	-	-	2/4/4/4	-
12	EDO	K	1106	-	-	0/1/1/1	-
9	GOL	I	701	-	-	2/4/4/4	-
9	GOL	H	505	-	-	0/4/4/4	-
9	GOL	E	1105	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SF4	K	1104	5	-	-	0/6/5/5
14	SF4	B	501	2	-	-	0/6/5/5
12	EDO	G	605	-	-	0/1/1/1	-
18	FAD	K	1103	-	-	1/34/50/50	0/6/6/6
12	EDO	E	1106	-	-	0/1/1/1	-
12	EDO	B	508	-	-	0/1/1/1	-

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	503	MGD	C16-C21	5.44	1.47	1.38
16	H	503	MGD	C16-C21	5.35	1.47	1.38
16	B	504	MGD	C16-C21	5.19	1.47	1.38
16	H	504	MGD	C16-C21	5.03	1.47	1.38
18	E	1103	FAD	C9A-C5X	5.01	1.49	1.41

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	1103	FAD	C5A-C4A-N3A	-5.92	118.56	126.72
18	E	1103	FAD	C5A-C4A-N3A	-5.84	118.68	126.72
16	H	504	MGD	C5-C4-N3	-5.81	119.15	128.39
16	B	503	MGD	C5-C4-N3	-5.77	119.20	128.39
16	H	503	MGD	C5-C4-N3	-5.77	119.20	128.39

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	611	GOL	O1-C1-C2-C3
9	A	611	GOL	C1-C2-C3-O3
9	H	508	GOL	O1-C1-C2-C3
9	I	703	GOL	C1-C2-C3-O3
16	B	504	MGD	C5'-O5'-PB-O2B

There are no ring outliers.

8 monomers are involved in 9 short contacts:

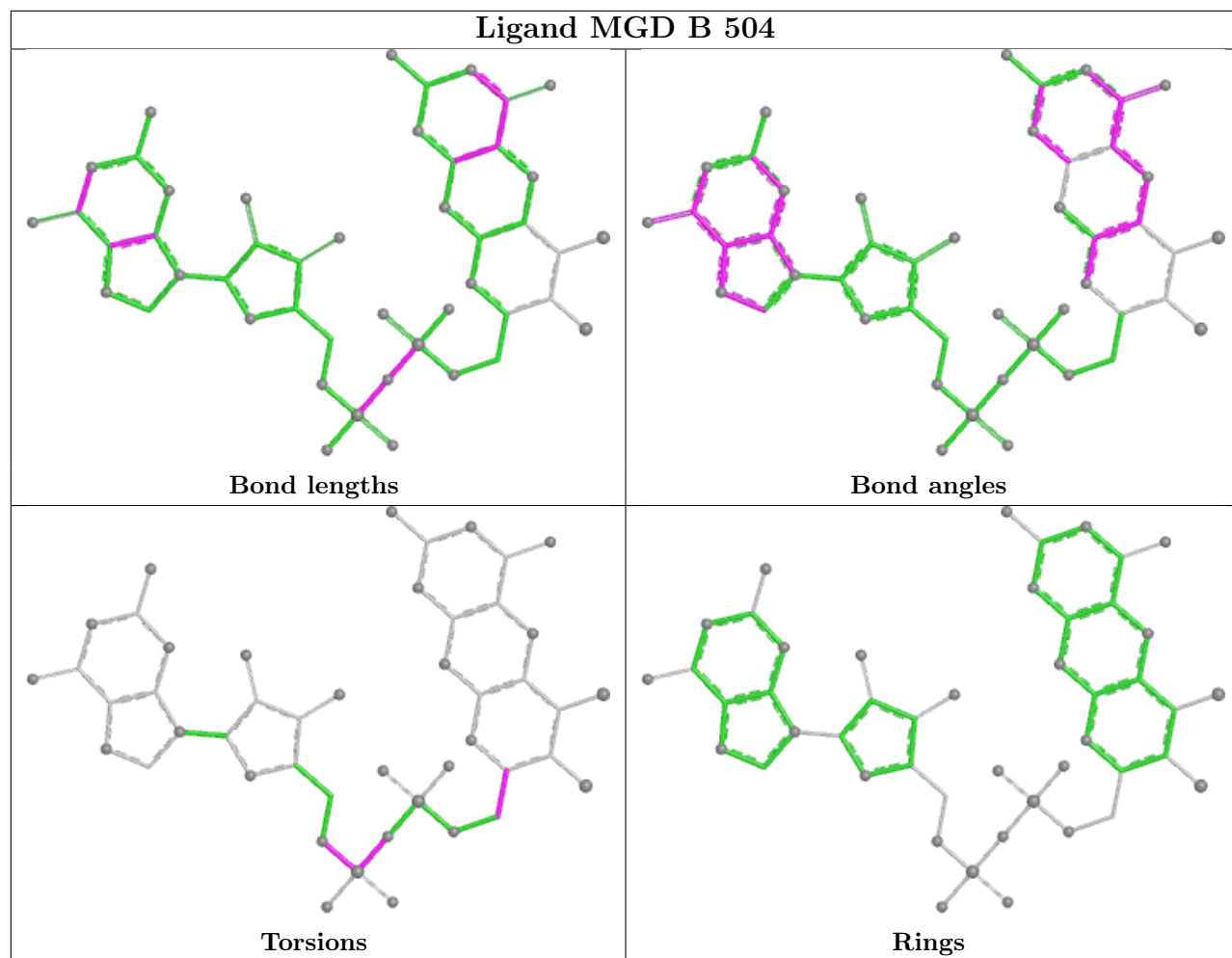
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	504	MGD	2	0
14	E	1101	SF4	1	0

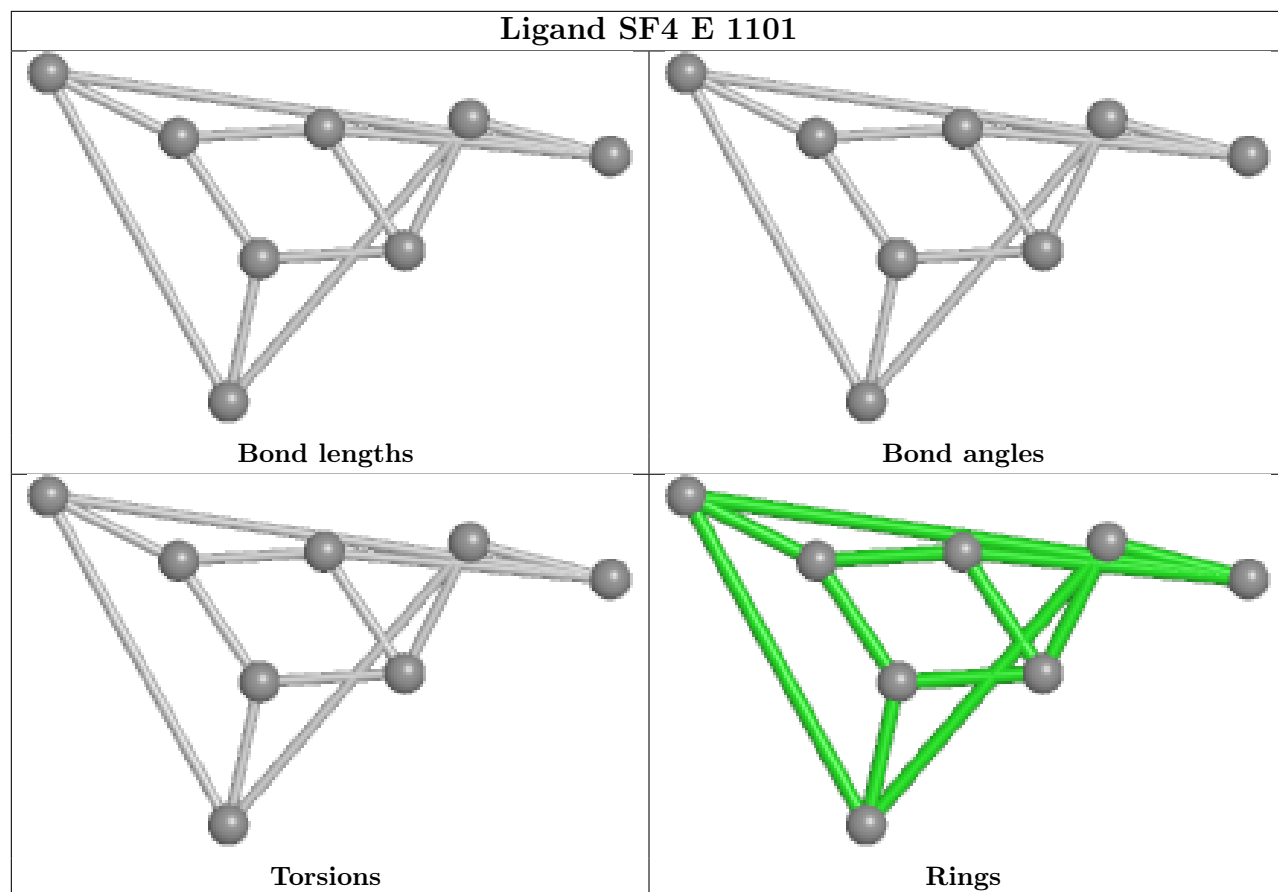
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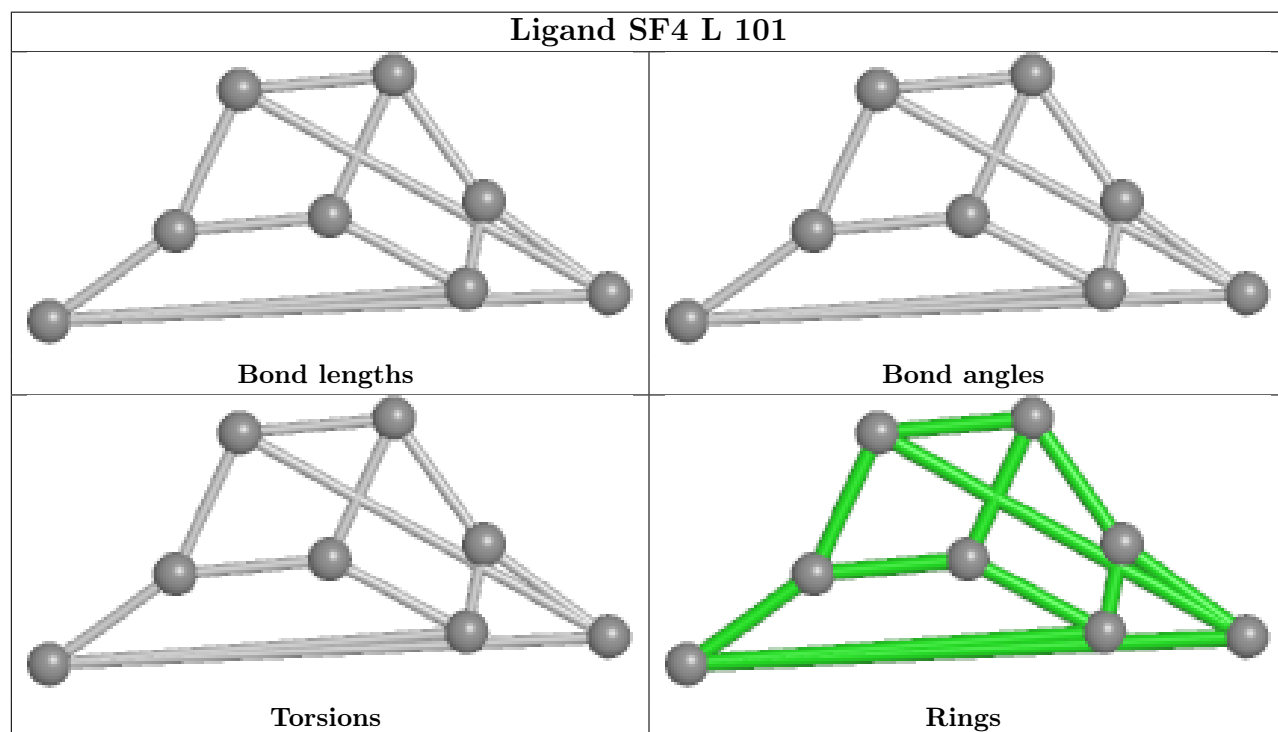
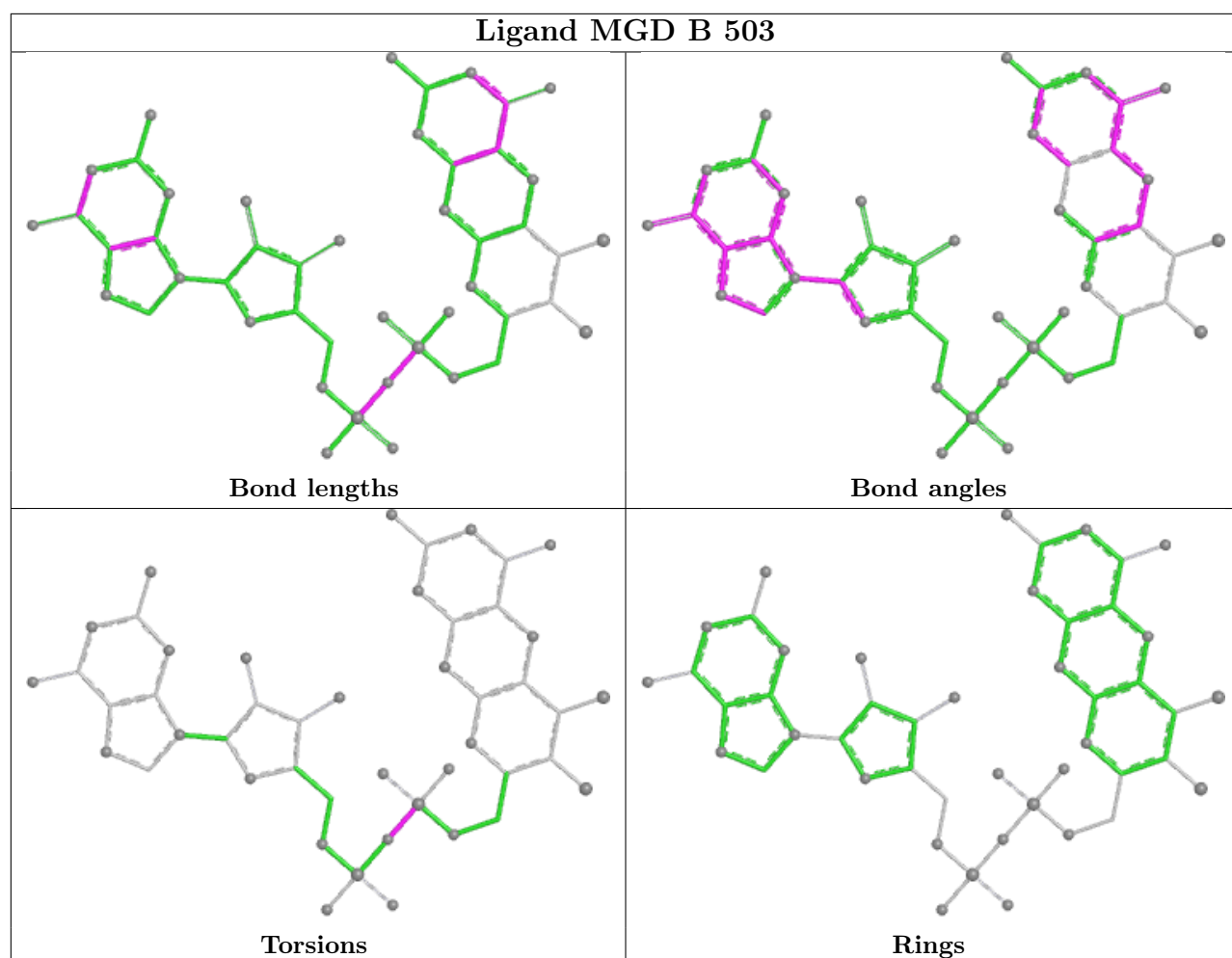
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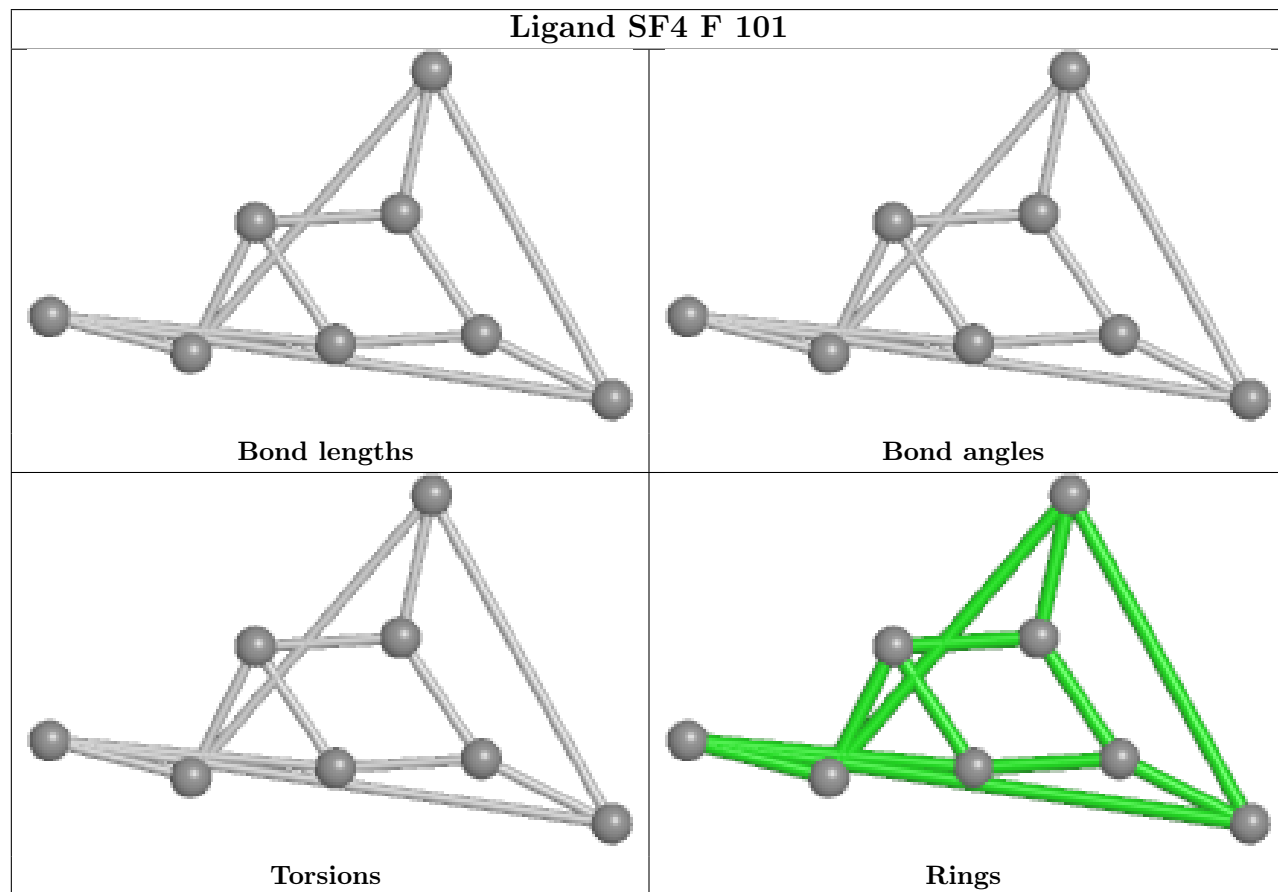
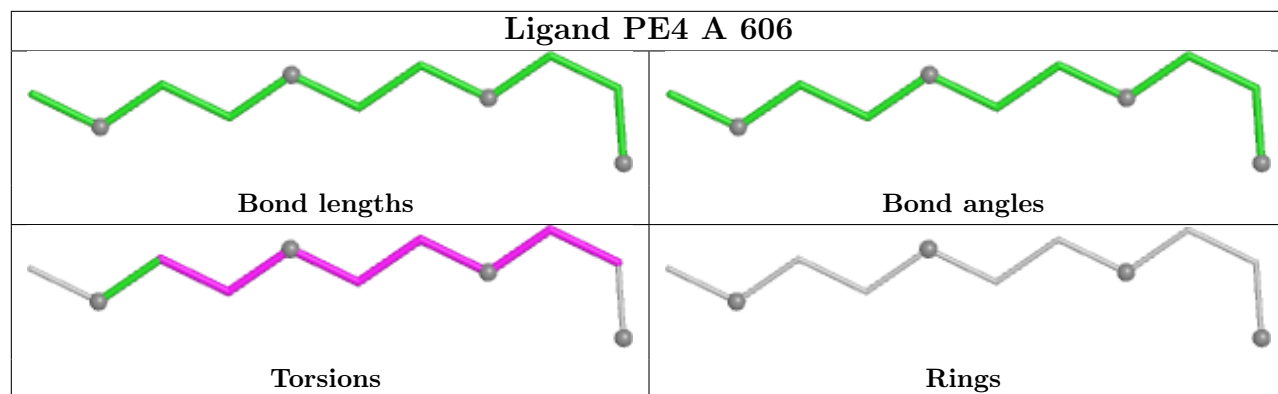
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	503	MGD	1	0
16	H	503	MGD	1	0
16	H	504	MGD	1	0
18	E	1103	FAD	1	0
10	A	607	ACT	1	0
18	K	1103	FAD	1	0

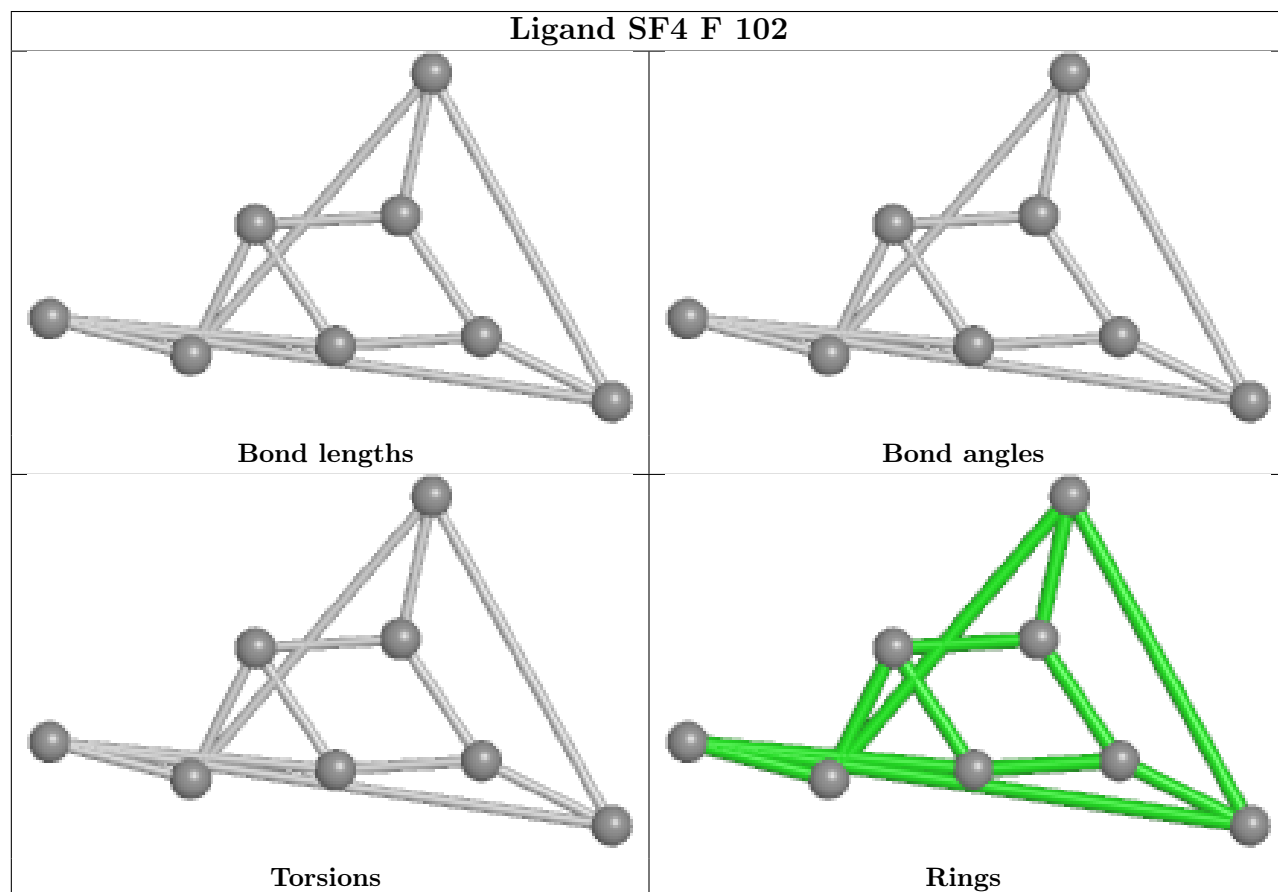
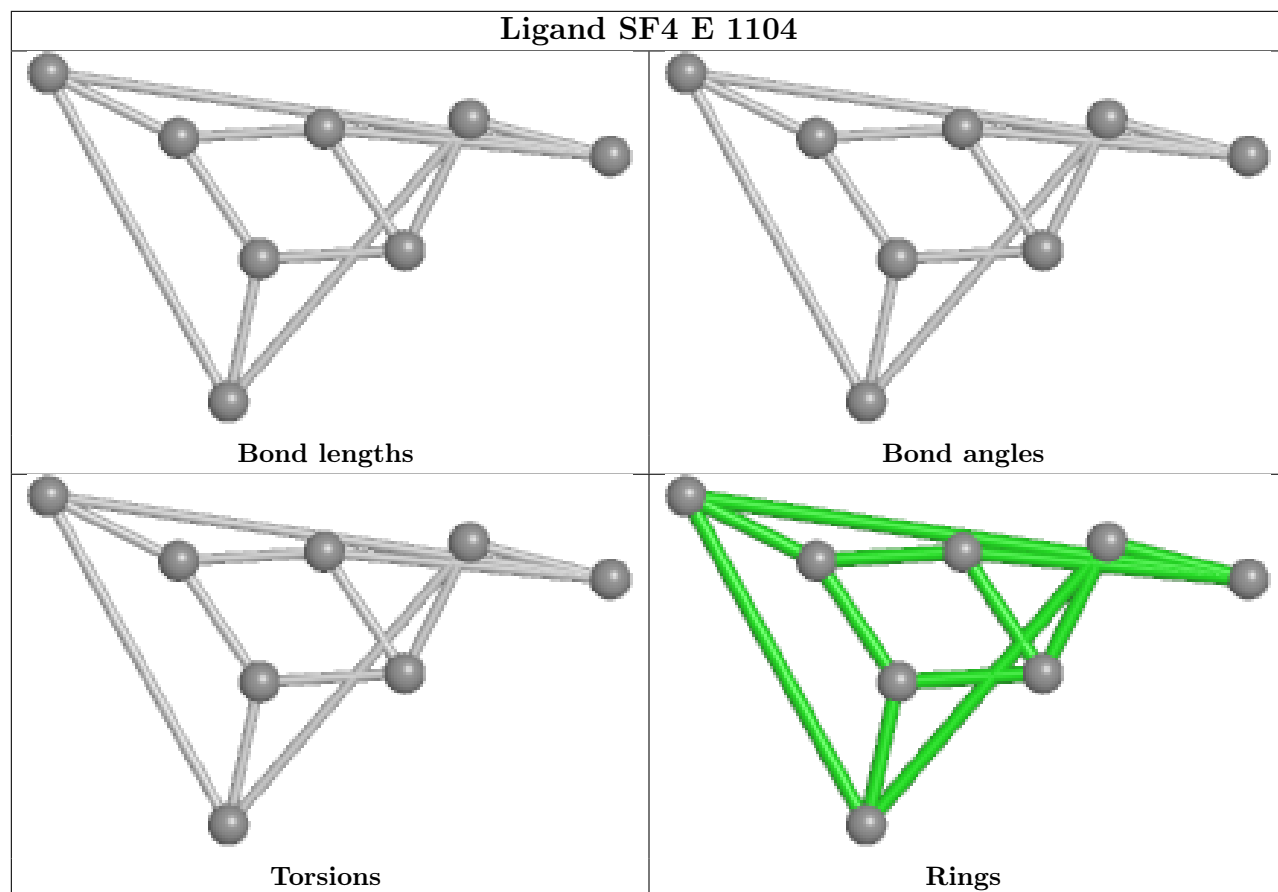
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

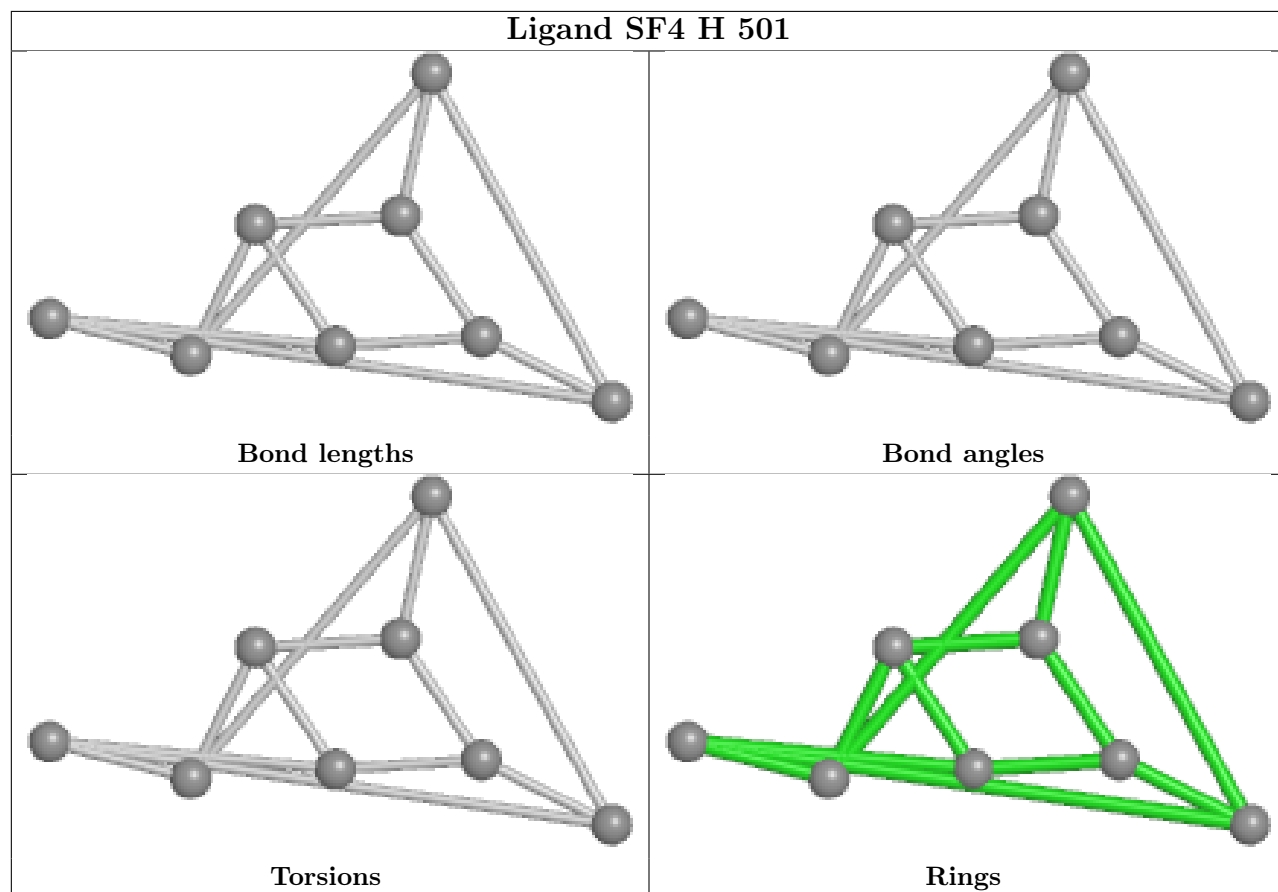
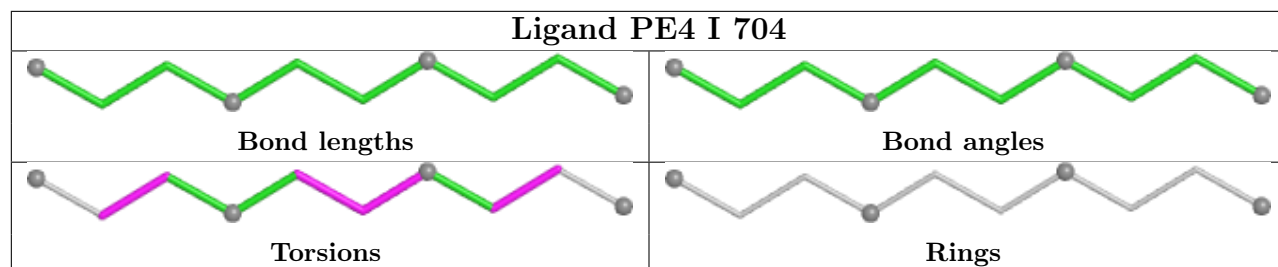




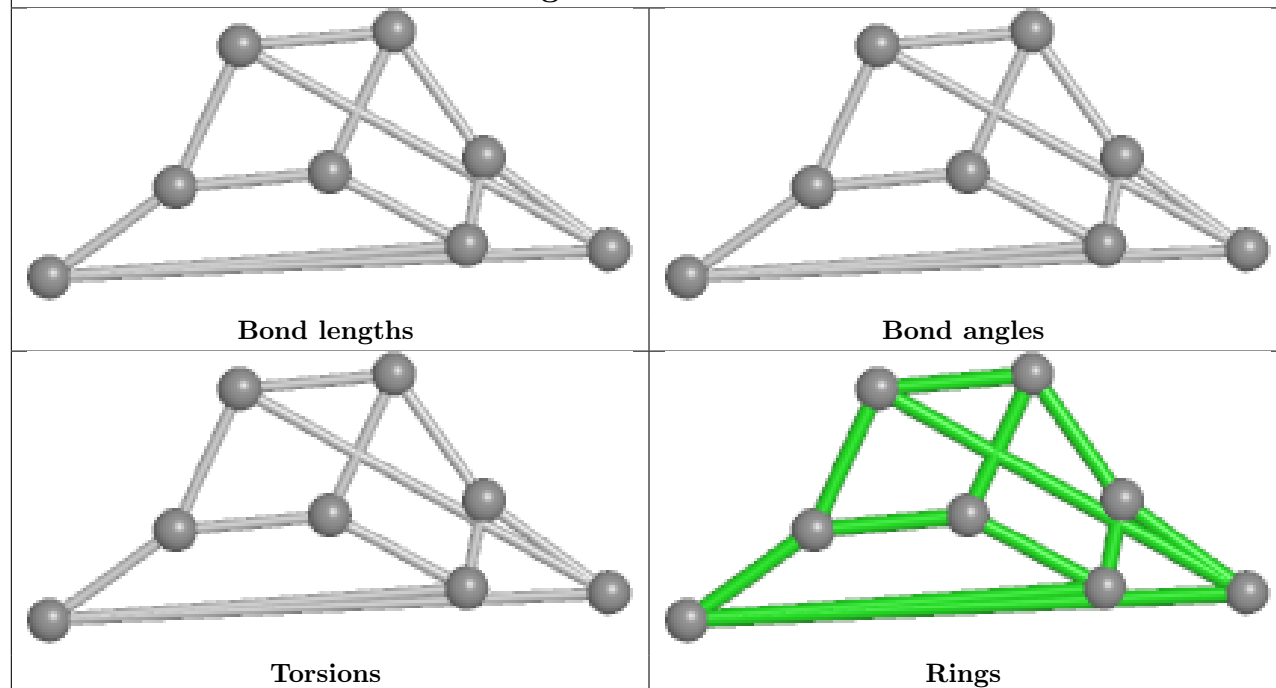




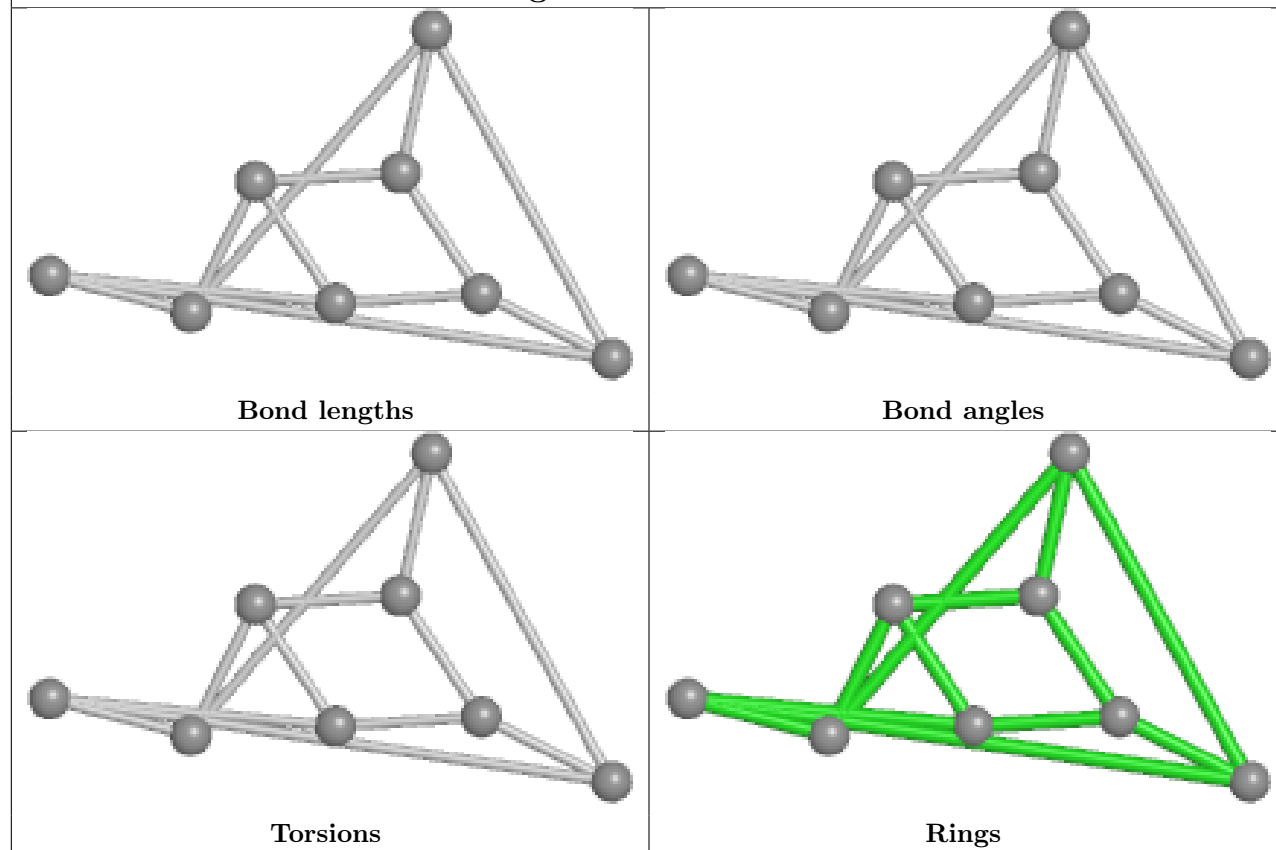


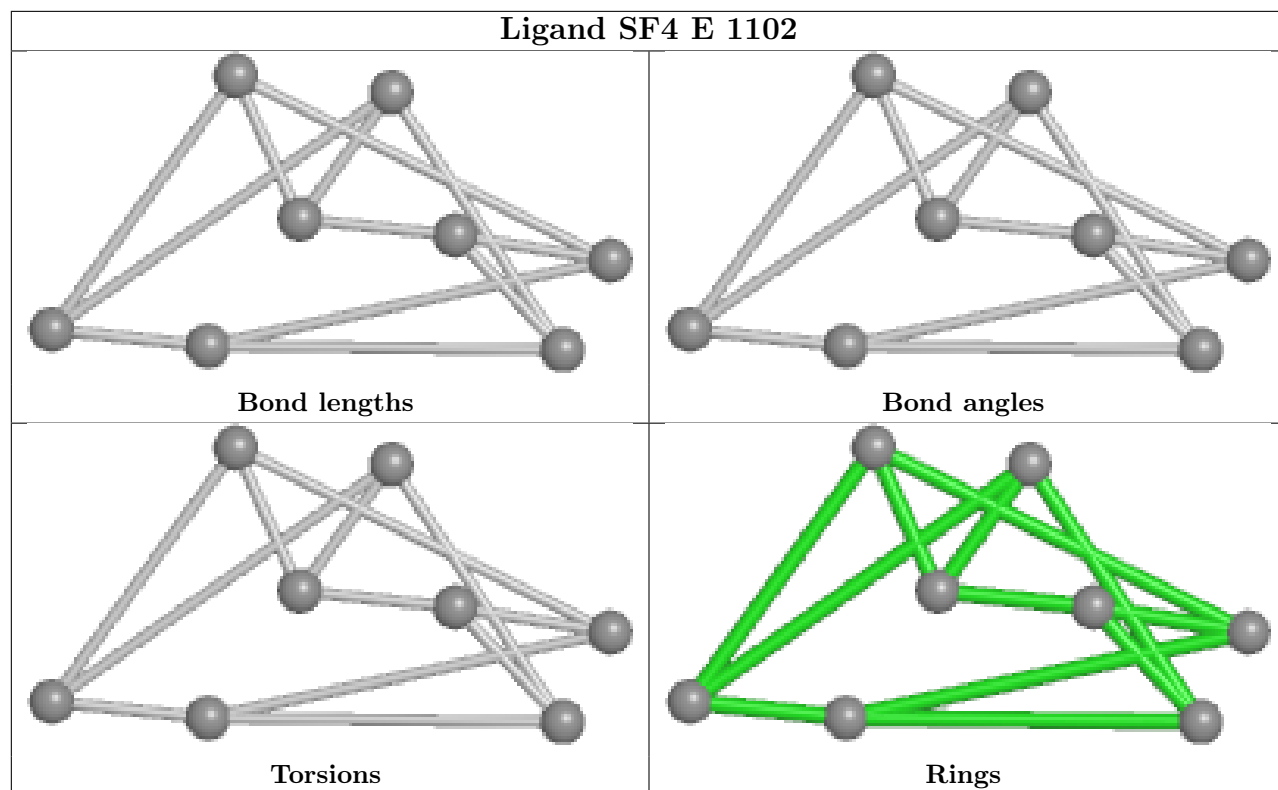
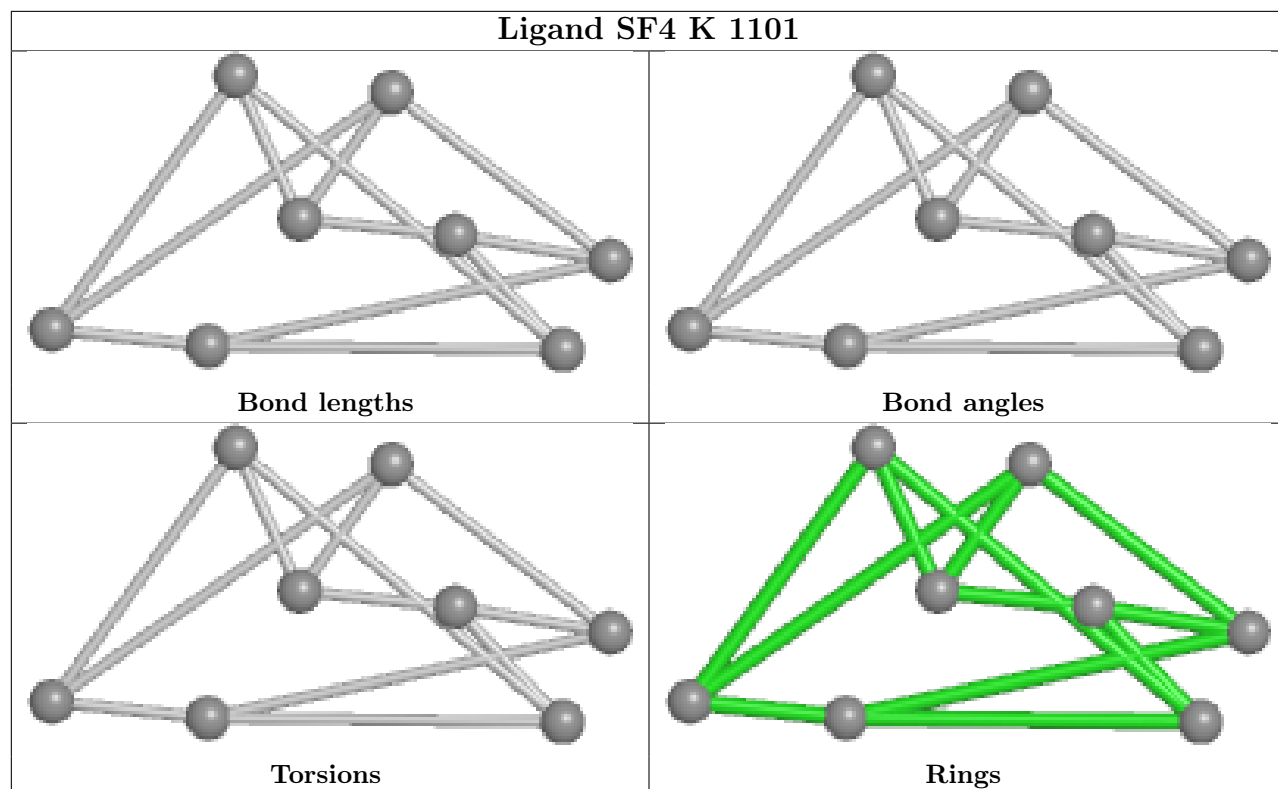


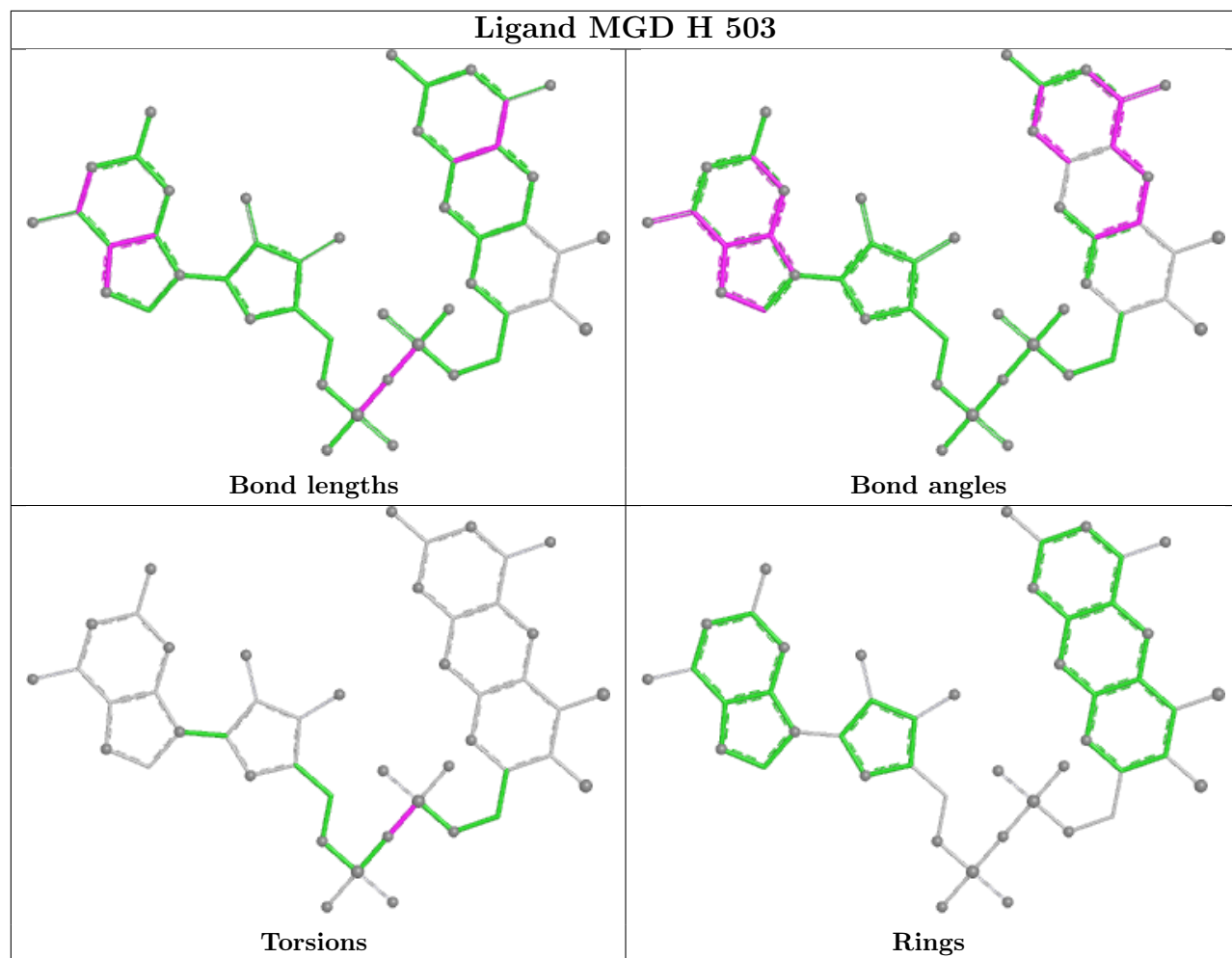
Ligand SF4 L 102

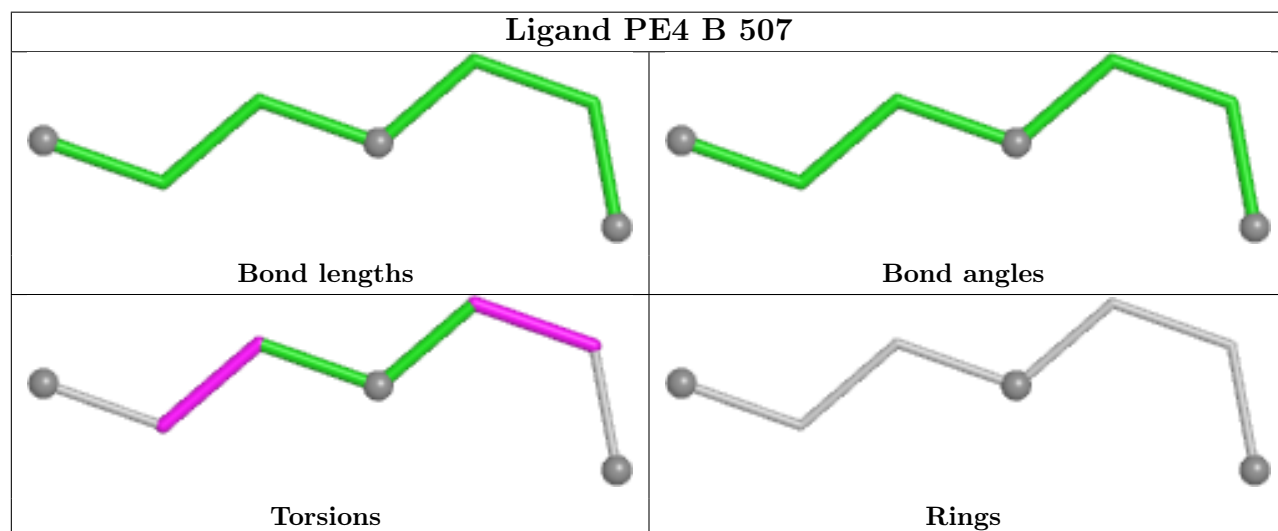
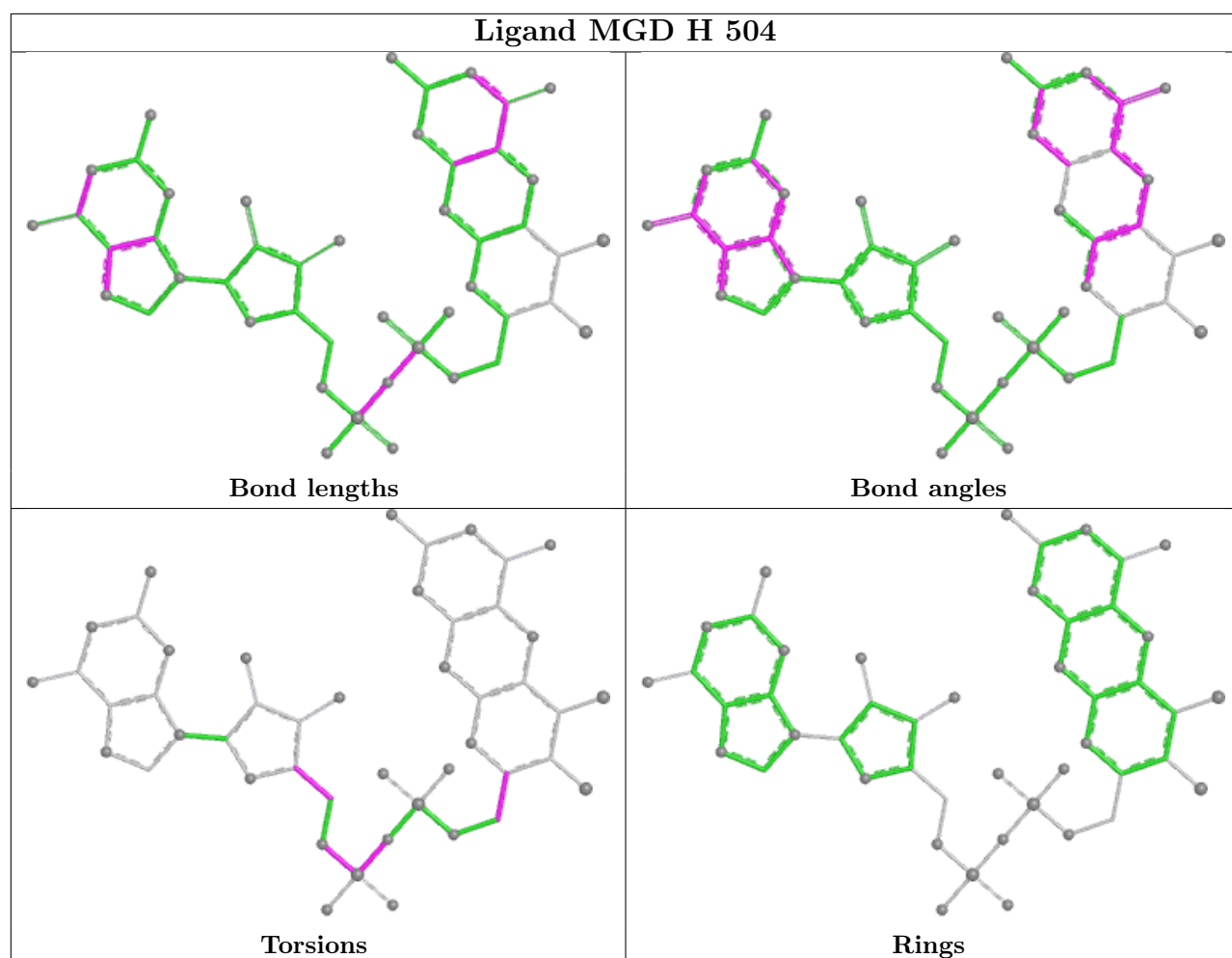


Ligand SF4 K 1102

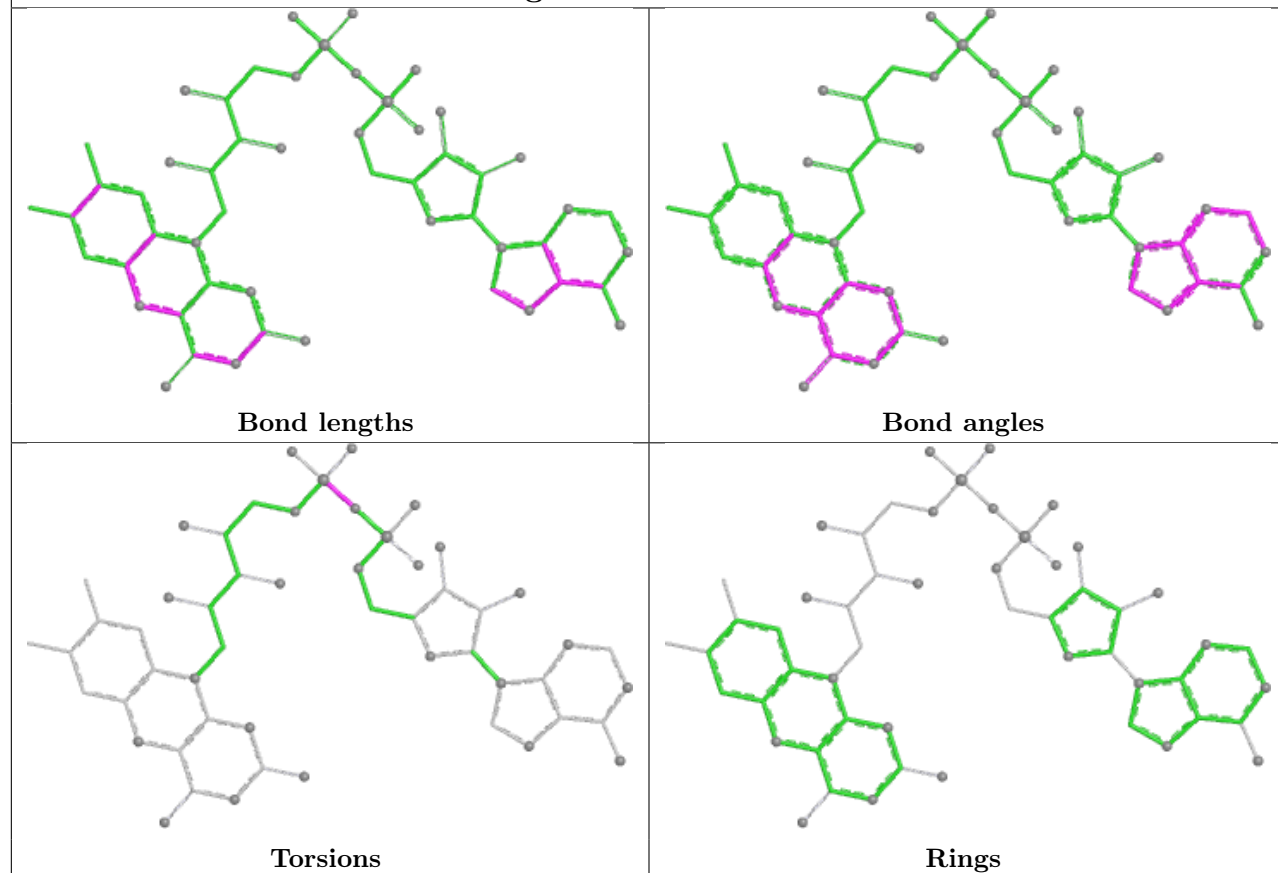




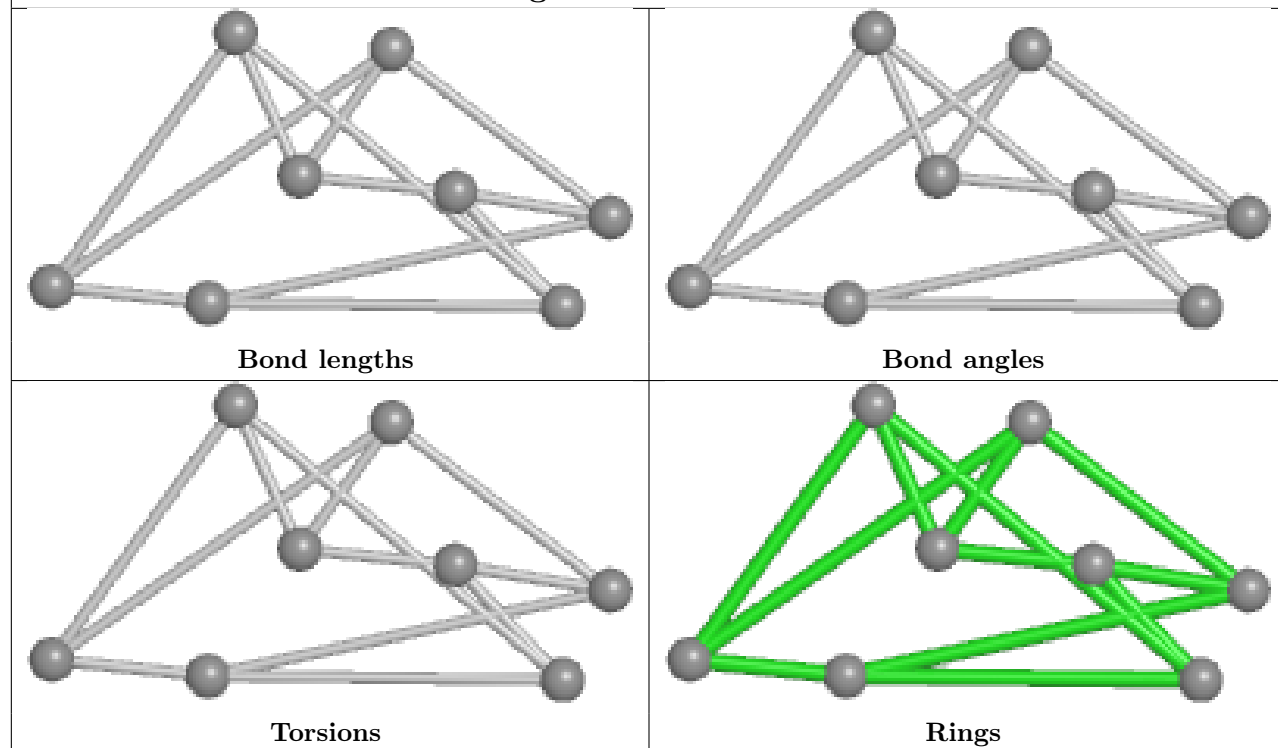


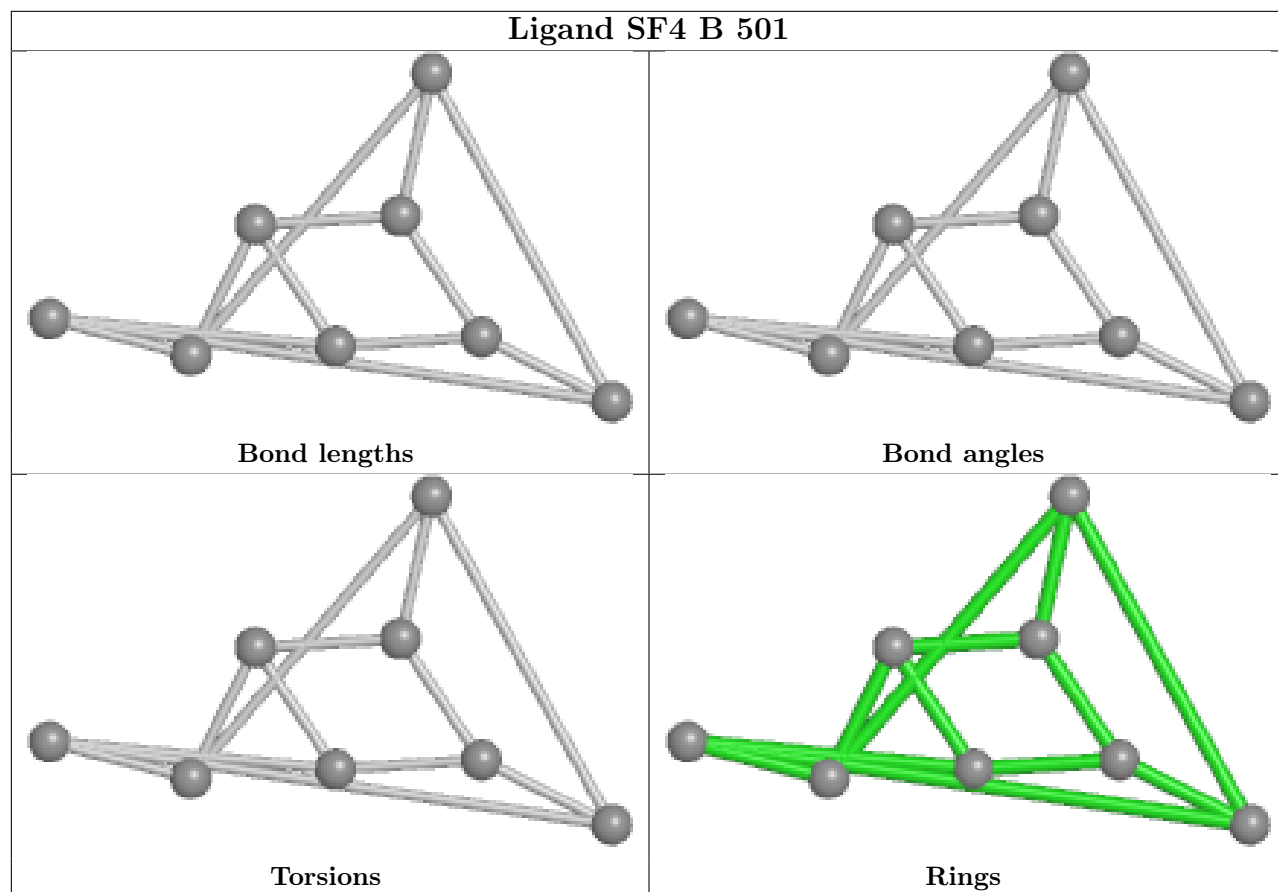


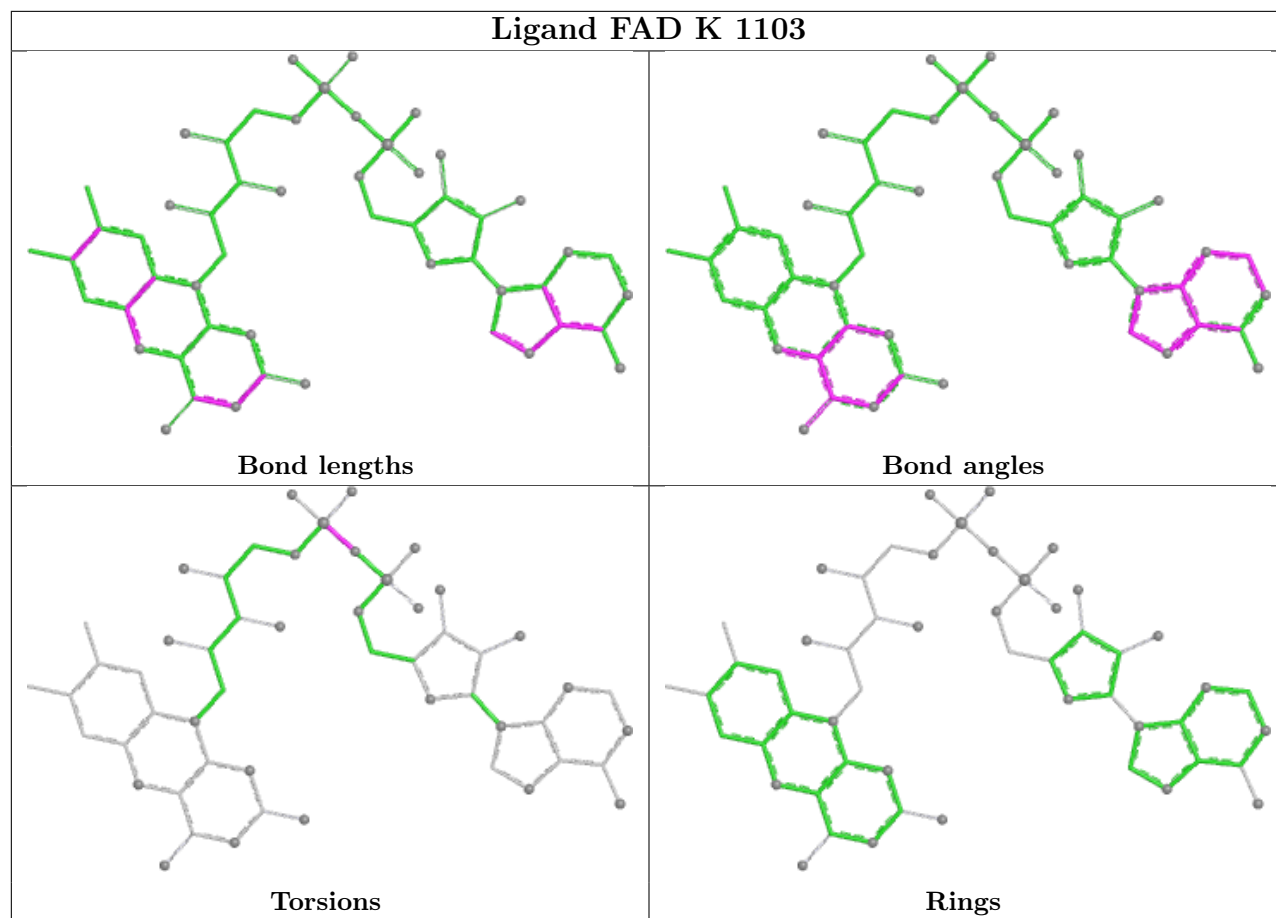
Ligand FAD E 1103



Ligand SF4 K 1104







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	565/567 (99%)	-0.25	3 (0%) 87 91	11, 18, 31, 63	0
1	G	565/567 (99%)	-0.29	1 (0%) 91 94	10, 17, 29, 64	1 (0%)
2	B	429/430 (99%)	-0.21	2 (0%) 87 91	10, 18, 31, 61	0
2	H	429/430 (99%)	-0.18	3 (0%) 84 89	10, 18, 36, 66	1 (0%)
3	C	253/253 (100%)	0.19	5 (1%) 65 74	15, 26, 51, 78	0
3	I	253/253 (100%)	-0.15	3 (1%) 76 83	11, 19, 37, 75	0
4	D	124/126 (98%)	0.12	2 (1%) 70 79	14, 25, 41, 67	0
4	J	125/126 (99%)	-0.07	1 (0%) 82 87	14, 23, 38, 74	0
5	E	351/359 (97%)	0.32	15 (4%) 40 49	18, 30, 55, 85	0
5	K	351/359 (97%)	0.85	38 (10%) 11 15	23, 41, 71, 100	0
6	F	77/85 (90%)	0.18	5 (6%) 25 33	17, 23, 51, 93	0
6	L	78/85 (91%)	0.10	5 (6%) 25 33	15, 24, 52, 75	0
All	All	3600/3640 (98%)	-0.01	83 (2%) 61 70	10, 21, 50, 100	2 (0%)

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	K	233	VAL	5.6
5	K	231	LEU	5.4
5	K	228	LEU	4.8
5	K	351	ARG	4.5
3	I	11	SER	4.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	G	180	12/13	0.92	0.09	11,14,26,27	0
1	KCX	A	180	12/13	0.95	0.08	11,14,28,31	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	EDO	E	1108	4/4	0.58	0.17	55,56,56,63	0
12	EDO	E	1109	4/4	0.65	0.23	48,48,49,52	0
12	EDO	K	1105	4/4	0.66	0.26	46,46,47,56	0
9	GOL	A	611	6/6	0.67	0.19	40,44,49,53	0
8	PEG	A	603	7/7	0.70	0.16	28,33,40,40	0
12	EDO	B	508	4/4	0.71	0.17	34,34,37,45	0
12	EDO	H	510	4/4	0.73	0.18	49,52,52,52	0
10	ACT	A	605	4/4	0.75	0.15	33,37,41,45	0
10	ACT	I	705	4/4	0.75	0.12	24,29,38,40	0
12	EDO	A	610	4/4	0.75	0.18	33,35,36,55	0
9	GOL	H	505	6/6	0.75	0.20	33,39,41,45	0
12	EDO	G	605	4/4	0.76	0.15	35,40,41,52	0
12	EDO	G	606	4/4	0.76	0.17	34,36,38,41	0
10	ACT	H	507	4/4	0.78	0.17	30,32,37,44	0
12	EDO	A	609	4/4	0.79	0.13	32,33,36,36	0
9	GOL	I	703	6/6	0.80	0.19	34,38,39,40	0
10	ACT	B	506	4/4	0.80	0.15	33,35,36,38	0
11	PE4	A	606	11/24	0.80	0.12	29,32,41,43	0
12	EDO	E	1107	4/4	0.80	0.18	33,38,43,44	0
11	PE4	B	507	7/24	0.80	0.14	26,30,40,51	0
20	PG4	I	702	10/13	0.80	0.17	32,48,57,65	0
19	NA	H	511	1/1	0.81	0.14	47,47,47,47	0
11	PE4	I	704	10/24	0.82	0.13	29,33,36,39	0
9	GOL	H	509	6/6	0.83	0.18	36,37,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	GOL	I	701	6/6	0.83	0.13	36,38,42,44	0
12	EDO	G	604	4/4	0.83	0.12	31,31,33,35	0
12	EDO	G	607	4/4	0.84	0.12	25,31,36,36	0
12	EDO	K	1106	4/4	0.84	0.13	43,45,45,48	0
13	CL	A	612	1/1	0.86	0.12	61,61,61,61	0
9	GOL	E	1105	6/6	0.86	0.12	27,37,41,43	0
12	EDO	E	1106	4/4	0.86	0.10	30,32,34,35	0
9	GOL	A	608	6/6	0.87	0.13	27,30,32,40	0
19	NA	E	1110	1/1	0.89	0.09	47,47,47,47	0
10	ACT	A	607	4/4	0.89	0.13	32,32,34,36	0
9	GOL	A	604	6/6	0.89	0.14	30,33,35,37	0
19	NA	K	1107	1/1	0.91	0.11	46,46,46,46	0
9	GOL	H	508	6/6	0.92	0.10	27,31,34,37	0
17	H2S	B	505	1/1	0.92	0.11	24,24,24,24	0
13	CL	C	301	1/1	0.93	0.12	62,62,62,62	0
18	FAD	K	1103	53/53	0.93	0.09	25,32,39,42	0
18	FAD	E	1103	53/53	0.95	0.07	15,22,27,32	0
17	H2S	H	506	1/1	0.96	0.10	13,13,13,13	0
19	NA	G	603	1/1	0.97	0.10	21,21,21,21	0
16	MGD	H	504	47/47	0.97	0.06	11,15,19,26	0
13	CL	F	103	1/1	0.97	0.07	31,31,31,31	0
13	CL	L	103	1/1	0.97	0.05	26,26,26,26	0
7	ZN	G	601	1/1	0.98	0.09	42,42,42,42	0
14	SF4	B	501	8/8	0.98	0.03	8,11,12,14	0
14	SF4	E	1101	8/8	0.98	0.04	21,23,24,28	0
14	SF4	E	1104	8/8	0.98	0.03	10,13,16,19	0
14	SF4	F	101	8/8	0.98	0.03	12,16,19,20	0
14	SF4	H	501	8/8	0.98	0.04	12,14,16,16	0
14	SF4	K	1101	8/8	0.98	0.05	20,26,27,28	0
16	MGD	B	503	47/47	0.98	0.05	8,12,14,18	0
16	MGD	B	504	47/47	0.98	0.05	8,13,18,18	0
16	MGD	H	503	47/47	0.98	0.05	8,15,19,20	0
14	SF4	E	1102	8/8	0.99	0.02	13,15,16,17	0
14	SF4	K	1102	8/8	0.99	0.03	16,17,22,23	0
14	SF4	K	1104	8/8	0.99	0.02	17,19,22,22	0
14	SF4	L	101	8/8	0.99	0.03	12,15,17,17	0
14	SF4	L	102	8/8	0.99	0.03	14,19,21,24	0
7	ZN	G	602	1/1	0.99	0.04	33,33,33,33	0
7	ZN	A	602	1/1	0.99	0.04	33,33,33,33	0
14	SF4	F	102	8/8	0.99	0.02	12,15,18,20	0
7	ZN	A	601	1/1	0.99	0.04	42,42,42,42	0
15	W	H	502	1/1	1.00	0.04	15,15,15,15	0

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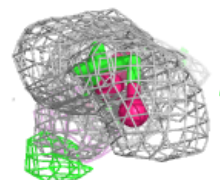
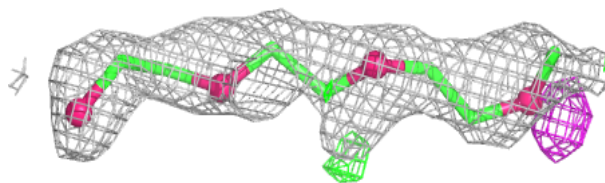
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	W	B	502	1/1	1.00	0.04	15,15,15,15	0

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

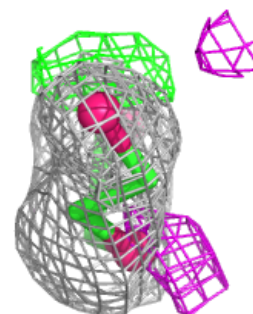
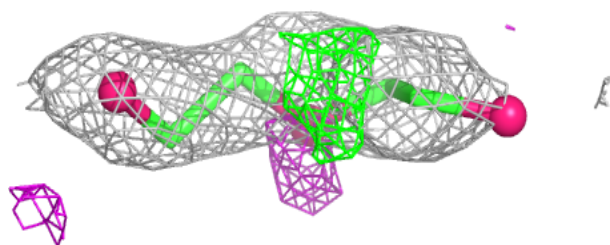
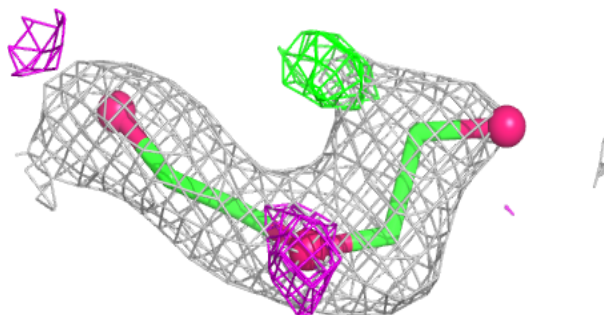
Electron density around PE4 A 606:

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

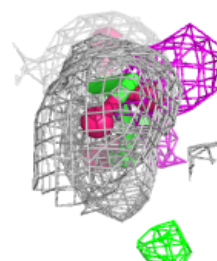
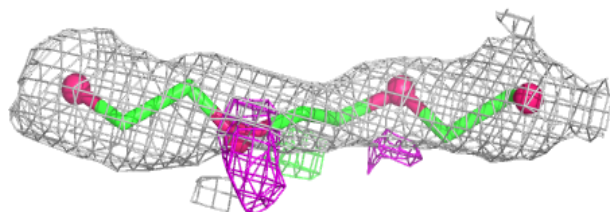
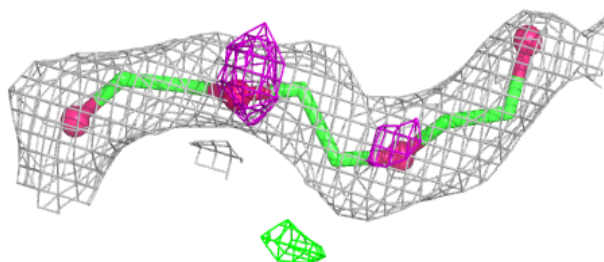


Electron density around PE4 B 507:

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and green (positive)

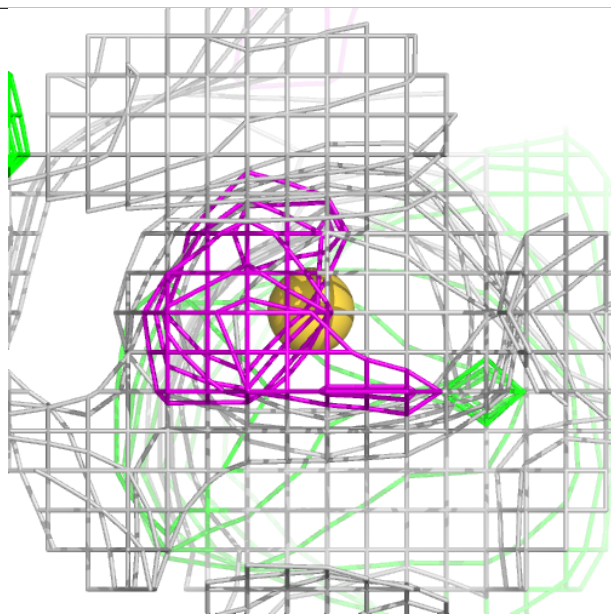
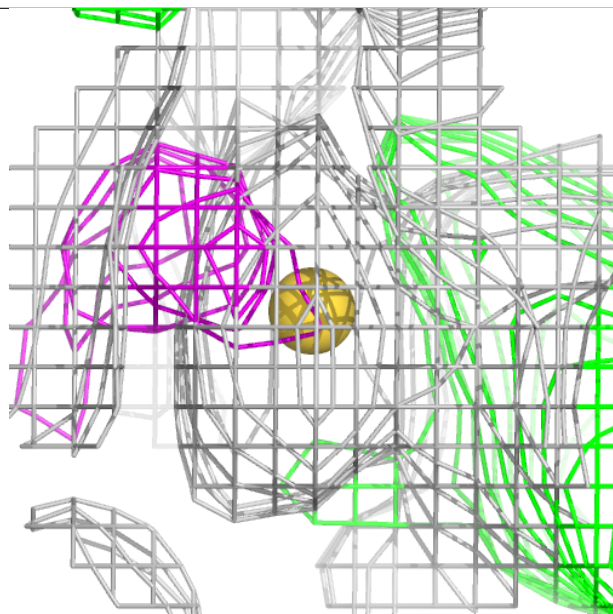
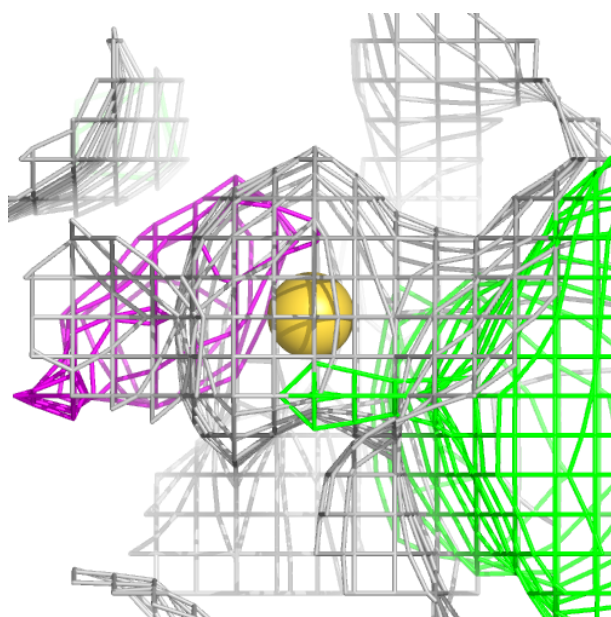
**Electron density around PE4 I 704:**

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



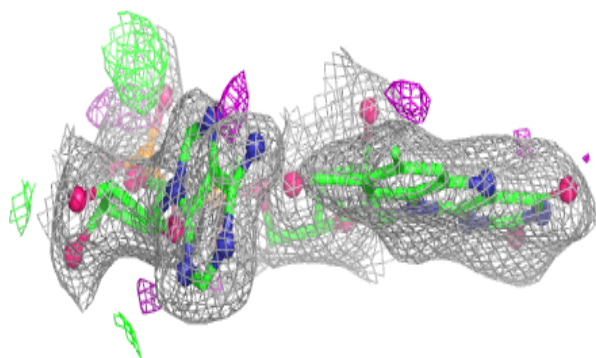
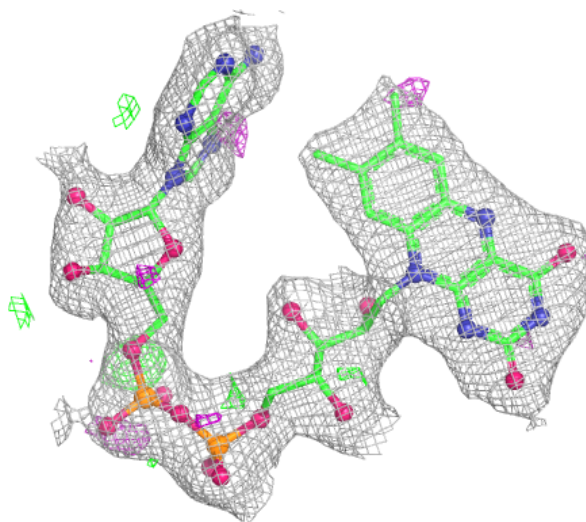
Electron density around H2S B 505:

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and green (positive)



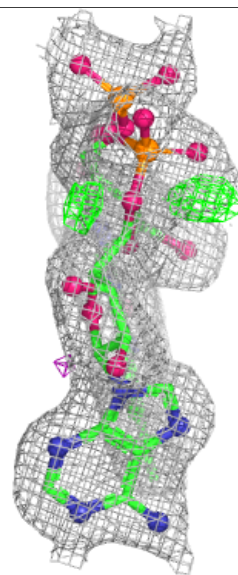
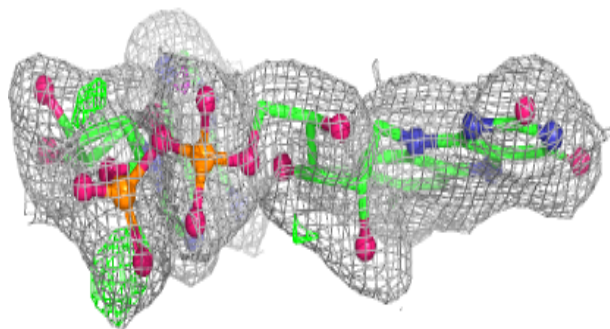
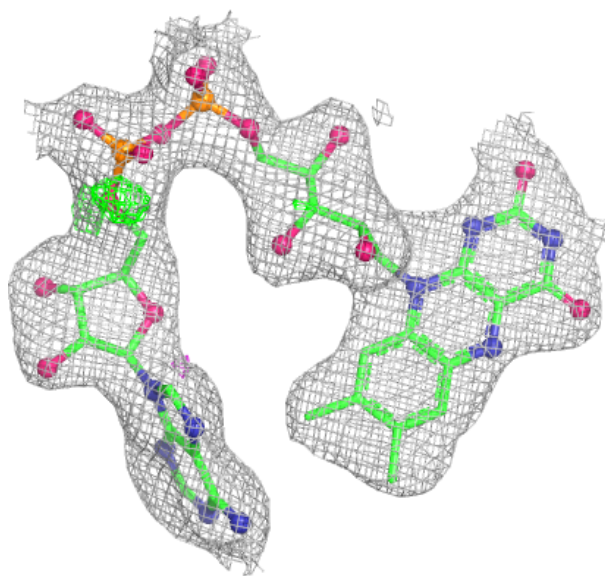
Electron density around FAD K 1103:

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



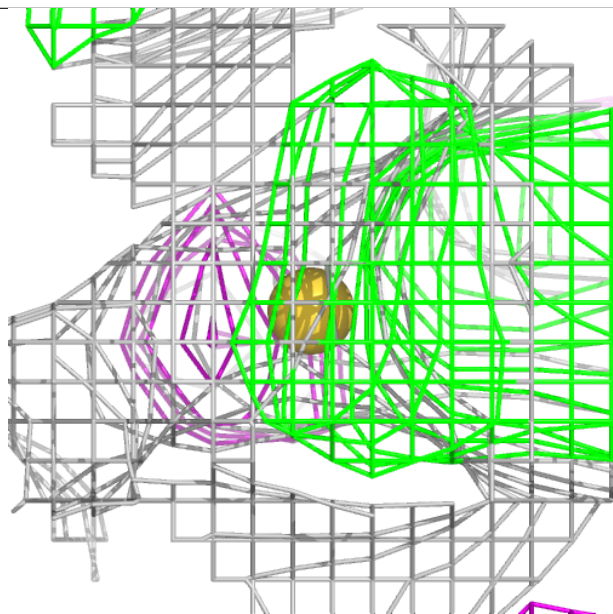
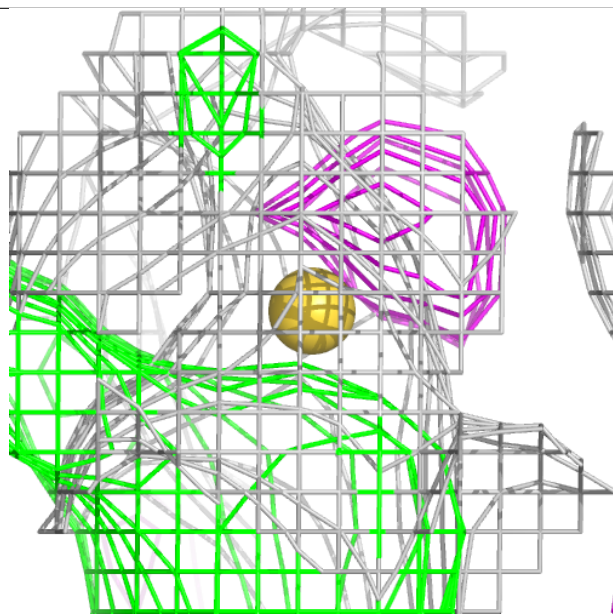
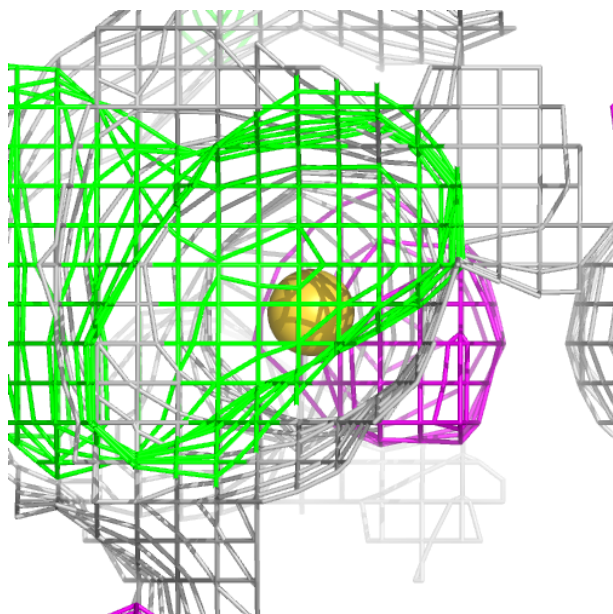
Electron density around FAD E 1103:

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



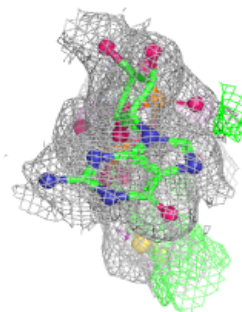
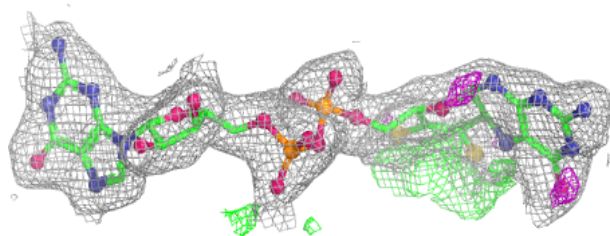
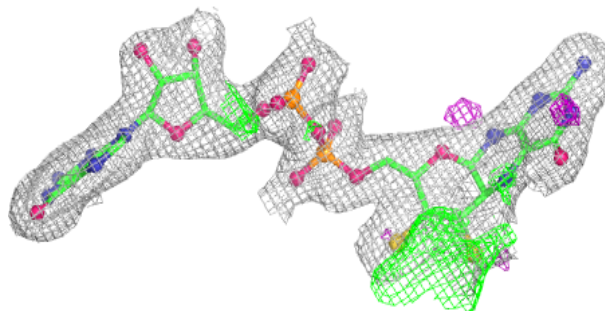
Electron density around H2S H 506:

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



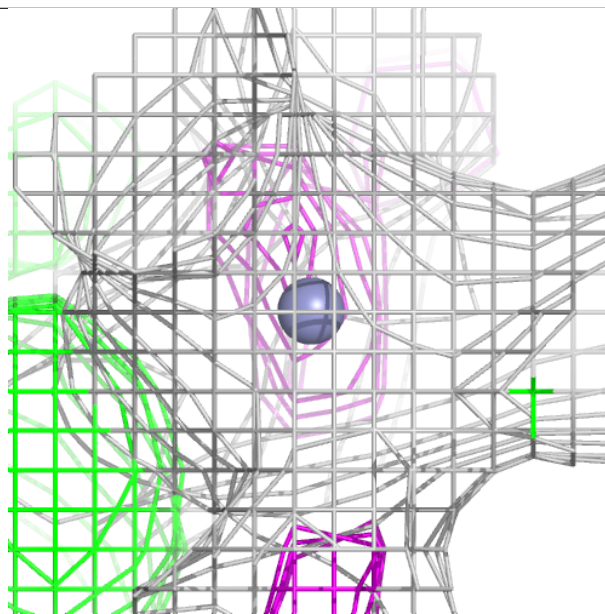
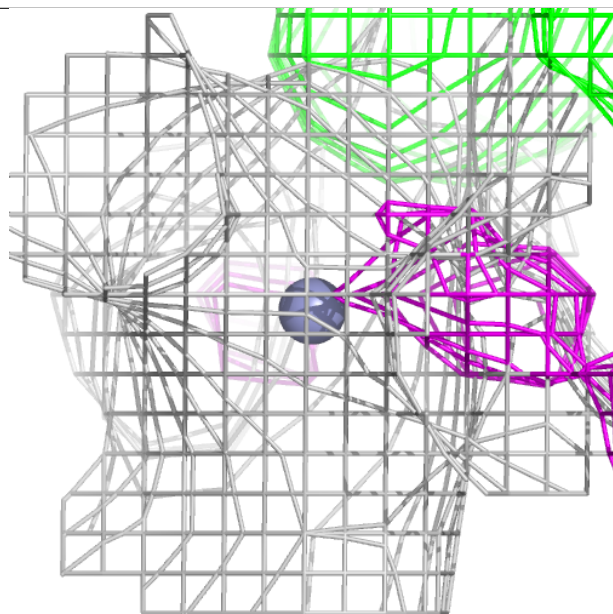
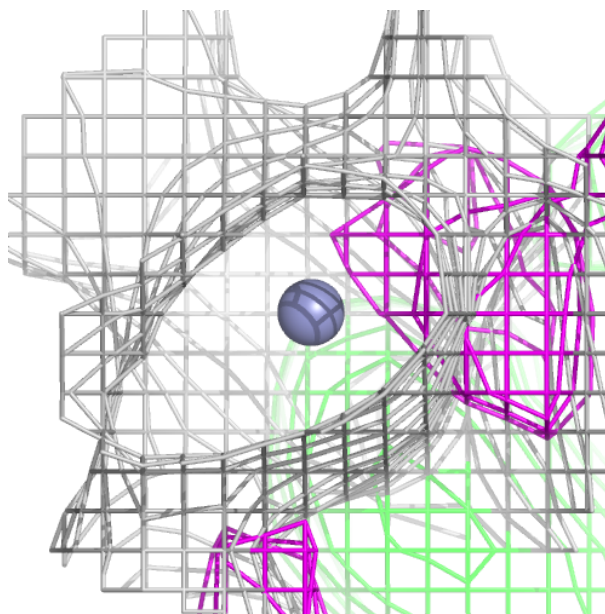
Electron density around MGD H 504:

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and green (positive)



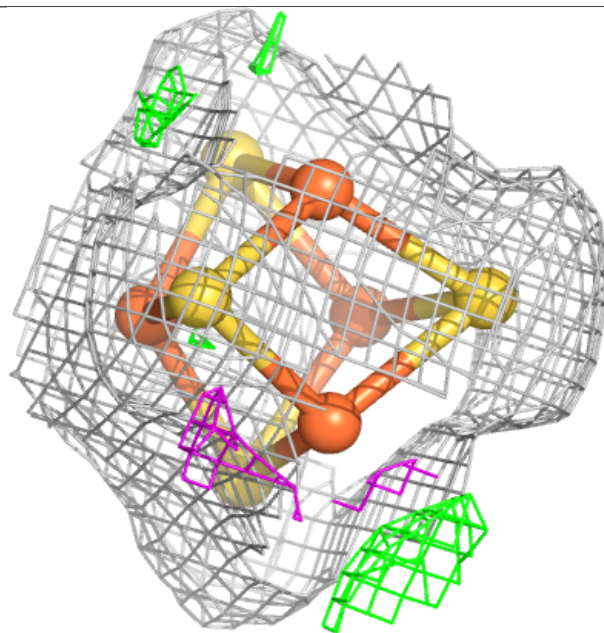
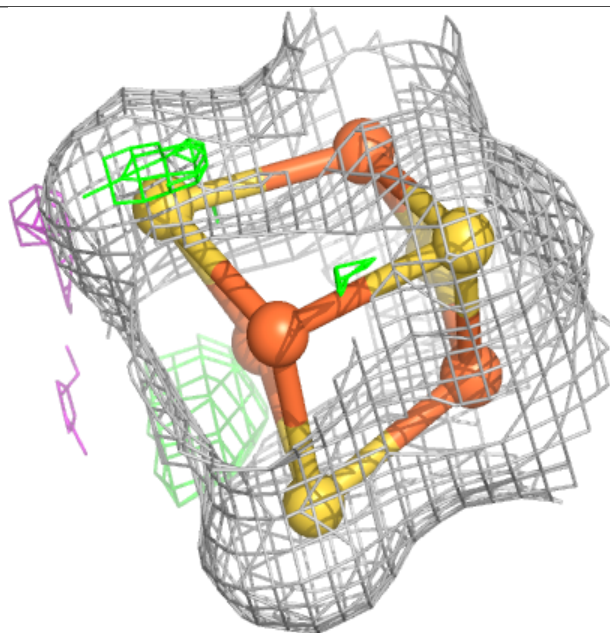
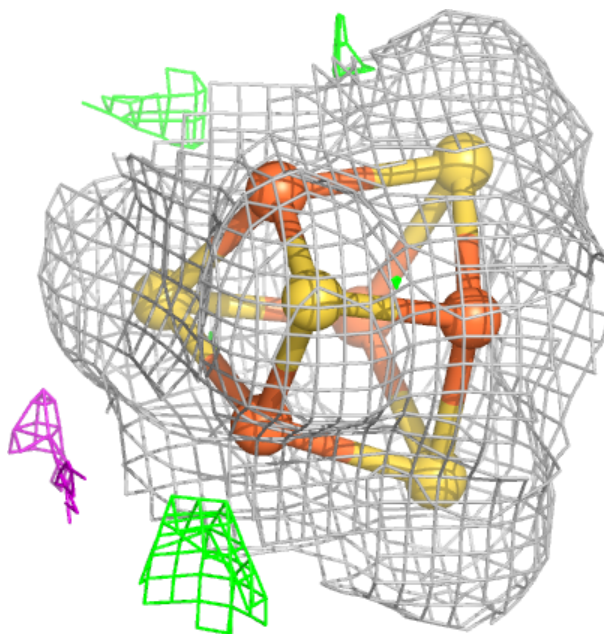
Electron density around ZN G 601:

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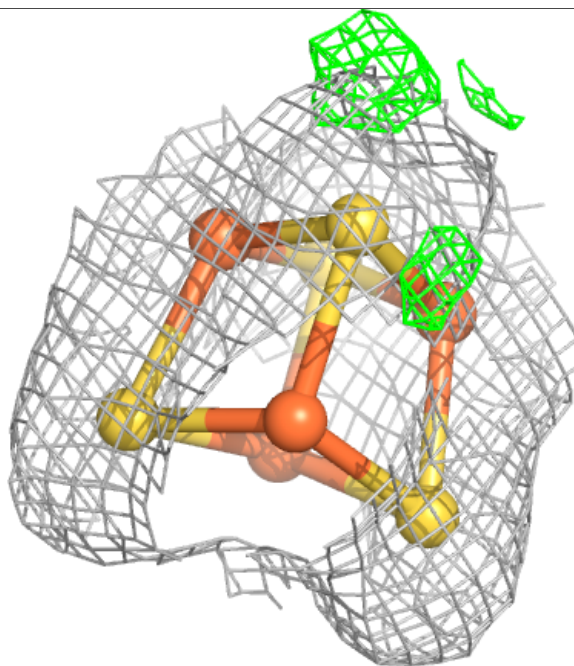
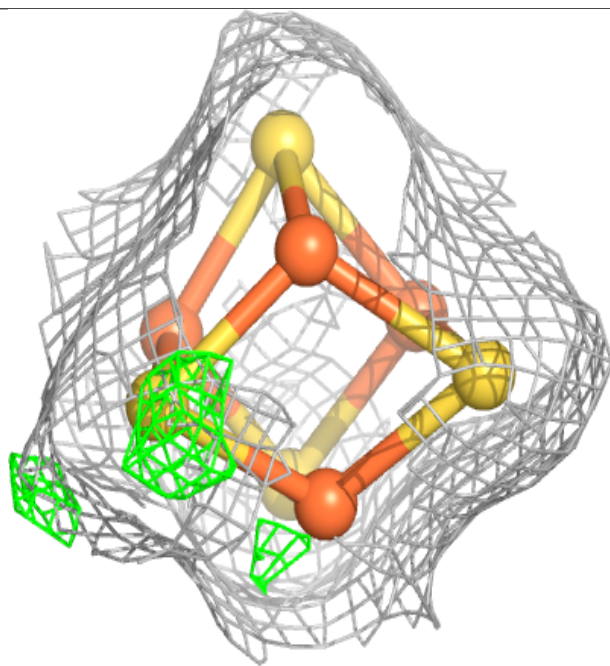
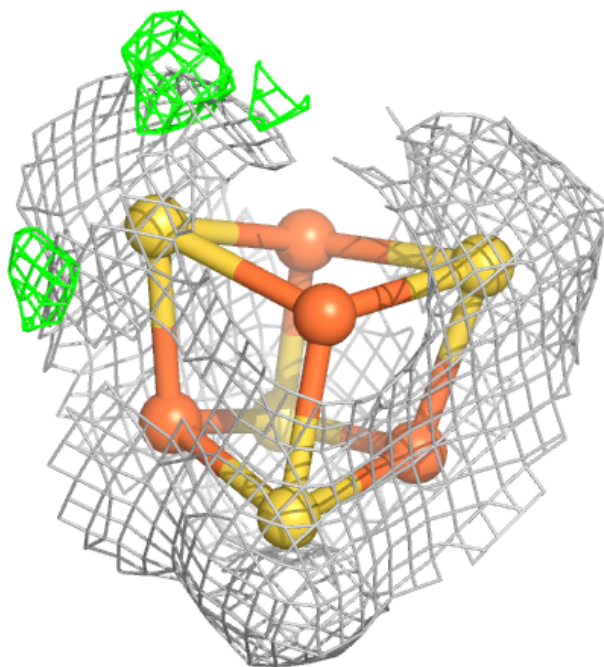
Electron density around SF4 B 501:

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



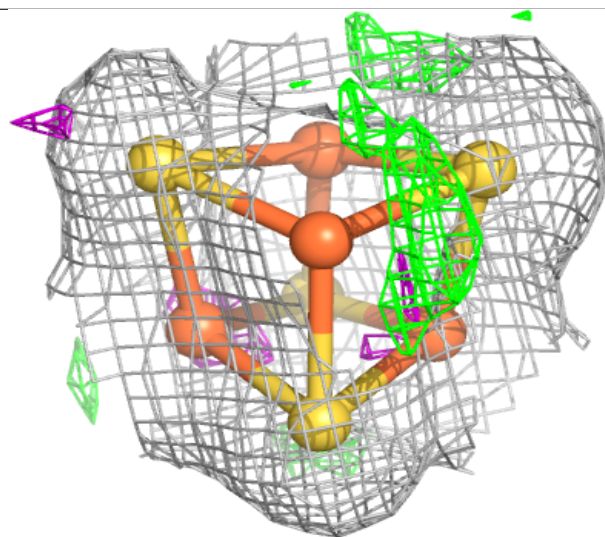
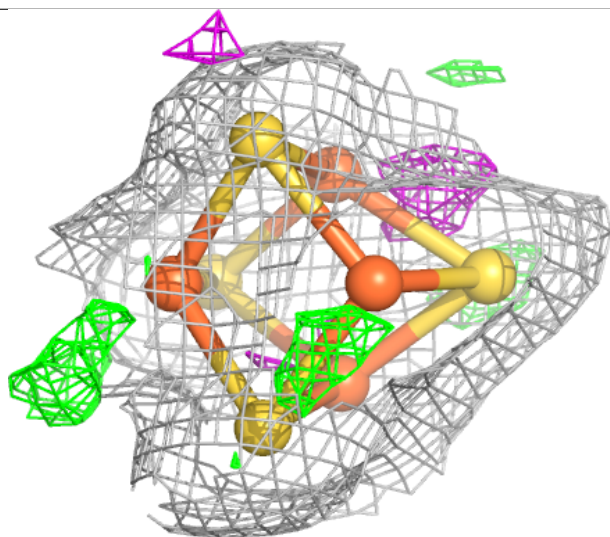
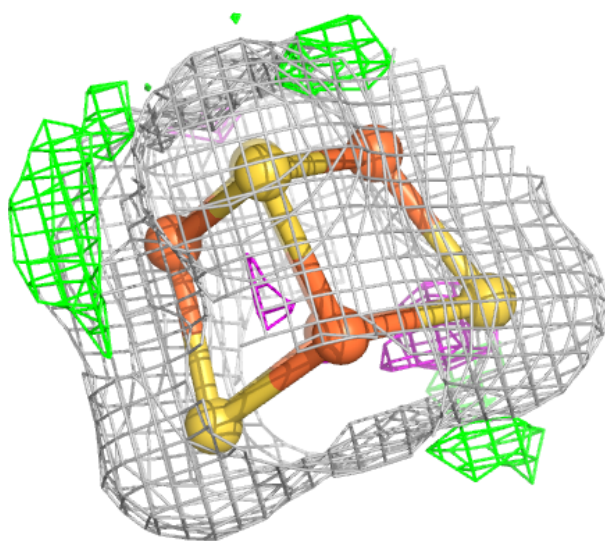
Electron density around SF4 E 1101:

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



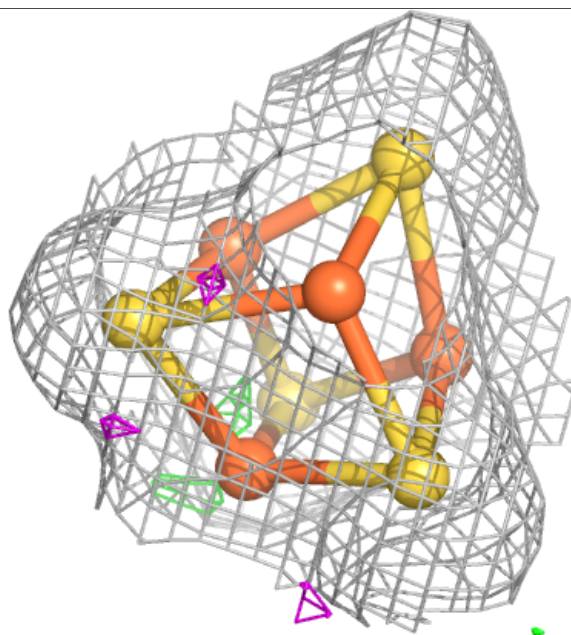
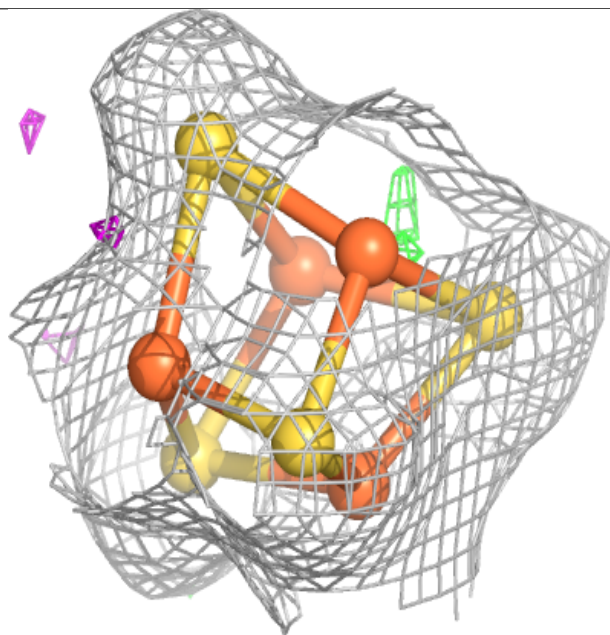
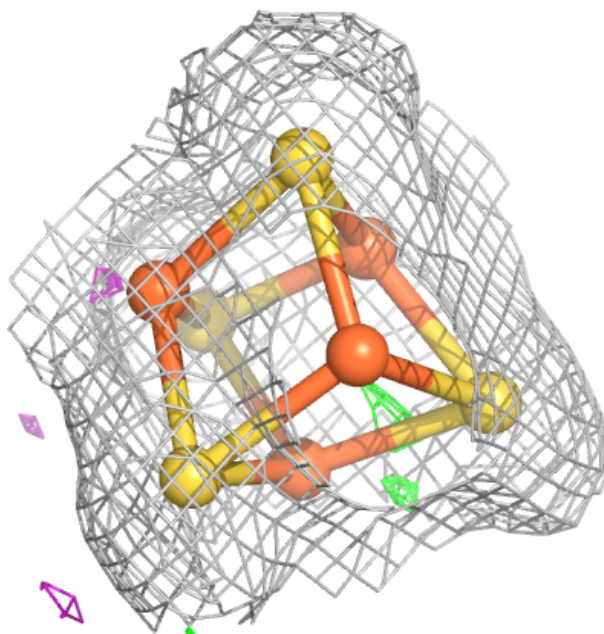
Electron density around SF4 E 1104:

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



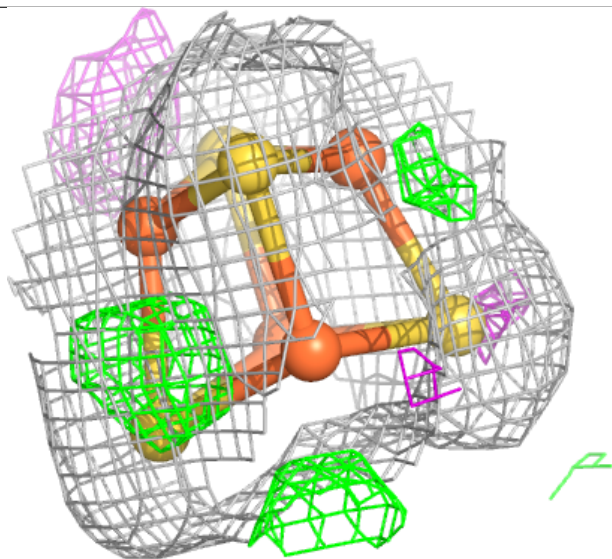
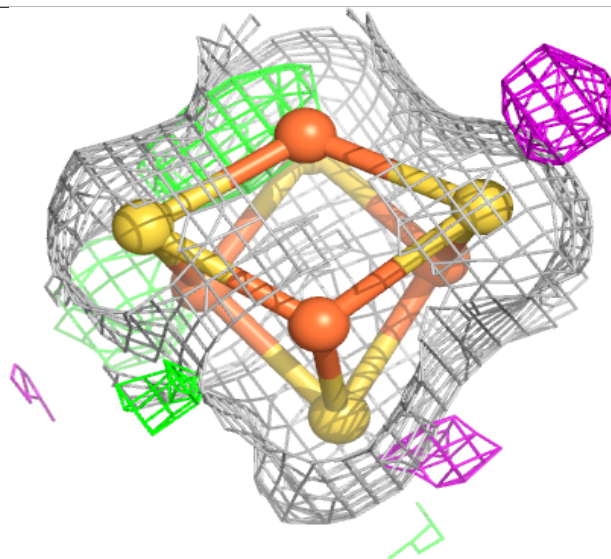
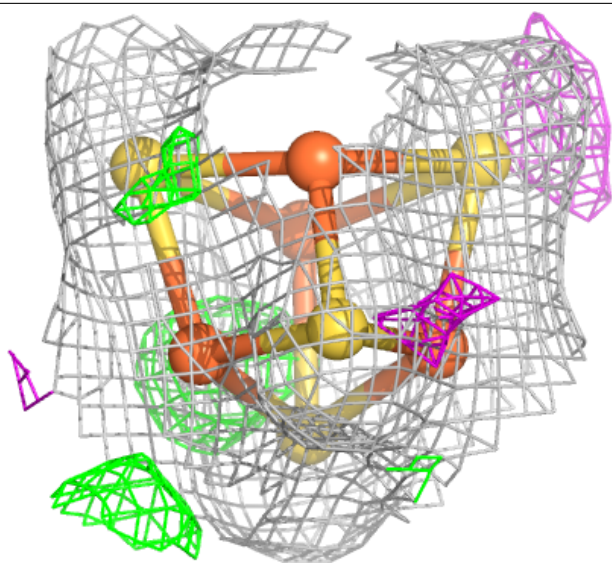
Electron density around SF4 F 101:

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



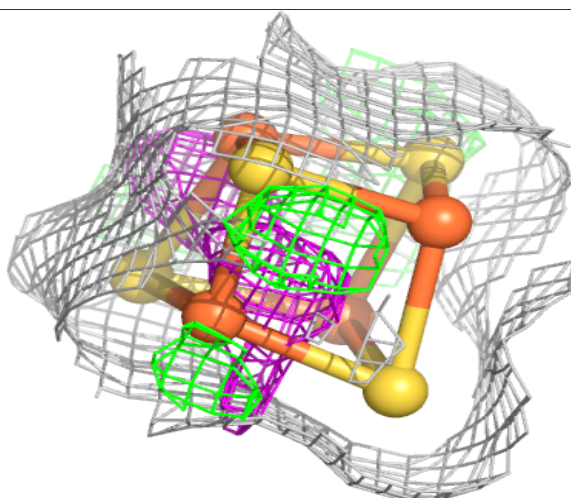
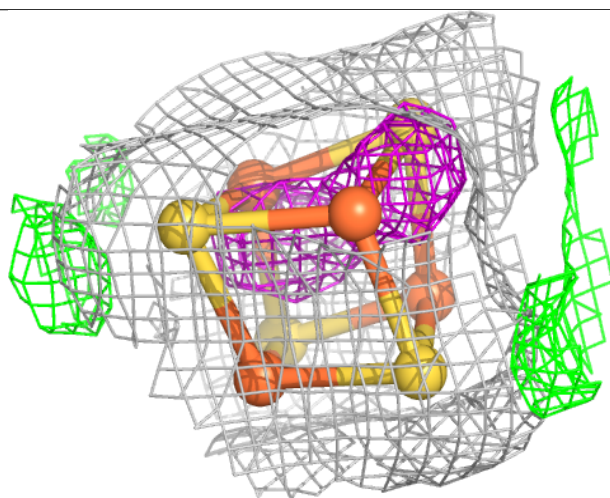
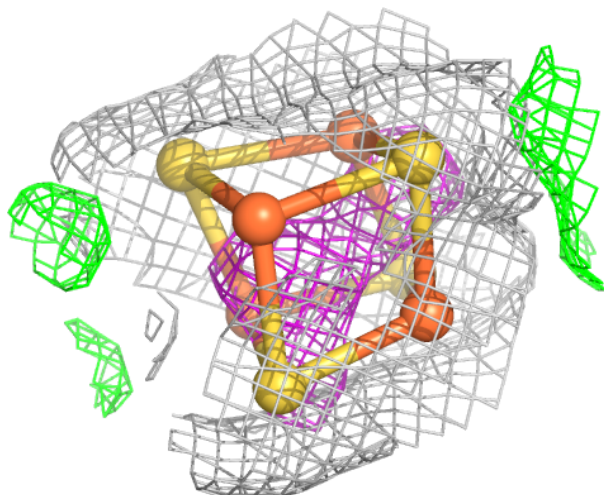
Electron density around SF4 H 501:

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



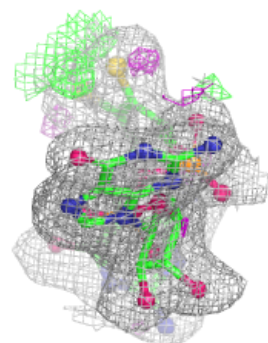
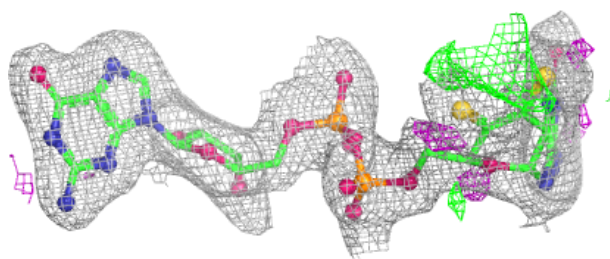
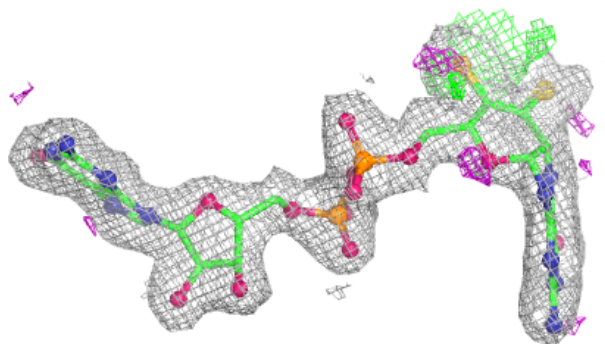
Electron density around SF4 K 1101:

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

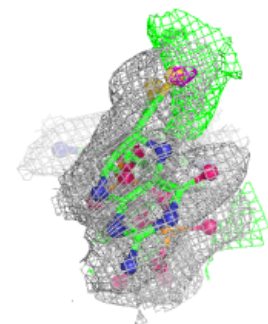
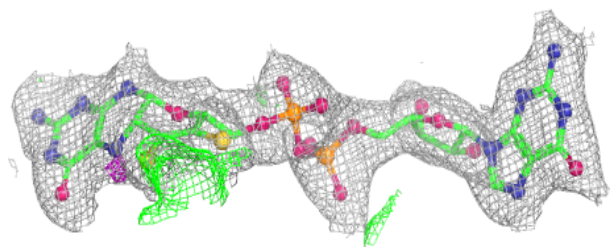
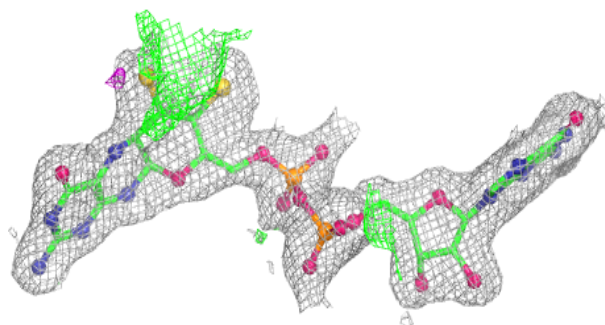


Electron density around MGD B 503:

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

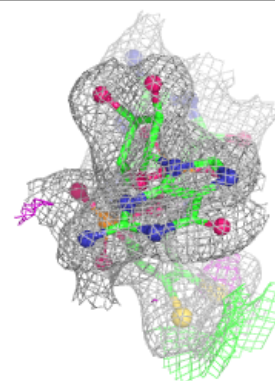
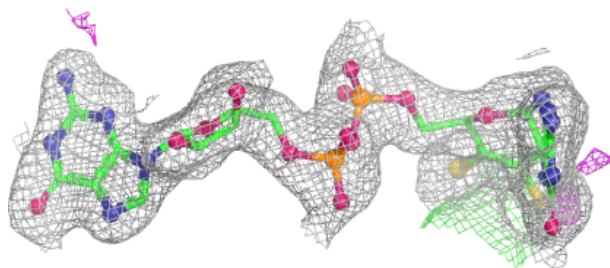
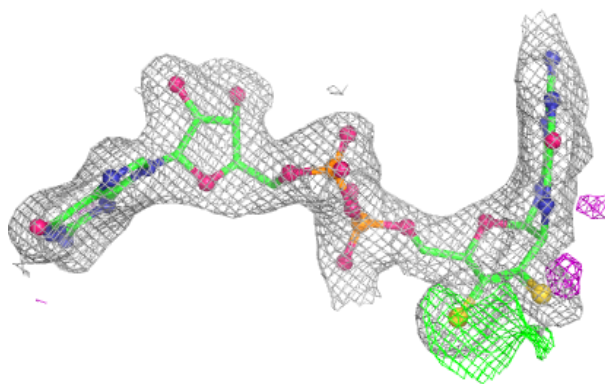
**Electron density around MGD B 504:**

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



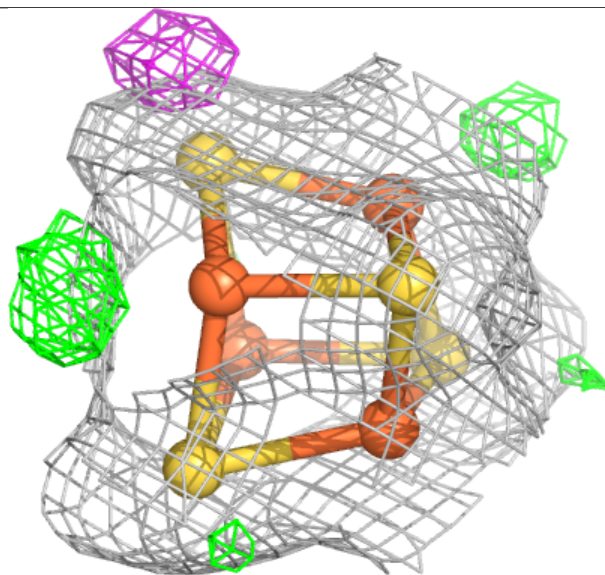
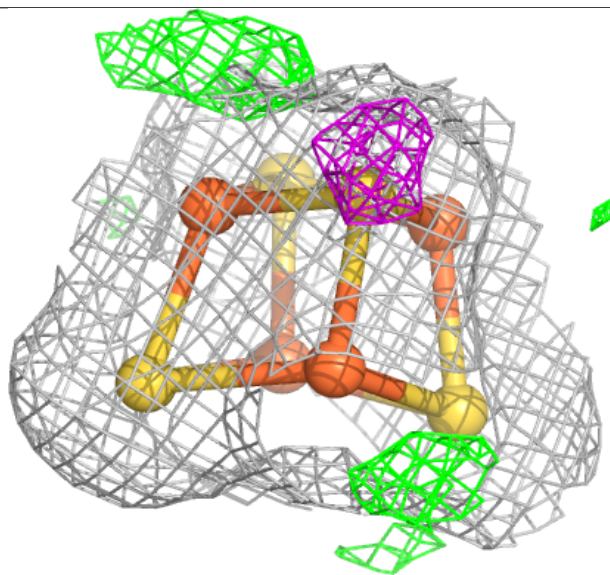
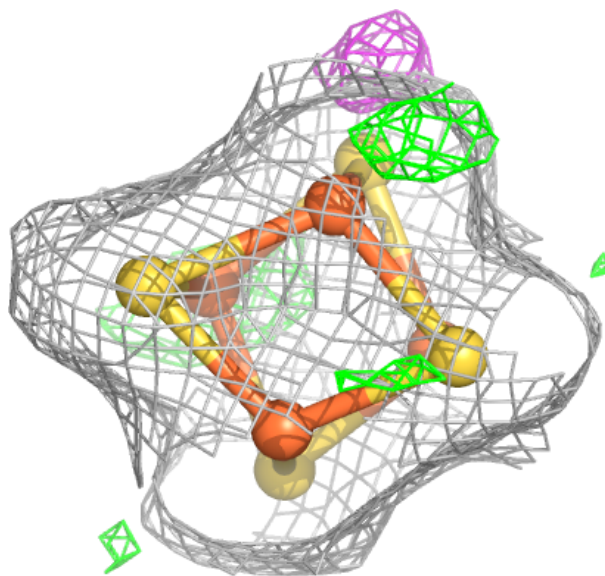
Electron density around MGD H 503:

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



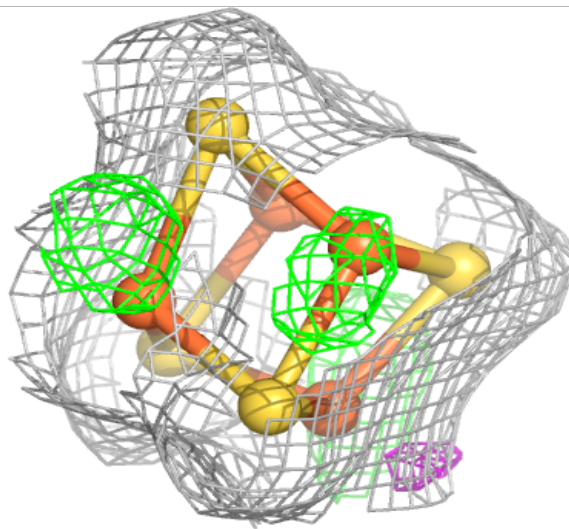
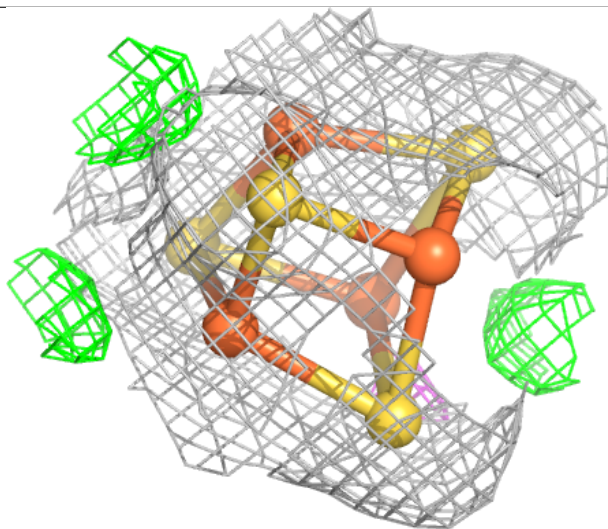
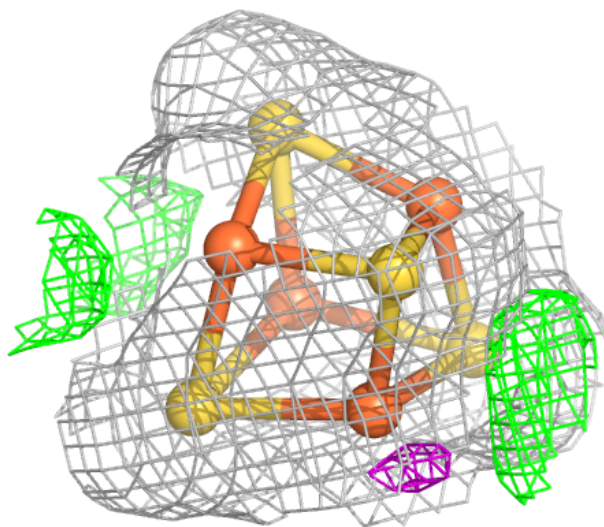
Electron density around SF4 E 1102:

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



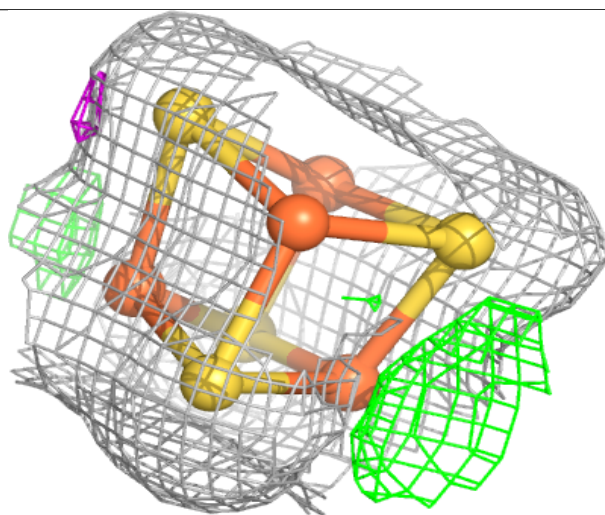
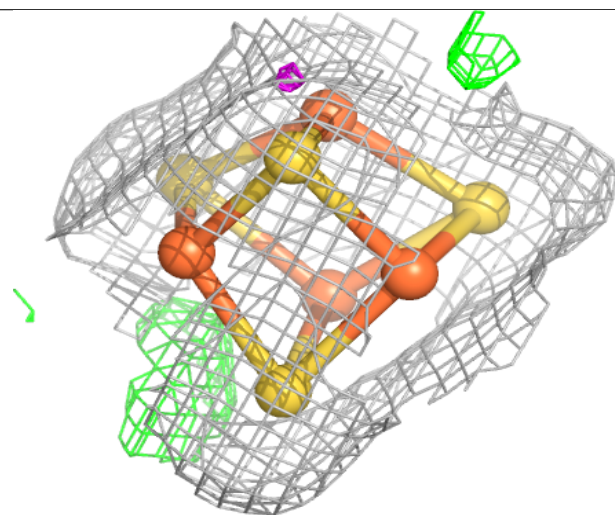
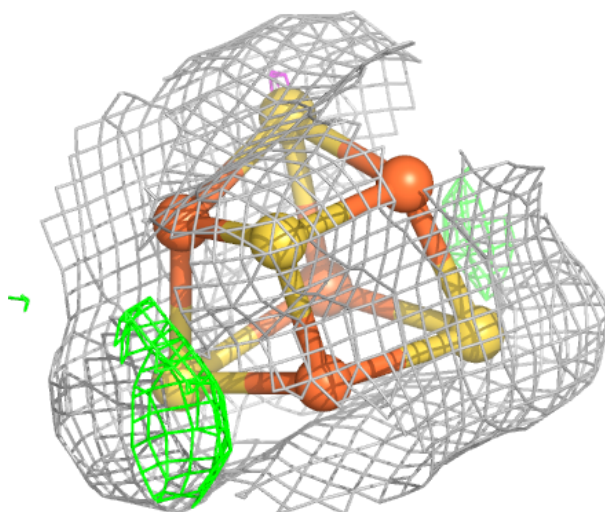
Electron density around SF4 K 1102:

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



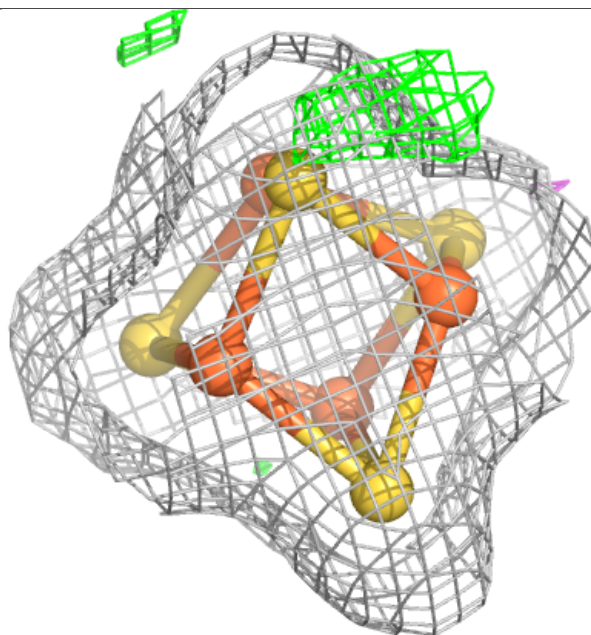
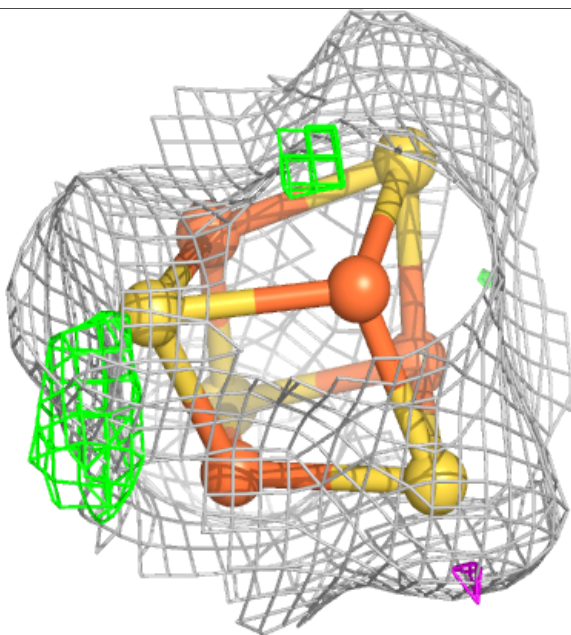
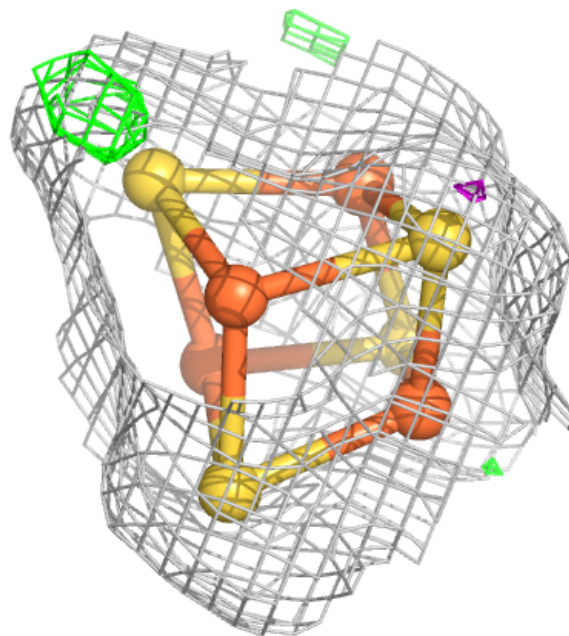
Electron density around SF4 K 1104:

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



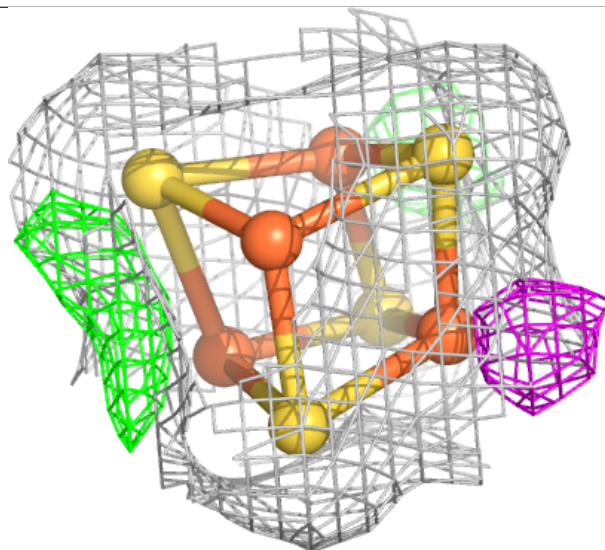
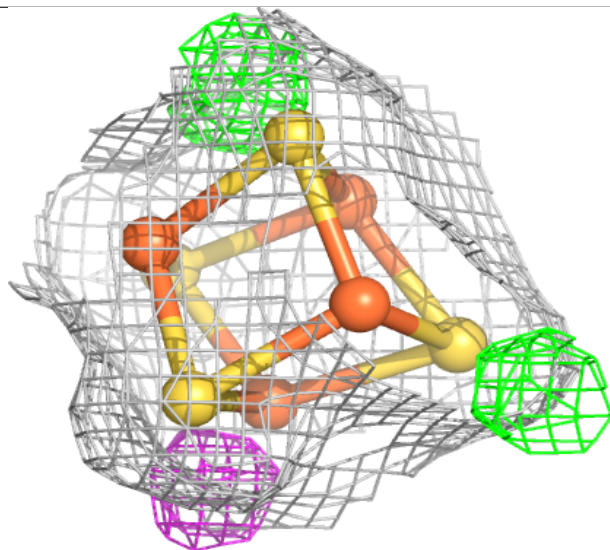
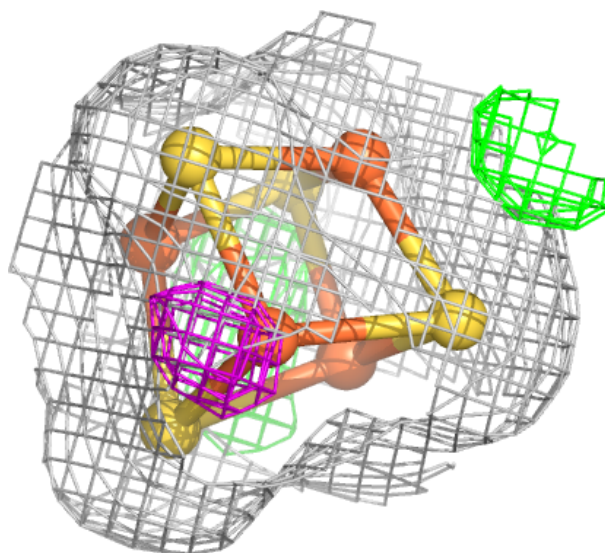
Electron density around SF4 L 101:

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



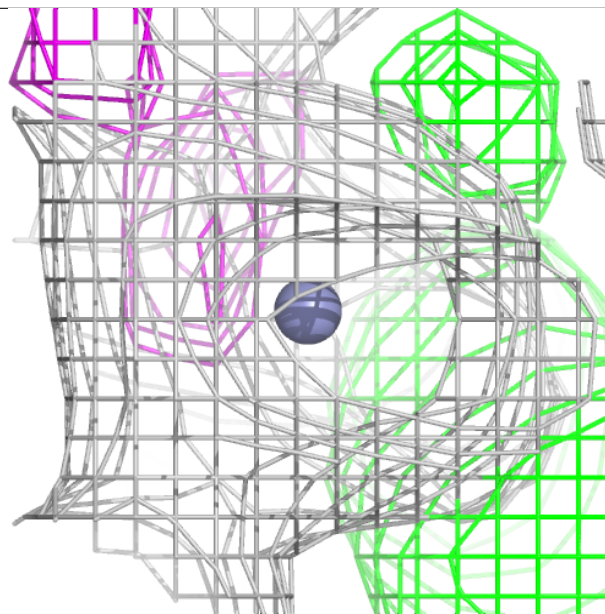
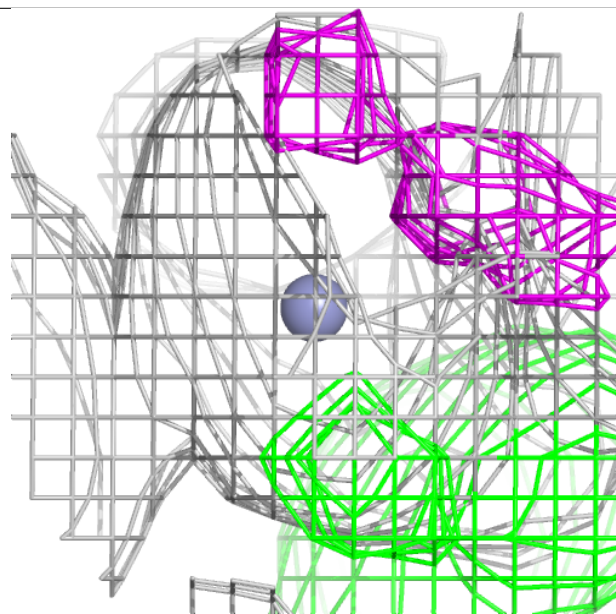
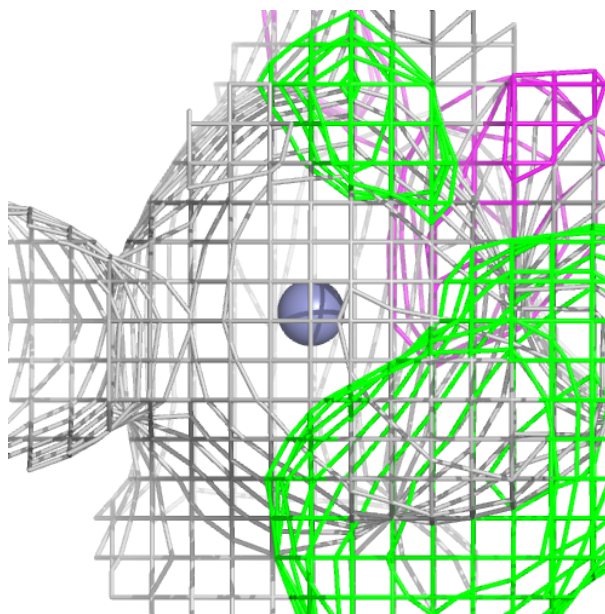
Electron density around SF4 L 102:

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



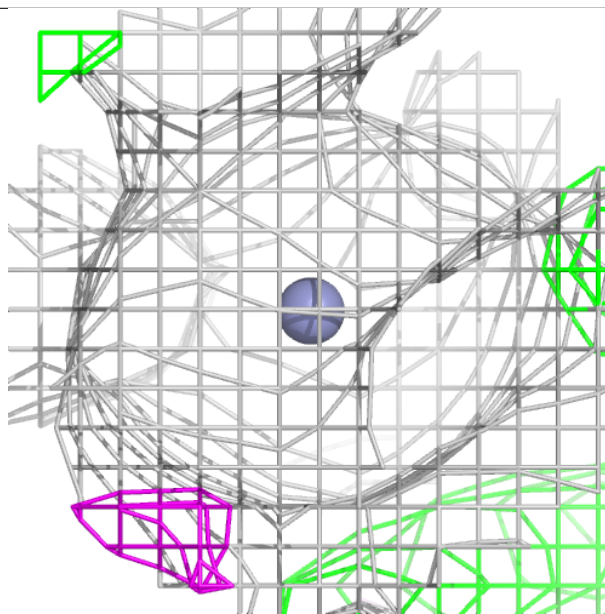
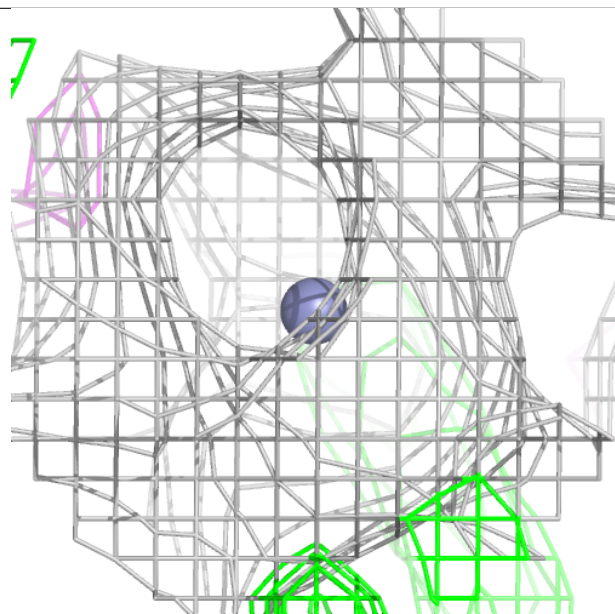
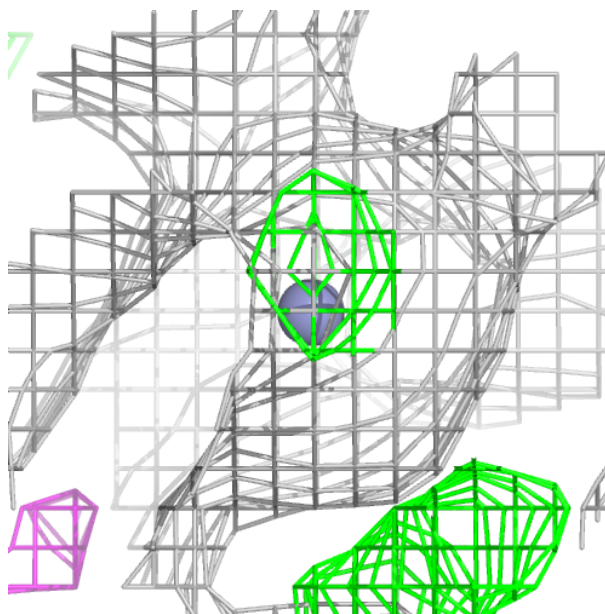
Electron density around ZN G 602:

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



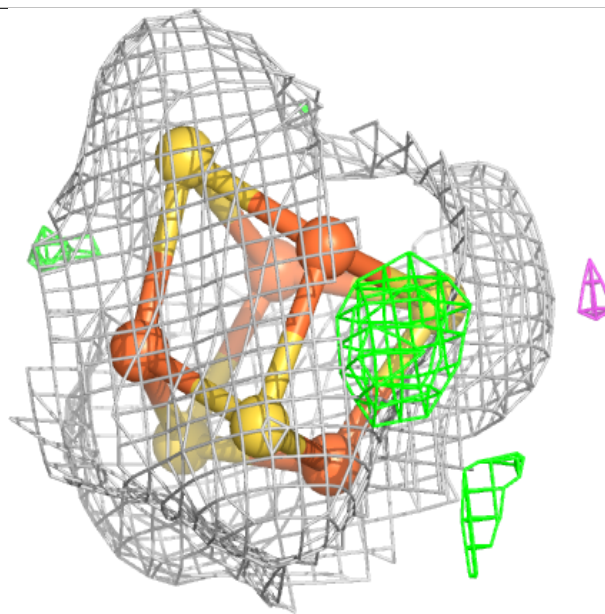
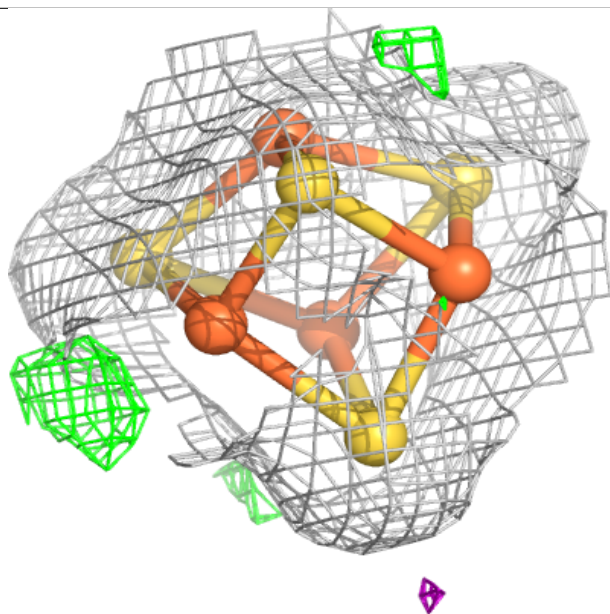
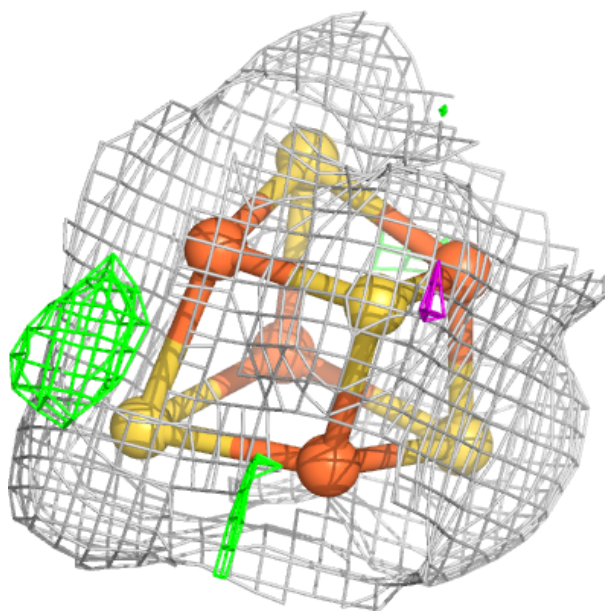
Electron density around ZN A 602:

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



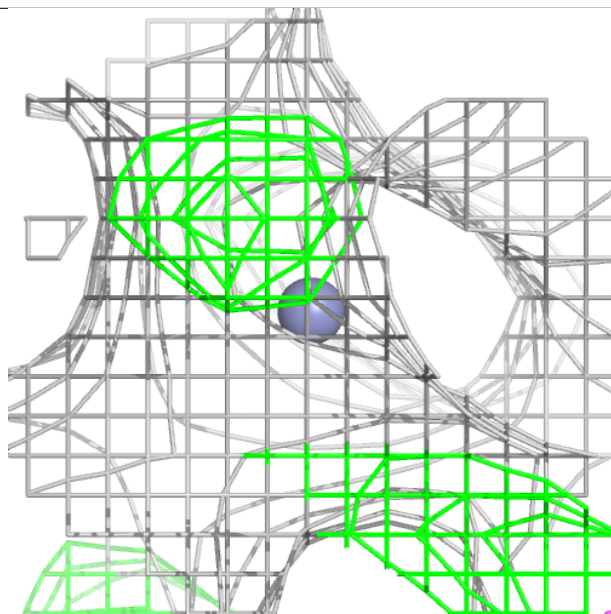
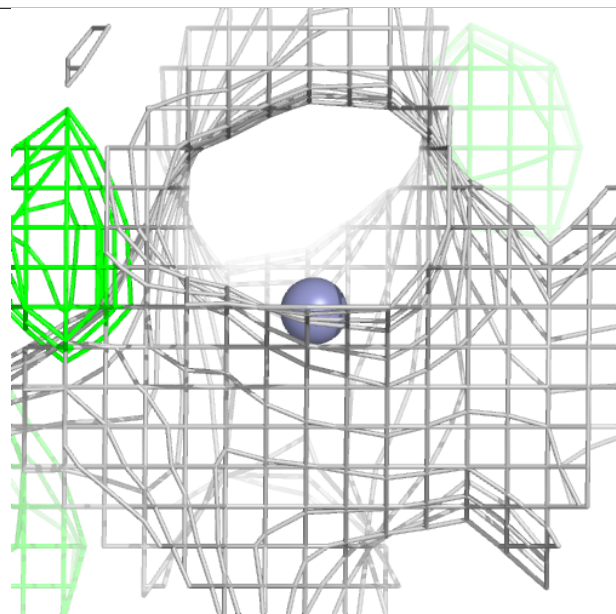
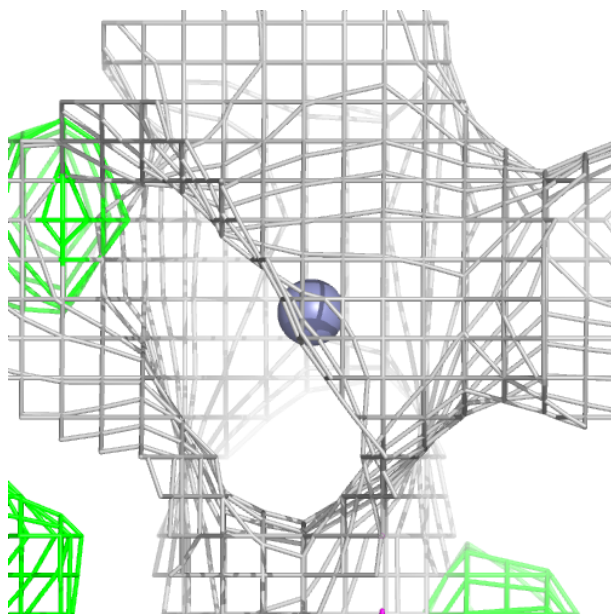
Electron density around SF4 F 102:

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



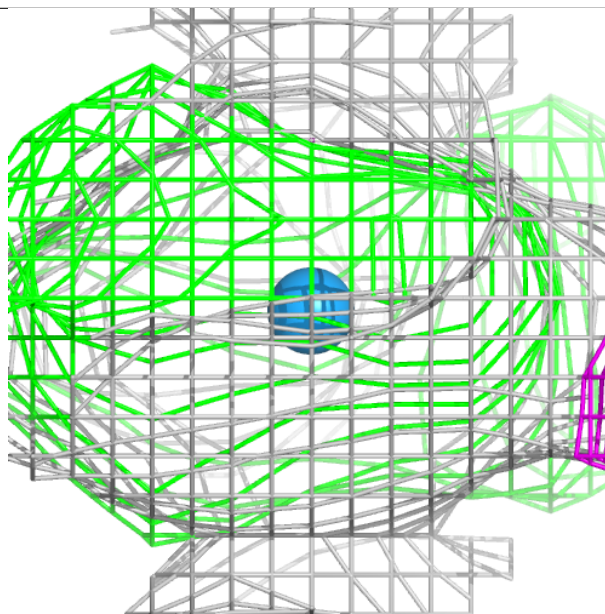
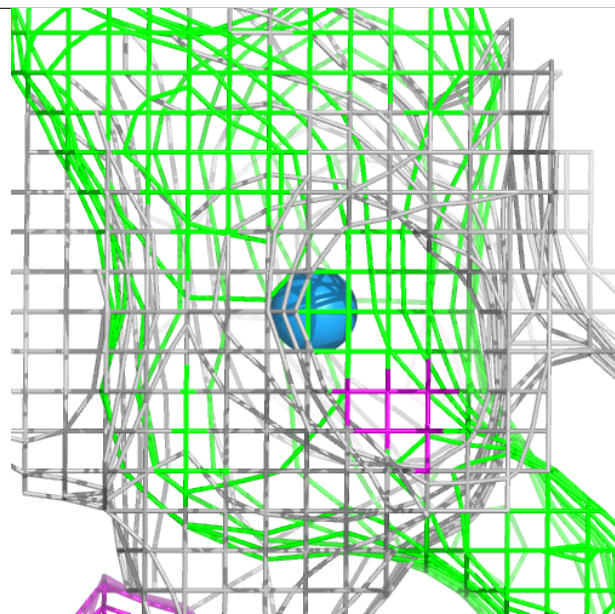
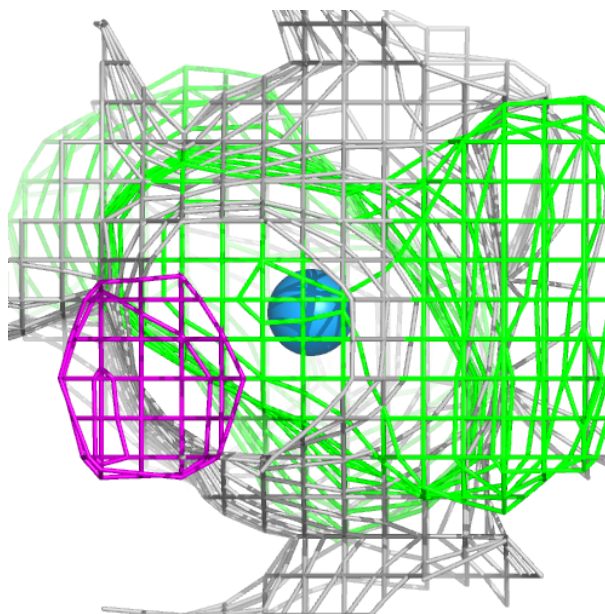
Electron density around ZN A 601:

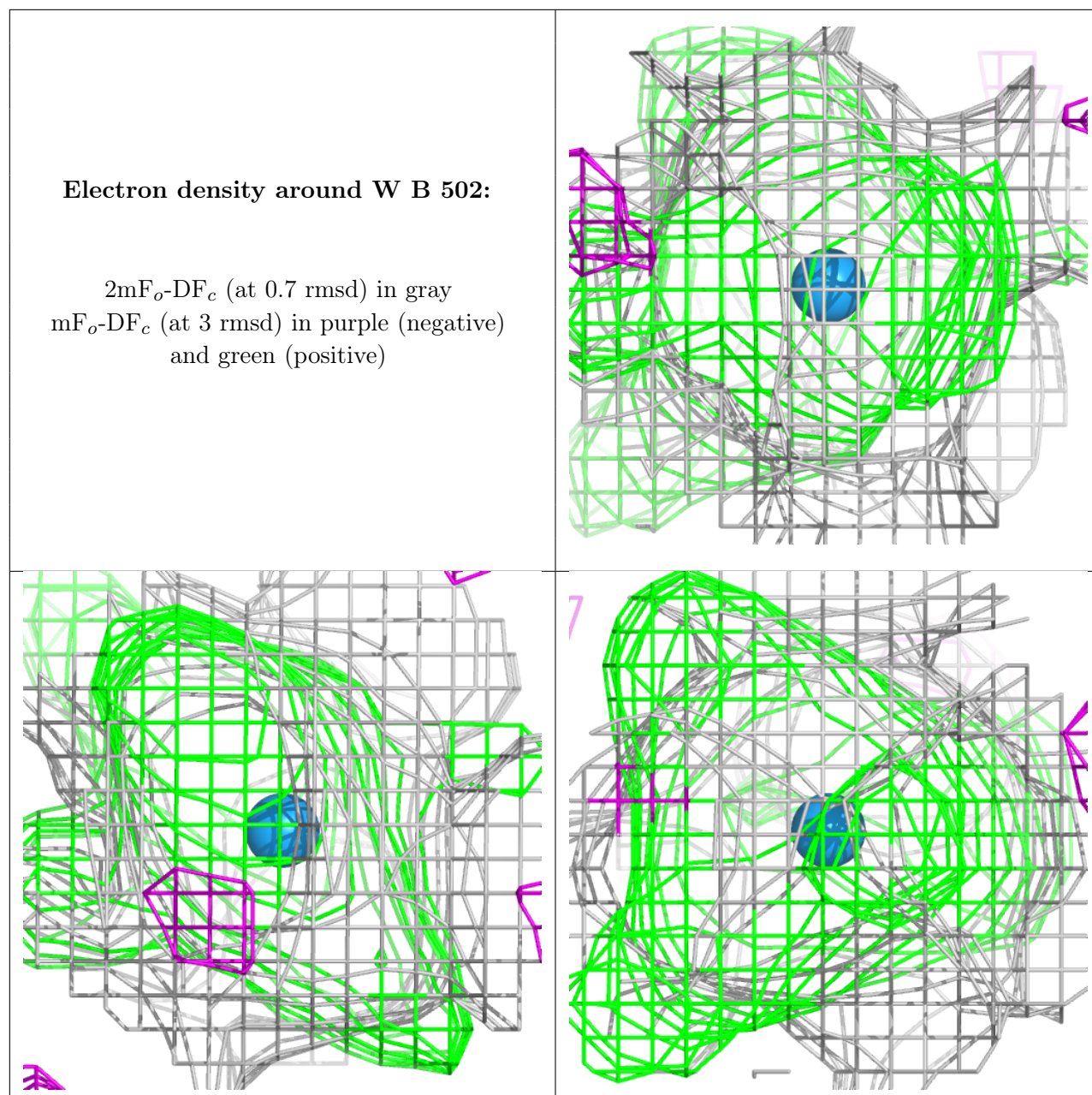
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around W H 502:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.