Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2024 – 07:24 pm BST

PDB ID	:	8RJA
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 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:

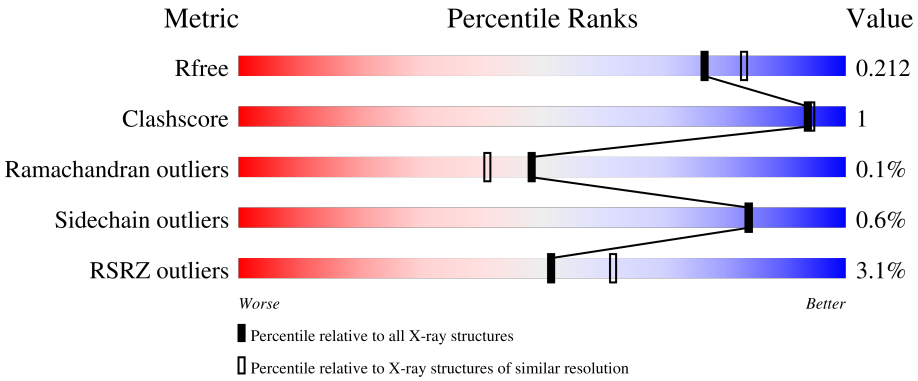
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

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}	164625	1356 (1.98-1.98)
Clashscore	180529	1437 (1.98-1.98)
Ramachandran outliers	177936	1426 (1.98-1.98)
Sidechain outliers	177891	1426 (1.98-1.98)
RSRZ outliers	164620	1356 (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 <=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	96% .
1	G	567	95% 5%
2	B	430	94% 6%
2	H	430	92% 7%
3	C	253	4% 98% .

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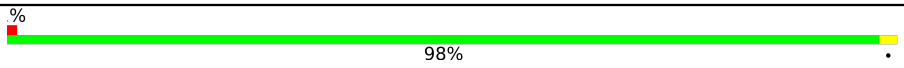
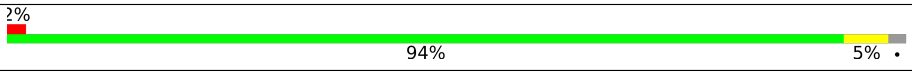
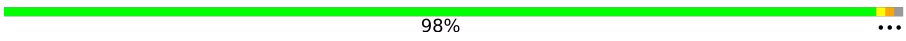
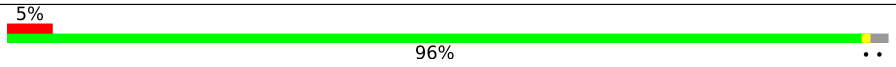
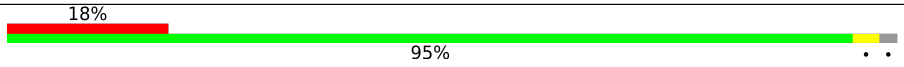
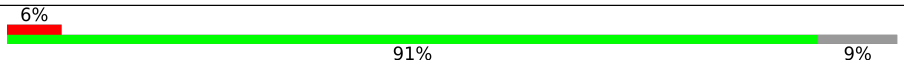
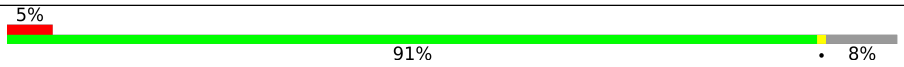
Mol	Chain	Length	Quality of chain
3	I	253	
4	D	126	
4	J	126	
5	E	359	
5	K	359	
6	F	85	
6	L	85	

2 Entry composition (i)

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			

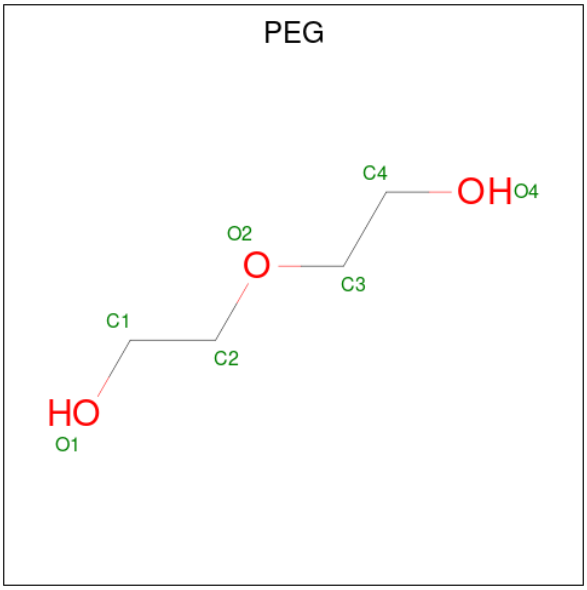
- Molecule 6 is a protein called NAD(P)H-quinone oxidoreductase subunit I, chloroplastic.

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 (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

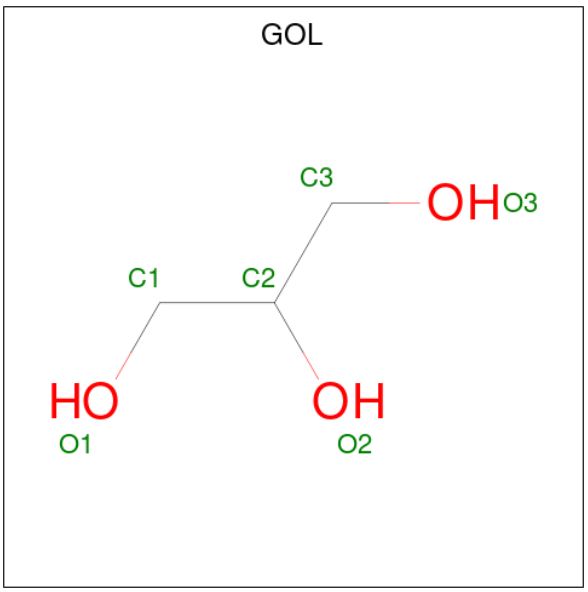
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Zn	0	0
			2	2		
7	G	2	Total	Zn	0	0
			2	2		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



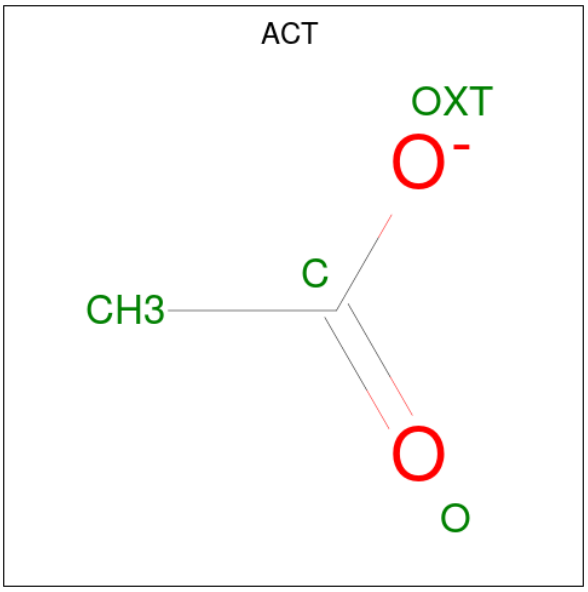
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



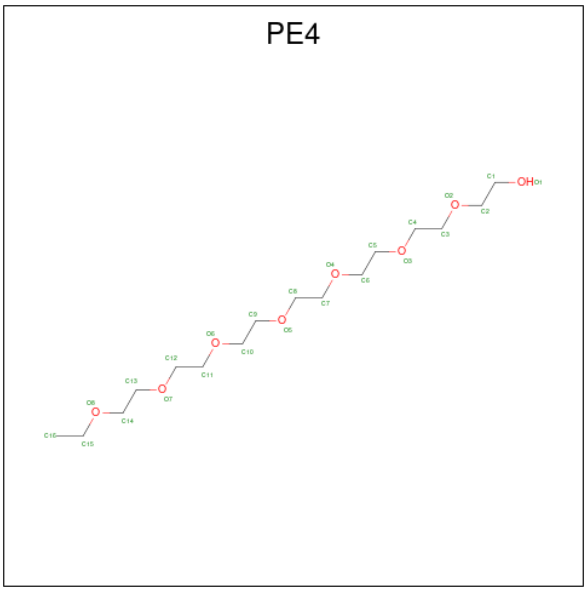
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 6 3 3	0	0
9	E	1	Total C O 6 3 3	0	0
9	H	1	Total C O 6 3 3	0	0
9	H	1	Total C O 6 3 3	0	0
9	H	1	Total C O 6 3 3	0	0
9	I	1	Total C O 6 3 3	0	0
9	I	1	Total C O 6 3 3	0	0

- Molecule 10 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



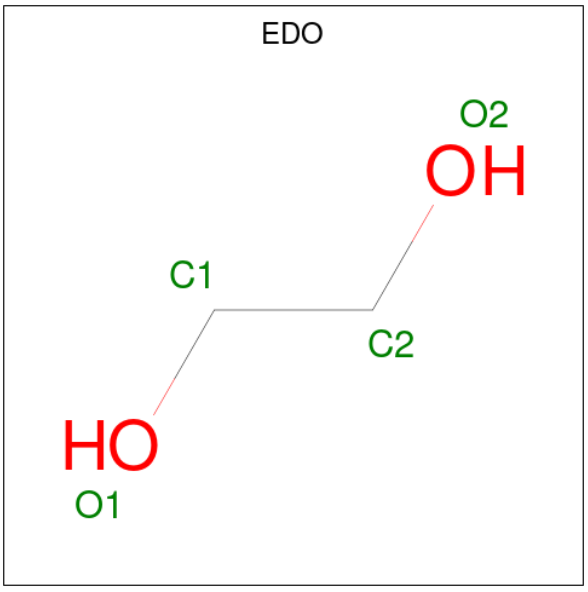
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		
10	H	1	Total	C	O	0	0
			4	2	2		
10	I	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: $C_{16}H_{34}O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 11 7 4	0	0
11	B	1	Total C O 7 4 3	0	0
11	I	1	Total C O 10 6 4	0	0

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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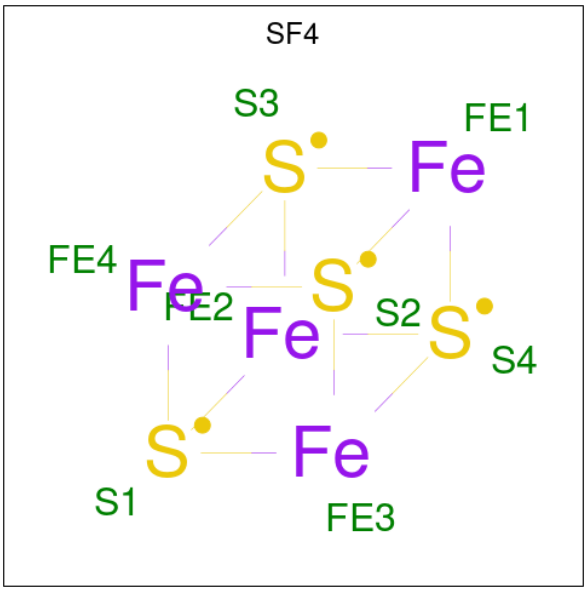
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 4 2 2	0	0
12	B	1	Total C O 4 2 2	0	0
12	E	1	Total C O 4 2 2	0	0
12	E	1	Total C O 4 2 2	0	0
12	E	1	Total C O 4 2 2	0	0
12	E	1	Total C O 4 2 2	0	0
12	G	1	Total C O 4 2 2	0	0
12	G	1	Total C O 4 2 2	0	0
12	G	1	Total C O 4 2 2	0	0
12	G	1	Total C O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

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

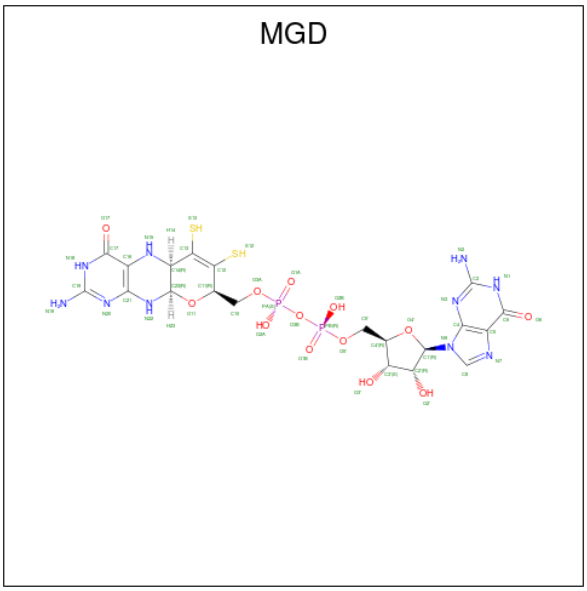


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total Fe S 8 4 4	0	0
14	E	1	Total Fe S 8 4 4	0	0
14	E	1	Total Fe S 8 4 4	0	0
14	E	1	Total Fe S 8 4 4	0	0
14	F	1	Total Fe S 8 4 4	0	0
14	F	1	Total Fe S 8 4 4	0	0
14	H	1	Total Fe S 8 4 4	0	0
14	K	1	Total Fe S 8 4 4	0	0
14	K	1	Total Fe S 8 4 4	0	0
14	K	1	Total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

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

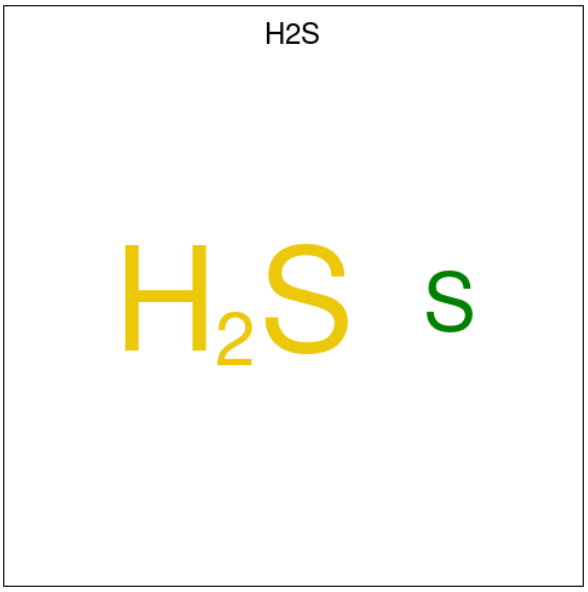
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total W 1 1	0	0
15	H	1	Total W 1 1	0	0

- 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 (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).



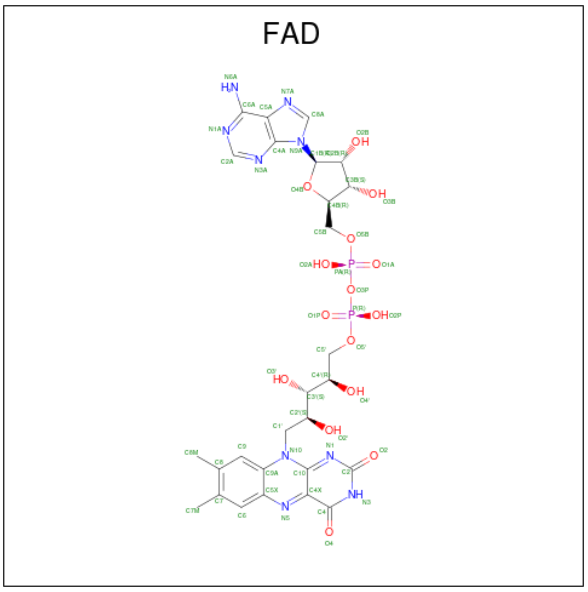
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total C N O P S 47 20 10 13 2 2	0	0
16	B	1	Total C N O P S 47 20 10 13 2 2	0	0
16	H	1	Total C N O P S 47 20 10 13 2 2	0	0
16	H	1	Total C N O P S 47 20 10 13 2 2	0	0

- Molecule 17 is HYDROSULFURIC ACID (three-letter code: 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 (three-letter code: 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 53 27 9 15 2	0	0

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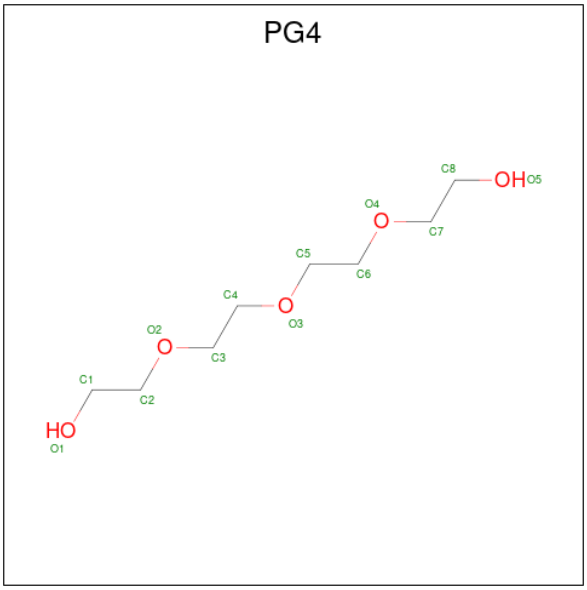
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	K	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 19 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 20 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 21 is water.

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

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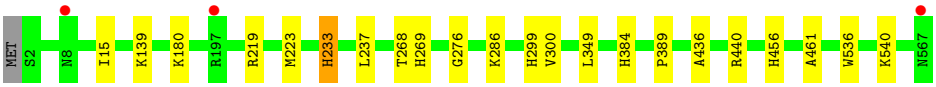
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	278	Total O 278 278	0	0
21	C	146	Total O 146 146	0	0
21	D	68	Total O 68 68	0	0
21	E	195	Total O 195 195	0	0
21	F	62	Total O 62 62	0	0
21	G	415	Total O 415 415	0	0
21	H	255	Total O 255 255	0	1
21	I	211	Total O 211 211	0	0
21	J	86	Total O 86 86	0	0
21	K	102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

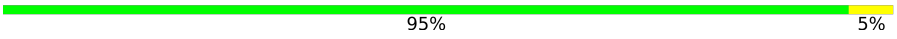
• Molecule 1: Formylmethanofuran dehydrogenase subunit A

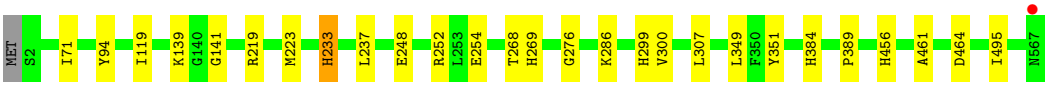
Chain A:



• Molecule 1: Formylmethanofuran dehydrogenase subunit A

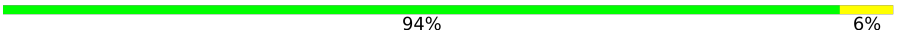
Chain G:

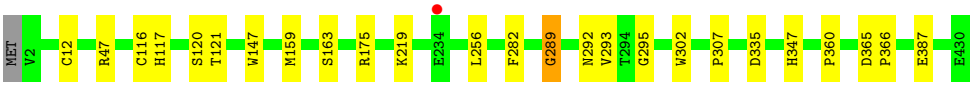




• Molecule 2: Formylmethanofuran dehydrogenase subunit B

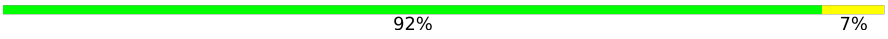
Chain B:

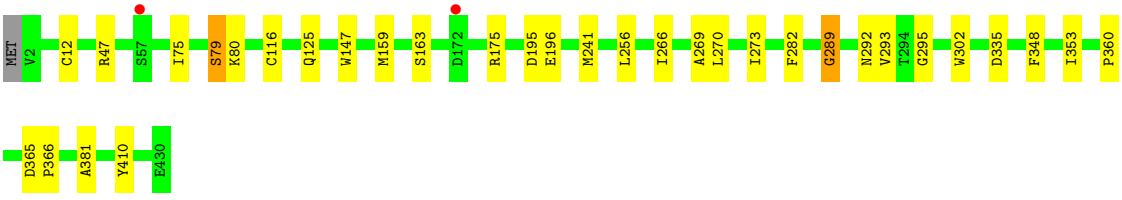




• Molecule 2: Formylmethanofuran dehydrogenase subunit B

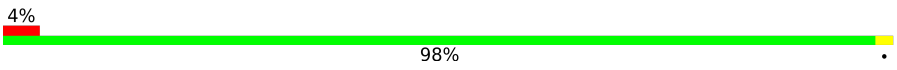
Chain H:

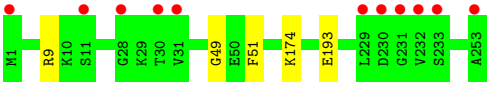




• Molecule 3: formylmethanofuran dehydrogenase

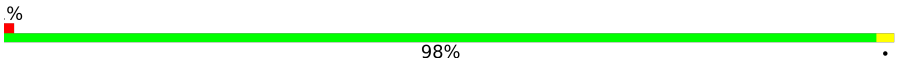
Chain C:

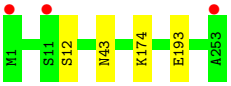




• Molecule 3: formylmethanofuran dehydrogenase

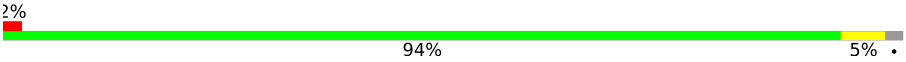
Chain I:

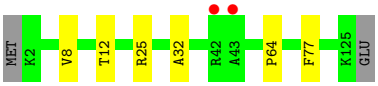




• Molecule 4: Formylmethanofuran dehydrogenase subunit D

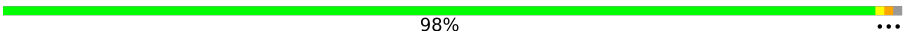
Chain D:

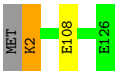




• Molecule 4: Formylmethanofuran dehydrogenase subunit D

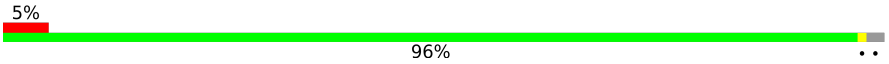
Chain J:

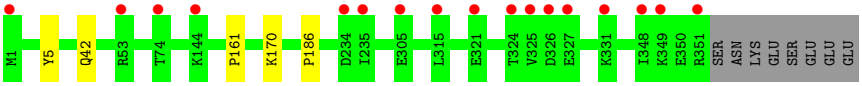




• Molecule 5: Coenzyme F420 hydrogenase/dehydrogenase, beta subunit C terminus

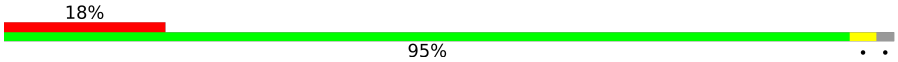
Chain E:

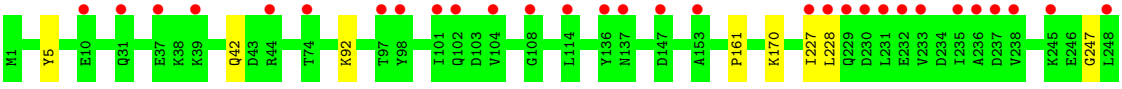


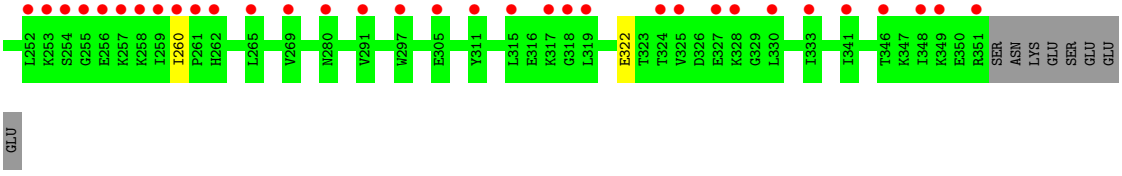


• Molecule 5: Coenzyme F420 hydrogenase/dehydrogenase, beta subunit C terminus

Chain K:

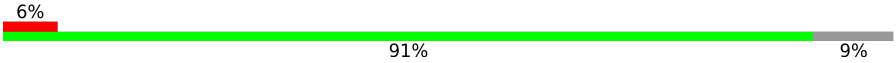


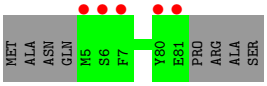




• Molecule 6: NAD(P)H-quinone oxidoreductase subunit I, chloroplastic

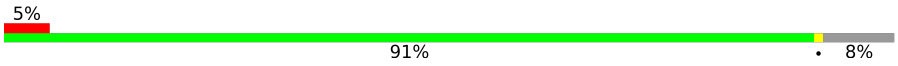
Chain F:

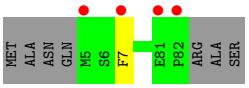




• Molecule 6: NAD(P)H-quinone oxidoreductase subunit I, chloroplastic

Chain L:





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.46 (at 1.97Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.176 , 0.210 0.176 , 0.212	Depositor DCC
R_{free} test set	89745 reflections (4.97%)	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 , 35.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: W, ACT, ZN, PG4, CL, PEG, NA, EDO, GOL, MGD, H2S, PE4, FAD, KCX, 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	0.32	0/4477	0.54	0/6068
1	G	0.32	0/4486	0.55	0/6080
2	B	0.31	0/3336	0.55	0/4515
2	H	0.32	0/3347	0.54	0/4529
3	C	0.29	0/1912	0.53	0/2568
3	I	0.30	0/1912	0.53	0/2568
4	D	0.28	0/945	0.51	0/1283
4	J	0.28	0/954	0.50	0/1295
5	E	0.29	0/2806	0.50	0/3788
5	K	0.30	0/2806	0.48	0/3788
6	F	0.24	0/573	0.48	0/776
6	L	0.26	0/581	0.46	0/788
All	All	0.30	0/28135	0.53	0/38046

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	4396	0	4341	14	0
2	B	3282	0	3306	12	0
2	H	3293	0	3318	18	0
3	C	1888	0	1887	3	0
3	I	1888	0	1887	3	0
4	D	927	0	927	3	0
4	J	936	0	933	1	0
5	E	2763	0	2769	3	0
5	K	2763	0	2769	6	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
18	K	53	0	31	0	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	72	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.

All (72) 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
1:A:456:HIS:CE1	1:A:461:ALA:HB2	2.48	0.49
1:G:456:HIS:CE1	1:G:461:ALA:HB2	2.48	0.49
5:K:170:LYS:HB2	6:L:7:PHE:CE2	2.47	0.48
5:K:227:ILE:HG23	5:K:228:LEU:HD12	1.95	0.48
1:A:384:HIS:ND1	1:A:389:PRO:HA	2.28	0.48
2:H:348:PHE:HB2	2:H:353:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:THR:HG23	1:A:269:HIS:CD2	2.49	0.47
1:G:384:HIS:ND1	1:G:389:PRO:HA	2.30	0.47
1:G:268:THR:HG23	1:G:269:HIS:CD2	2.50	0.47
3:C:174:LYS:HA	3:C:193:GLU:HG3	1.97	0.47
2:B:147:TRP:CD1	2:B:256:LEU:HD21	2.49	0.47
2:H:365:ASP:OD1	2:H:366:PRO:HD2	2.14	0.47
2:B:365:ASP:OD1	2:B:366:PRO:HD2	2.14	0.46
5:E:186:PRO:HD2	14:E:1101:SF4:S2	2.55	0.46
1:G:276:GLY:HA3	1:G:286:LYS:HG2	1.96	0.46
2:B:121:THR:HG21	2:B:307:PRO:HG2	1.98	0.46
2:H:159:MET:HA	2:H:163:SER:OG	2.15	0.46
2:B:159:MET:HA	2:B:163:SER:OG	2.15	0.46
2:H:293:VAL:HG21	17:H:506:H2S:S	2.56	0.46
1:G:71:ILE:O	2:H:125:GLN:HG2	2.15	0.45
1:G:299:HIS:CE1	1:G:300:VAL:HG23	2.52	0.45
1:G:248:GLU:O	1:G:252:ARG:HG3	2.17	0.45
1:A:536:TRP:CZ2	1:A:540:LYS:NZ	2.78	0.45
1:A:299:HIS:CE1	1:A:300:VAL:HG23	2.53	0.44
2:H:75:ILE:O	2:H:79:SER:OG	2.35	0.44
3:I:12:SER:HB3	21:I:803:HOH:O	2.17	0.44
1:A:219:ARG:O	1:A:223:MET:HG3	2.18	0.43
1:A:286:LYS:HD2	1:A:286:LYS:HA	1.65	0.43
1:G:307:LEU:HD11	1:G:351:TYR:CD1	2.54	0.43
4:J:2:LYS:HG3	4:J:108:GLU:HB3	2.01	0.43
1:A:276:GLY:HA3	1:A:286:LYS:HG2	2.01	0.43
4:D:8:VAL:O	4:D:77:PHE:HA	2.19	0.43
5:E:5:TYR:CE2	5:E:42:GLN:HB2	2.54	0.43
2:H:195:ASP:O	2:H:196:GLU:HG3	2.18	0.42
3:I:174:LYS:HA	3:I:193:GLU:HG3	2.00	0.42
1:G:119:ILE:HD11	1:G:141:GLY:HA3	2.01	0.42
1:G:254:GLU:HG2	1:G:299:HIS:CE1	2.55	0.42
2:H:196:GLU:OE1	2:H:241:MET:HE1	2.20	0.42
1:A:233:HIS:CE1	1:A:237:LEU:HD13	2.53	0.42
3:C:9:ARG:HG2	3:C:51:PHE:C	2.40	0.42
2:H:47:ARG:NH1	2:H:410:TYR:CZ	2.87	0.42
3:C:9:ARG:HD3	3:C:49:GLY:O	2.18	0.42
1:G:94:TYR:CZ	1:G:389:PRO:HG2	2.55	0.42
1:G:219:ARG:O	1:G:223:MET:HG3	2.18	0.42
2:H:292:ASN:OD1	2:H:295:GLY:HA3	2.20	0.42
4:D:12:THR:HG23	21:D:259:HOH:O	2.19	0.42
5:K:5:TYR:CE2	5:K:42:GLN:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:289:GLY:HA2	16:H:503:MGD:C12	2.50	0.41
5:K:247:GLY:HA3	5:K:260:ILE:O	2.20	0.41
2:B:289:GLY:HA2	16:B:503:MGD:C12	2.50	0.41
4:D:32:ALA:O	4:D:64:PRO:HD2	2.21	0.41
1:G:464:ASP:HA	1:G:495:ILE:O	2.21	0.41
5:K:92:LYS:HD3	5:K:322:GLU:OE1	2.21	0.41
2:B:117:HIS:O	2:B:120:SER:HB2	2.21	0.41
1:A:436:ALA:O	1:A:440:ARG:HG2	2.21	0.41
2:B:335:ASP:O	2:B:360:PRO:HD2	2.21	0.41
1:G:233:HIS:CE1	1:G:237:LEU:HD13	2.56	0.41
2:H:335:ASP:O	2:H:360:PRO:HD2	2.20	0.41
1:A:15:ILE:CG2	10:A:607:ACT:H2	2.51	0.40
2:B:292:ASN:OD1	2:B:295:GLY:HA3	2.21	0.40
5:E:170:LYS:HE3	21:E:1256:HOH:O	2.21	0.40
2:H:147:TRP:CD1	2:H:256:LEU:HD21	2.56	0.40
2:H:269:ALA:O	2:H:273:ILE:HG12	2.21	0.40
5:K:227:ILE:HG23	5:K:228:LEU:N	2.36	0.40
2:B:347:HIS:HE1	16:B:504:MGD:O1B	2.03	0.40
2:H:266:ILE:O	2:H:270:LEU:HG	2.21	0.40
2:B:47:ARG:NH1	2:B:387:GLU:OE2	2.50	0.40
2:H:47:ARG:NH2	2:H:381:ALA:O	2.55	0.40
2:H:80:LYS:HA	3:I:43:ASN:OD1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	44	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	428/430 (100%)	409 (96%)	18 (4%)	1 (0%)	44 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%)	37 27
5	K	349/359 (97%)	335 (96%)	13 (4%)	1 (0%)	37 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
2	H	289	GLY
5	K	161	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	458/459 (100%)	455 (99%)	3 (1%)	81 82
1	G	459/459 (100%)	456 (99%)	3 (1%)	81 82
2	B	355/356 (100%)	350 (99%)	5 (1%)	62 60
2	H	356/356 (100%)	351 (99%)	5 (1%)	62 60
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%)	102 (99%)	1 (1%)	73 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	J	104/105 (99%)	103 (99%)	1 (1%)	73 72
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%)	2956 (99%)	18 (1%)	84 84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	LYS
1	A	233	HIS
1	A	349	LEU
2	B	12	CYS
2	B	175	ARG
2	B	219	LYS
2	B	282	PHE
2	B	302	TRP
4	D	25	ARG
1	G	139	LYS
1	G	233	HIS
1	G	349	LEU
2	H	12	CYS
2	H	79	SER
2	H	175	ARG
2	H	282	PHE
2	H	302	TRP
4	J	2	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	1,7	9,11,12	0.56	0	5,12,14	0.73	0
1	KCX	A	180	1,7	9,11,12	2.25	1 (11%)	5,12,14	1.80	1 (20%)

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	1,7	-	0/9/10/12	-
1	KCX	A	180	1,7	-	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	6.61	1.33	1.21

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	180	KCX	OQ1-CX-NZ	-4.01	118.75	124.96

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	K	1106	-	3,3,3	0.05	0	2,2,2	0.17	0
12	EDO	G	607	-	3,3,3	0.06	0	2,2,2	0.17	0
14	SF4	K	1104	5	0,12,12	-	-	-		
16	MGD	B	503	15	41,52,52	1.26	4 (9%)	40,81,81	1.48	7 (17%)
18	FAD	E	1103	-	53,58,58	1.30	6 (11%)	68,89,89	1.28	10 (14%)
9	GOL	H	505	-	5,5,5	0.36	0	5,5,5	0.38	0
14	SF4	L	102	6	0,12,12	-	-	-		
9	GOL	A	611	-	5,5,5	0.09	0	5,5,5	0.34	0
18	FAD	K	1103	-	53,58,58	1.28	5 (9%)	68,89,89	1.27	11 (16%)
9	GOL	I	703	-	5,5,5	0.34	0	5,5,5	0.31	0
10	ACT	A	607	-	3,3,3	0.82	0	3,3,3	1.66	1 (33%)
12	EDO	A	610	-	3,3,3	0.06	0	2,2,2	0.21	0
12	EDO	G	606	-	3,3,3	0.07	0	2,2,2	0.18	0
14	SF4	F	102	6	0,12,12	-	-	-		
9	GOL	H	509	-	5,5,5	0.08	0	5,5,5	0.34	0
9	GOL	A	608	-	5,5,5	0.27	0	5,5,5	0.22	0
12	EDO	G	605	-	3,3,3	0.07	0	2,2,2	0.22	0
14	SF4	E	1102	5	0,12,12	-	-	-		
10	ACT	B	506	-	3,3,3	0.79	0	3,3,3	1.62	1 (33%)
14	SF4	K	1102	5	0,12,12	-	-	-		
20	PG4	I	702	-	9,9,12	0.22	0	8,8,11	0.23	0
11	PE4	B	507	-	6,6,23	0.40	0	5,5,22	0.31	0
12	EDO	B	508	-	3,3,3	0.06	0	2,2,2	0.14	0
16	MGD	B	504	15	41,52,52	1.26	4 (9%)	40,81,81	1.48	8 (20%)
12	EDO	E	1107	-	3,3,3	0.06	0	2,2,2	0.14	0
12	EDO	K	1105	-	3,3,3	0.05	0	2,2,2	0.15	0
12	EDO	E	1109	-	3,3,3	0.06	0	2,2,2	0.16	0
14	SF4	H	501	2	0,12,12	-	-	-		
14	SF4	E	1101	5	0,12,12	-	-	-		
12	EDO	H	510	-	3,3,3	0.06	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	SF4	E	1104	5	0,12,12	-	-	-		
16	MGD	H	504	15	41,52,52	1.24	4 (9%)	40,81,81	1.48	7 (17%)
9	GOL	H	508	-	5,5,5	0.31	0	5,5,5	0.27	0
10	ACT	A	605	-	3,3,3	0.89	0	3,3,3	1.54	1 (33%)
10	ACT	H	507	-	3,3,3	1.02	0	3,3,3	0.84	0
12	EDO	G	604	-	3,3,3	0.07	0	2,2,2	0.22	0
14	SF4	B	501	2	0,12,12	-	-	-		
14	SF4	F	101	6	0,12,12	-	-	-		
8	PEG	A	603	-	6,6,6	0.23	0	5,5,5	0.35	0
10	ACT	I	705	-	3,3,3	0.73	0	3,3,3	1.73	1 (33%)
11	PE4	A	606	-	10,10,23	0.46	0	9,9,22	0.46	0
14	SF4	K	1101	5	0,12,12	-	-	-		
12	EDO	E	1108	-	3,3,3	0.05	0	2,2,2	0.17	0
9	GOL	A	604	-	5,5,5	0.28	0	5,5,5	0.09	0
14	SF4	L	101	6	0,12,12	-	-	-		
12	EDO	A	609	-	3,3,3	0.35	0	2,2,2	0.15	0
9	GOL	I	701	-	5,5,5	0.32	0	5,5,5	0.28	0
12	EDO	E	1106	-	3,3,3	0.22	0	2,2,2	0.27	0
9	GOL	E	1105	-	5,5,5	0.25	0	5,5,5	0.12	0
16	MGD	H	503	15	41,52,52	1.27	3 (7%)	40,81,81	1.45	7 (17%)
11	PE4	I	704	-	9,9,23	0.47	0	8,8,22	0.30	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	K	1106	-	-	0/1/1/1	-
12	EDO	G	607	-	-	0/1/1/1	-
14	SF4	K	1104	5	-	-	0/6/5/5
16	MGD	B	503	15	-	2/18/66/66	0/6/6/6
18	FAD	E	1103	-	-	1/30/50/50	0/6/6/6
9	GOL	H	505	-	-	0/4/4/4	-
14	SF4	L	102	6	-	-	0/6/5/5
9	GOL	A	611	-	-	4/4/4/4	-
18	FAD	K	1103	-	-	1/30/50/50	0/6/6/6
9	GOL	I	703	-	-	2/4/4/4	-
12	EDO	A	610	-	-	0/1/1/1	-
12	EDO	G	606	-	-	1/1/1/1	-
14	SF4	F	102	6	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	H	509	-	-	1/4/4/4	-
9	GOL	A	608	-	-	1/4/4/4	-
12	EDO	G	605	-	-	0/1/1/1	-
14	SF4	E	1102	5	-	-	0/6/5/5
14	SF4	K	1102	5	-	-	0/6/5/5
20	PG4	I	702	-	-	1/7/7/10	-
11	PE4	B	507	-	-	2/4/4/21	-
12	EDO	B	508	-	-	0/1/1/1	-
16	MGD	B	504	15	-	7/18/66/66	0/6/6/6
12	EDO	E	1107	-	-	0/1/1/1	-
12	EDO	K	1105	-	-	1/1/1/1	-
12	EDO	E	1109	-	-	0/1/1/1	-
14	SF4	H	501	2	-	-	0/6/5/5
14	SF4	E	1101	5	-	-	0/6/5/5
12	EDO	H	510	-	-	0/1/1/1	-
14	SF4	E	1104	5	-	-	0/6/5/5
16	MGD	H	504	15	-	7/18/66/66	0/6/6/6
9	GOL	H	508	-	-	2/4/4/4	-
12	EDO	G	604	-	-	0/1/1/1	-
14	SF4	B	501	2	-	-	0/6/5/5
14	SF4	F	101	6	-	-	0/6/5/5
8	PEG	A	603	-	-	2/4/4/4	-
11	PE4	A	606	-	-	7/8/8/21	-
14	SF4	K	1101	5	-	-	0/6/5/5
12	EDO	E	1108	-	-	1/1/1/1	-
9	GOL	A	604	-	-	1/4/4/4	-
14	SF4	L	101	6	-	-	0/6/5/5
12	EDO	A	609	-	-	1/1/1/1	-
9	GOL	I	701	-	-	2/4/4/4	-
12	EDO	E	1106	-	-	0/1/1/1	-
9	GOL	E	1105	-	-	2/4/4/4	-
16	MGD	H	503	15	-	2/18/66/66	0/6/6/6
11	PE4	I	704	-	-	4/7/7/21	-

All (26) 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	504	MGD	C16-C21	5.03	1.47	1.38
18	E	1103	FAD	C9A-C5X	4.81	1.49	1.41
18	K	1103	FAD	C9A-C5X	4.79	1.49	1.41
18	E	1103	FAD	C8-C7	3.45	1.49	1.40
18	K	1103	FAD	C8-C7	3.42	1.49	1.40
18	K	1103	FAD	C4-N3	-2.69	1.33	1.38
18	E	1103	FAD	C5A-C4A	2.64	1.47	1.40
18	E	1103	FAD	C4-N3	-2.51	1.34	1.38
18	K	1103	FAD	C5A-C4A	2.48	1.47	1.40
16	H	503	MGD	C16-C17	2.46	1.48	1.42
16	B	503	MGD	C16-C17	2.44	1.48	1.42
18	E	1103	FAD	C4X-N5	2.41	1.35	1.30
16	H	503	MGD	C6-N1	-2.36	1.34	1.37
16	H	504	MGD	C6-N1	-2.35	1.34	1.37
16	B	504	MGD	C17-N18	-2.34	1.34	1.38
16	B	504	MGD	C16-C17	2.29	1.48	1.42
16	B	504	MGD	C6-N1	-2.25	1.34	1.37
16	H	504	MGD	C16-C17	2.25	1.48	1.42
18	K	1103	FAD	C4X-N5	2.19	1.35	1.30
16	H	504	MGD	C17-N18	-2.15	1.34	1.38
16	B	503	MGD	C6-N1	-2.09	1.34	1.37
18	E	1103	FAD	C5X-N5	-2.08	1.35	1.39
16	B	503	MGD	C17-N18	-2.07	1.35	1.38

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	503	MGD	C19-N20-C21	4.42	121.42	113.43
16	H	503	MGD	C19-N20-C21	4.41	121.40	113.43
16	H	504	MGD	C19-N20-C21	4.41	121.38	113.43
16	B	504	MGD	C19-N20-C21	4.24	121.08	113.43
18	E	1103	FAD	N3A-C2A-N1A	-3.43	123.31	128.68
18	K	1103	FAD	N3A-C2A-N1A	-3.29	123.54	128.68
16	B	503	MGD	O17-C17-C16	-3.22	119.86	127.24
16	H	503	MGD	O17-C17-C16	-3.09	120.15	127.24
18	K	1103	FAD	C4X-C10-N1	-2.90	118.01	124.73
18	E	1103	FAD	C4X-C10-N1	-2.86	118.10	124.73
16	H	504	MGD	O17-C17-C16	-2.84	120.72	127.24
16	B	504	MGD	C5-C6-N1	2.79	118.88	113.95
18	K	1103	FAD	C4A-C5A-N7A	-2.76	106.52	109.40
16	B	504	MGD	O17-C17-C16	-2.68	121.10	127.24
16	B	503	MGD	C5-C6-N1	2.63	118.60	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	E	1103	FAD	O4-C4-C4X	-2.63	119.64	126.60
16	B	503	MGD	C8-N7-C5	2.58	107.91	102.99
16	H	503	MGD	C17-C16-N15	2.58	123.68	116.76
16	H	503	MGD	C8-N7-C5	2.57	107.89	102.99
16	B	504	MGD	C8-N7-C5	2.56	107.86	102.99
16	H	504	MGD	C5-C6-N1	2.54	118.44	113.95
18	E	1103	FAD	P-O3P-PA	-2.51	124.21	132.83
16	B	503	MGD	C17-C16-N15	2.51	123.50	116.76
18	K	1103	FAD	C3B-C2B-C1B	2.51	104.75	100.98
16	H	504	MGD	C8-N7-C5	2.50	107.75	102.99
16	H	504	MGD	C17-C16-N15	2.48	123.42	116.76
18	E	1103	FAD	C3B-C2B-C1B	2.45	104.67	100.98
18	K	1103	FAD	P-O3P-PA	-2.44	124.45	132.83
16	H	503	MGD	C5-C6-N1	2.44	118.26	113.95
18	K	1103	FAD	O4-C4-C4X	-2.43	120.14	126.60
18	E	1103	FAD	C4A-C5A-N7A	-2.43	106.87	109.40
18	E	1103	FAD	C4X-C4-N3	2.38	119.25	113.19
16	H	504	MGD	PA-O3B-PB	-2.38	124.67	132.83
16	B	504	MGD	PA-O3B-PB	-2.36	124.74	132.83
16	B	504	MGD	C17-C16-N15	2.35	123.08	116.76
18	E	1103	FAD	C10-N1-C2	2.35	121.60	116.90
18	E	1103	FAD	C4-C4X-N5	2.30	121.51	118.23
10	I	705	ACT	OXT-C-O	2.27	130.43	122.05
18	K	1103	FAD	C4-N3-C2	-2.24	121.50	125.64
18	K	1103	FAD	C4X-C4-N3	2.22	118.83	113.19
10	A	607	ACT	OXT-C-O	2.21	130.18	122.05
16	B	504	MGD	O6-C6-C5	-2.18	120.11	124.37
18	E	1103	FAD	C4-N3-C2	-2.16	121.64	125.64
16	H	504	MGD	O11-C23-C14	-2.12	107.55	108.96
16	B	504	MGD	O11-C23-C14	-2.12	107.55	108.96
10	B	506	ACT	OXT-C-O	2.11	129.83	122.05
18	K	1103	FAD	N3-C2-N1	2.10	123.51	119.38
18	K	1103	FAD	C10-N1-C2	2.10	121.10	116.90
16	H	503	MGD	C16-C17-N18	2.10	118.56	112.31
18	K	1103	FAD	C4-C4X-N5	2.06	121.17	118.23
16	B	503	MGD	C16-C17-N18	2.06	118.44	112.31
10	A	605	ACT	OXT-C-O	2.05	129.60	122.05
16	H	503	MGD	O6-C6-C5	-2.01	120.44	124.37
16	B	503	MGD	O6-C6-C5	-2.01	120.45	124.37

There are no chirality outliers.

All (55) 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
16	B	504	MGD	O3A-C10-C11-C12
16	H	504	MGD	C5'-O5'-PB-O2B
16	H	504	MGD	O3A-C10-C11-C12
11	A	606	PE4	O2-C3-C4-O3
11	A	606	PE4	O1-C1-C2-O2
11	I	704	PE4	O4-C7-C8-O5
11	I	704	PE4	O6-C11-C12-O7
9	E	1105	GOL	O1-C1-C2-C3
9	I	701	GOL	C1-C2-C3-O3
11	A	606	PE4	O3-C5-C6-O4
9	I	703	GOL	O2-C2-C3-O3
12	E	1108	EDO	O1-C1-C2-O2
11	B	507	PE4	O2-C3-C4-O3
9	A	611	GOL	O2-C2-C3-O3
12	K	1105	EDO	O1-C1-C2-O2
9	I	701	GOL	O2-C2-C3-O3
16	B	504	MGD	PA-O3B-PB-O5'
16	H	504	MGD	PA-O3B-PB-O5'
11	A	606	PE4	C1-C2-O2-C3
8	A	603	PEG	C4-C3-O2-C2
16	B	504	MGD	C5'-O5'-PB-O3B
16	H	504	MGD	C5'-O5'-PB-O3B
16	B	503	MGD	PB-O3B-PA-O1A
16	H	503	MGD	PB-O3B-PA-O1A
11	I	704	PE4	C10-C9-O5-C8
8	A	603	PEG	O2-C3-C4-O4
20	I	702	PG4	C3-C4-O3-C5
9	H	508	GOL	O1-C1-C2-O2
11	B	507	PE4	O1-C1-C2-O2
11	A	606	PE4	C3-C4-O3-C5
12	A	609	EDO	O1-C1-C2-O2
11	A	606	PE4	C6-C5-O3-C4
11	A	606	PE4	C4-C3-O2-C2
16	B	504	MGD	O3A-C10-C11-O11
16	H	504	MGD	O3A-C10-C11-O11
16	H	504	MGD	O4'-C4'-C5'-O5'
9	A	611	GOL	O1-C1-C2-O2
9	E	1105	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
16	B	504	MGD	O4'-C4'-C5'-O5'
12	G	606	EDO	O1-C1-C2-O2
9	H	509	GOL	O2-C2-C3-O3
16	B	503	MGD	PB-O3B-PA-O2A
16	H	503	MGD	PB-O3B-PA-O2A
9	A	604	GOL	C1-C2-C3-O3
9	A	608	GOL	O1-C1-C2-C3
11	I	704	PE4	O6-C10-C9-O5
16	B	504	MGD	C5'-O5'-PB-O1B
16	H	504	MGD	C5'-O5'-PB-O1B
18	E	1103	FAD	O4B-C4B-C5B-O5B
18	K	1103	FAD	O4B-C4B-C5B-O5B

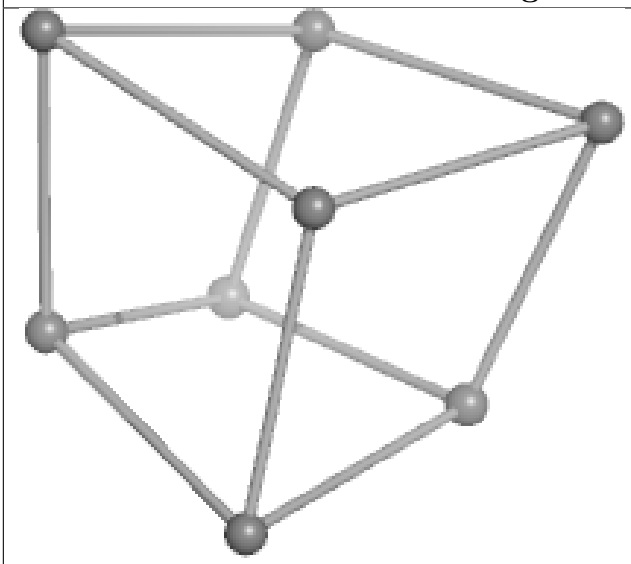
There are no ring outliers.

6 monomers are involved in 7 short contacts:

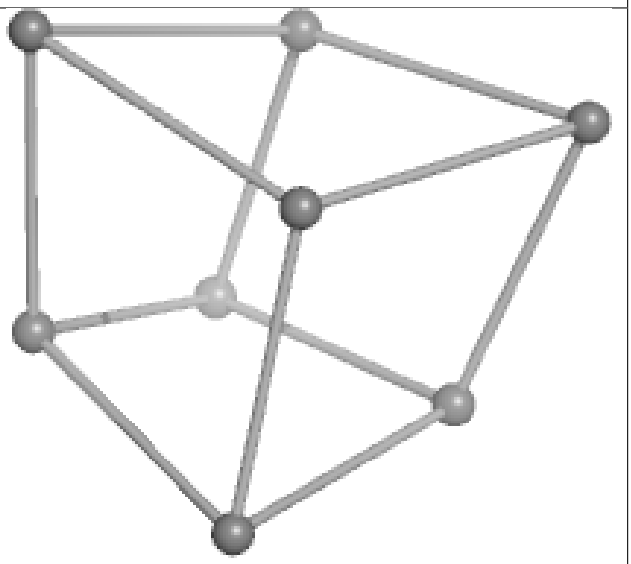
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	503	MGD	1	0
10	A	607	ACT	1	0
16	B	504	MGD	2	0
14	E	1101	SF4	1	0
16	H	504	MGD	1	0
16	H	503	MGD	1	0

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 then 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.

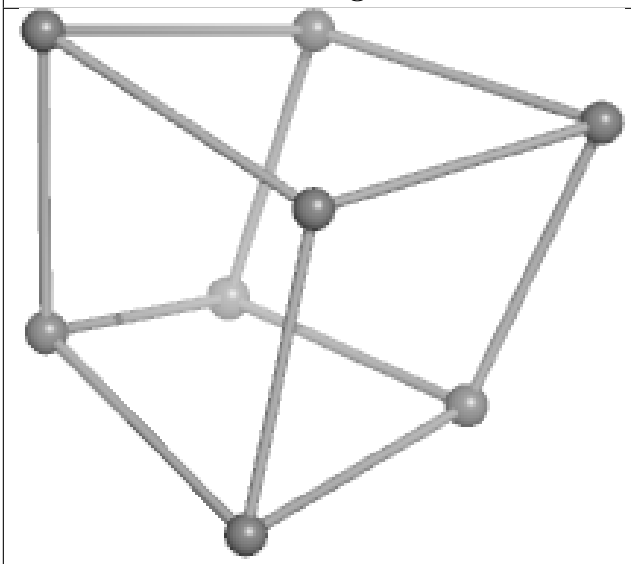
Ligand SF4 K 1104



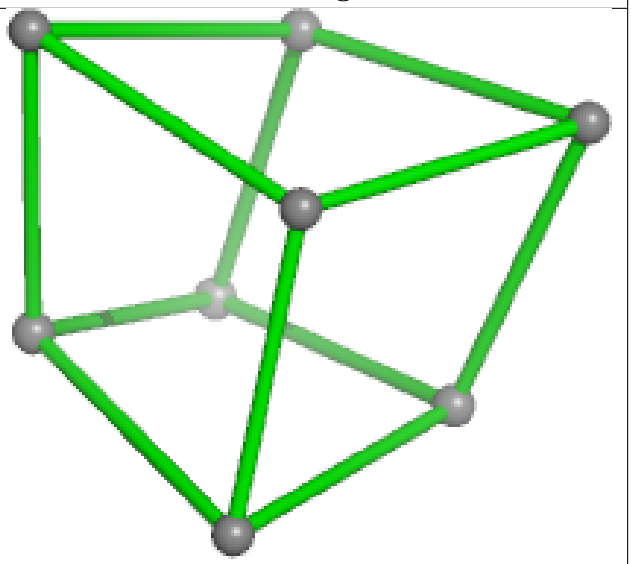
Bond lengths



Bond angles

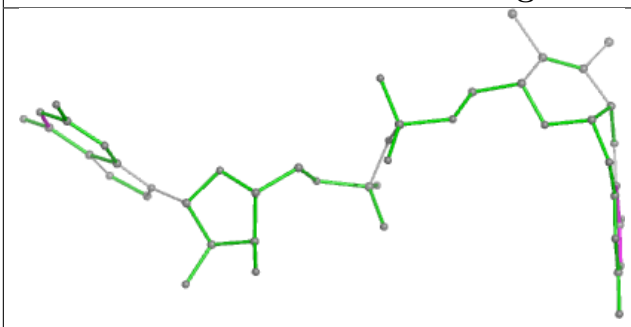


Torsions



Rings

Ligand MGD B 503



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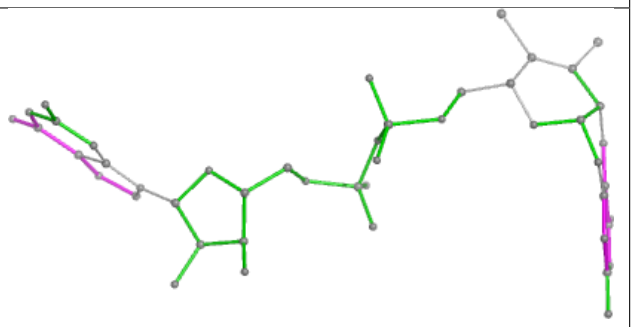

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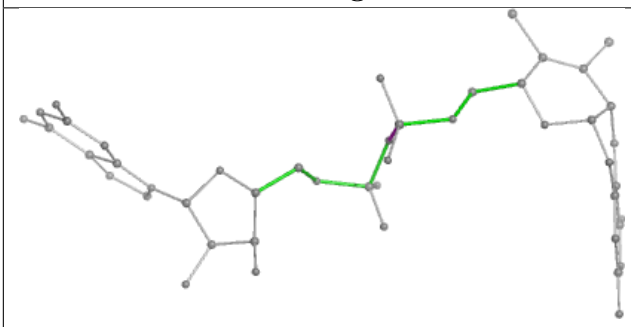

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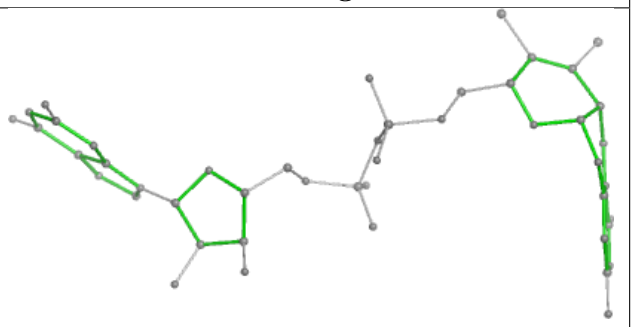
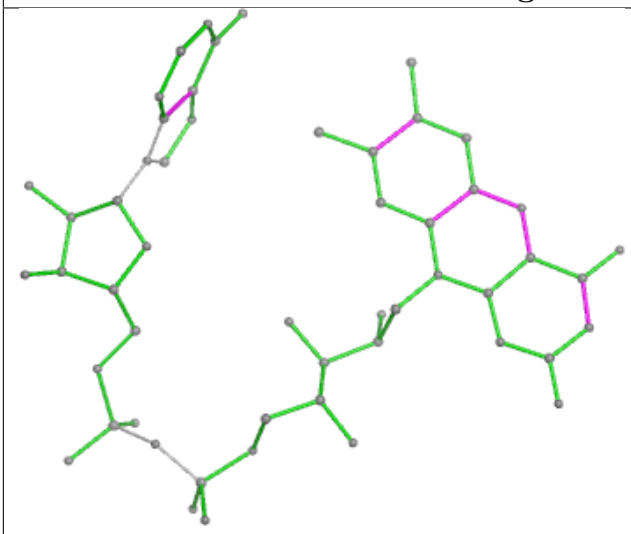
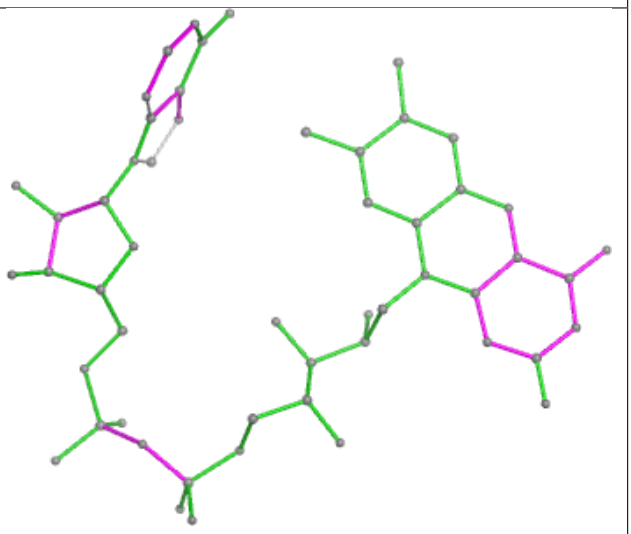


Rings

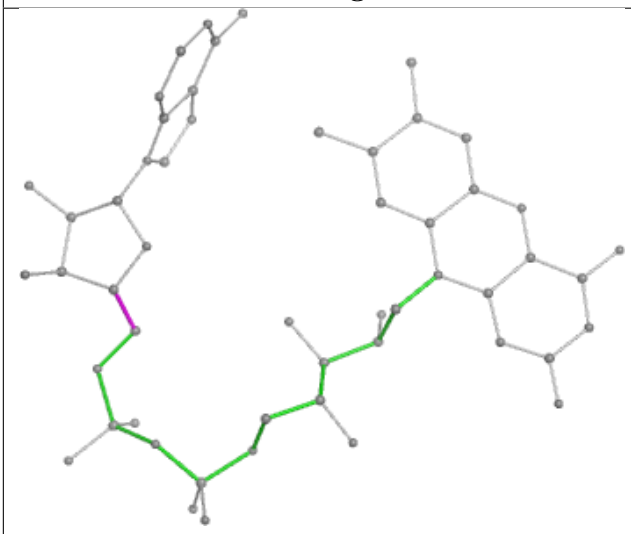
Ligand FAD E 1103



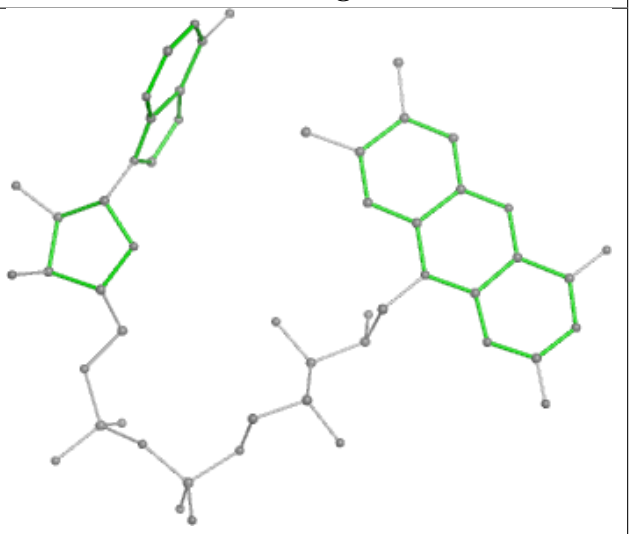
Bond lengths



Bond angles

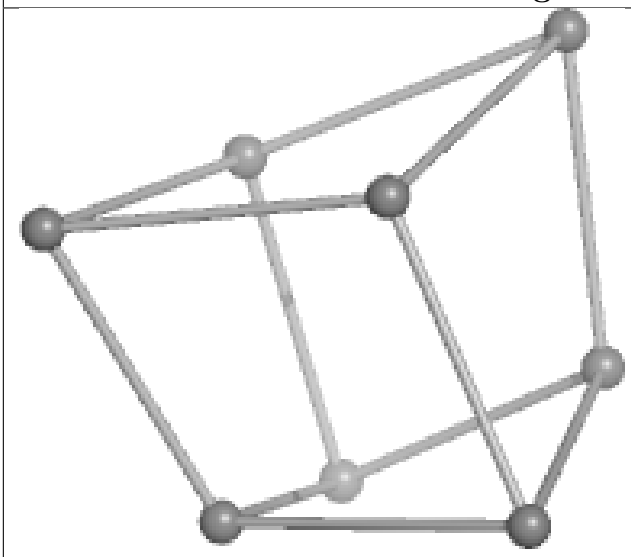


Torsions



Rings

Ligand SF4 L 102



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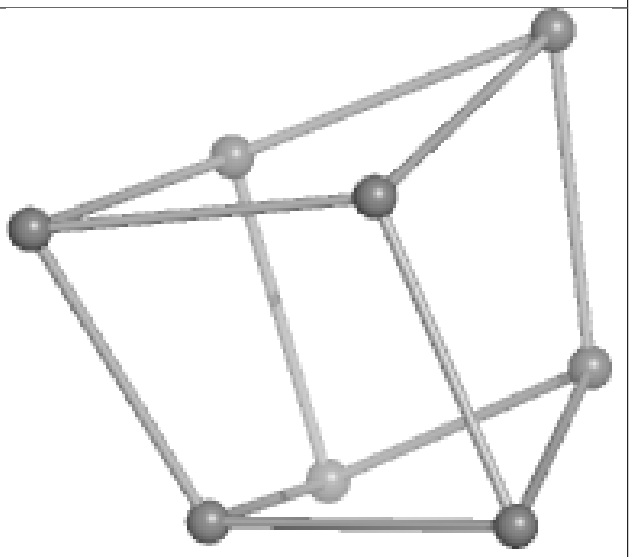

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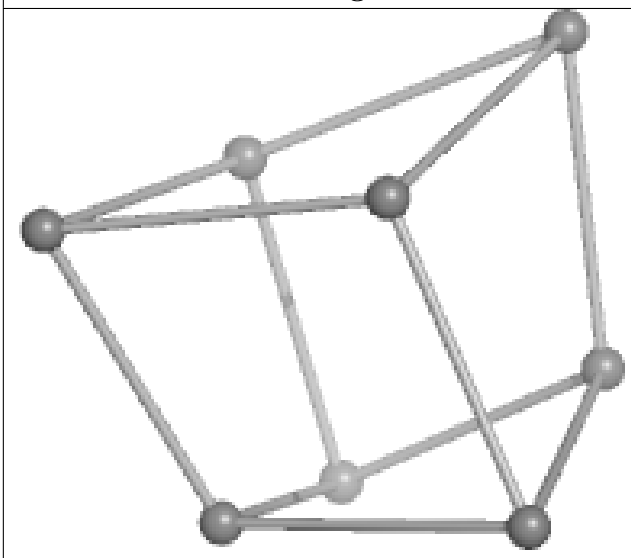

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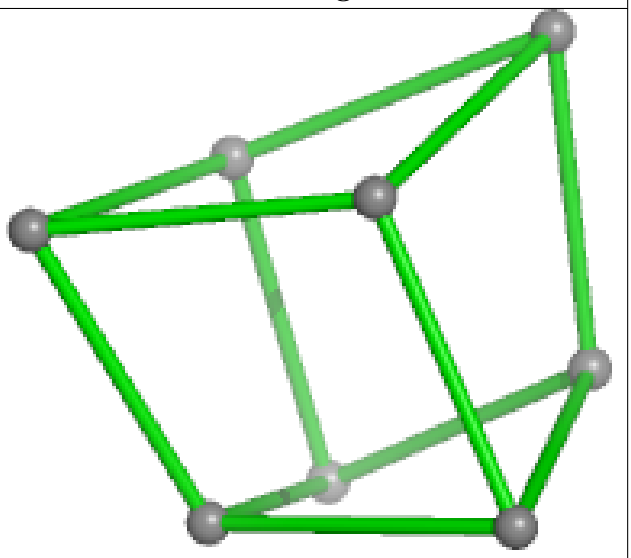
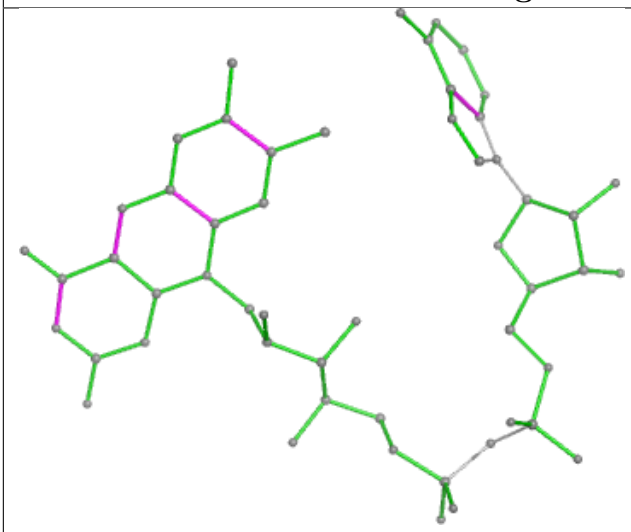


Rings

Ligand FAD K 1103



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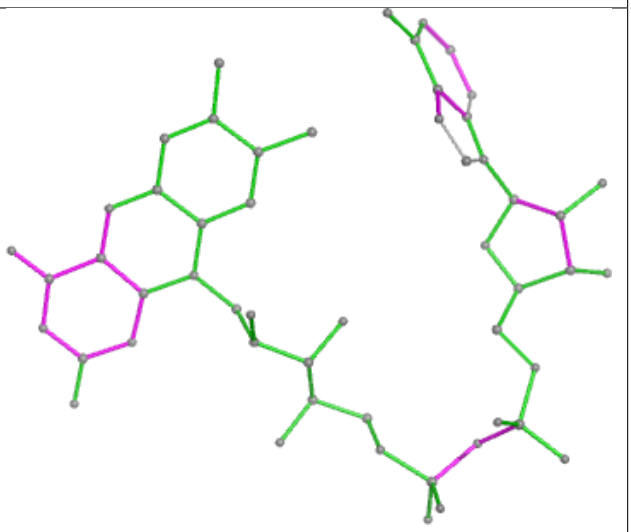
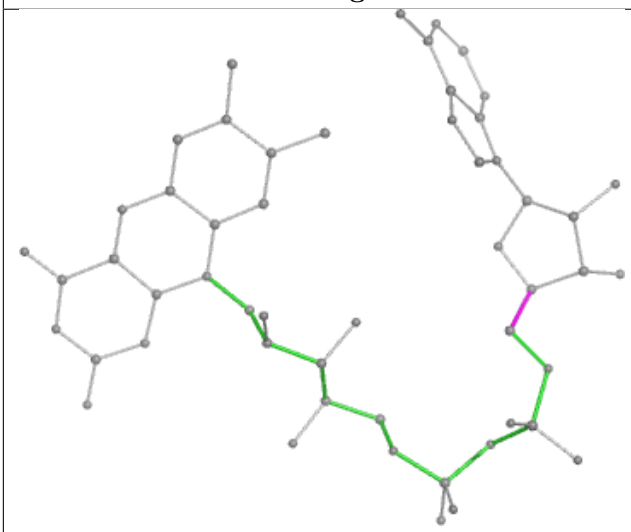


Bond angles



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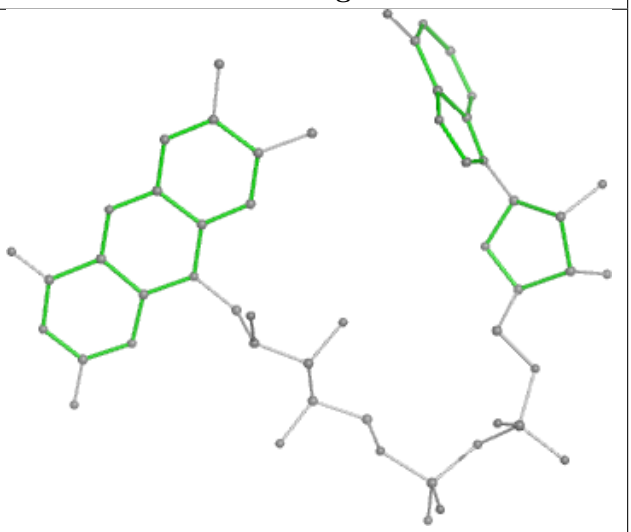
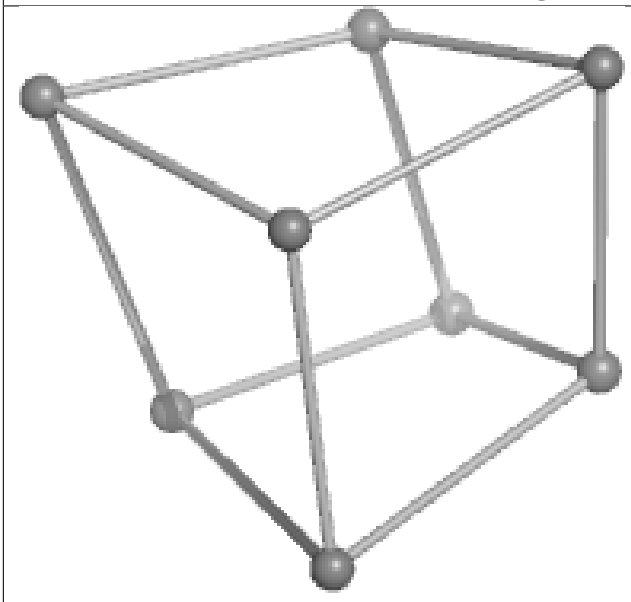


Rings

Ligand SF4 F 102



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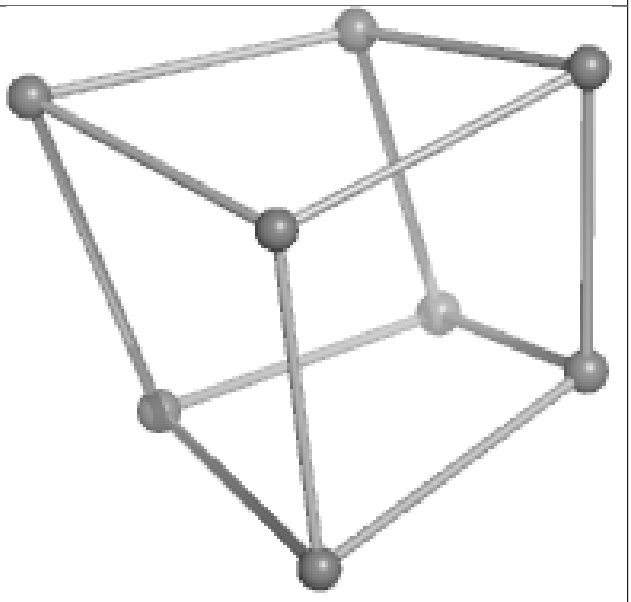
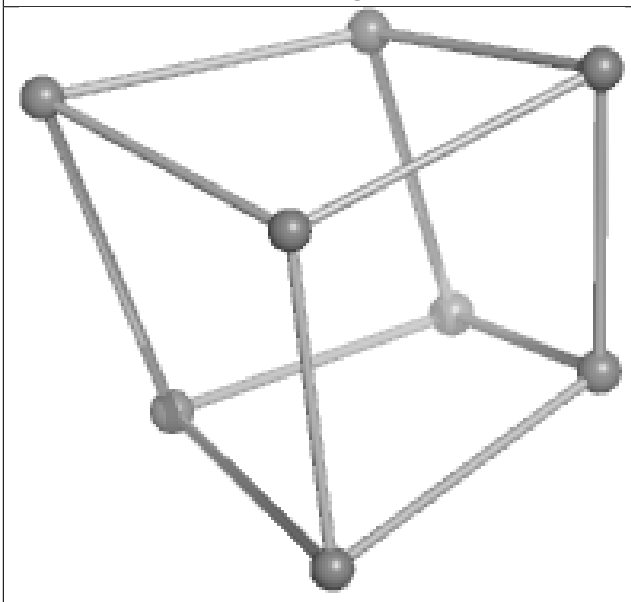


Bond angles



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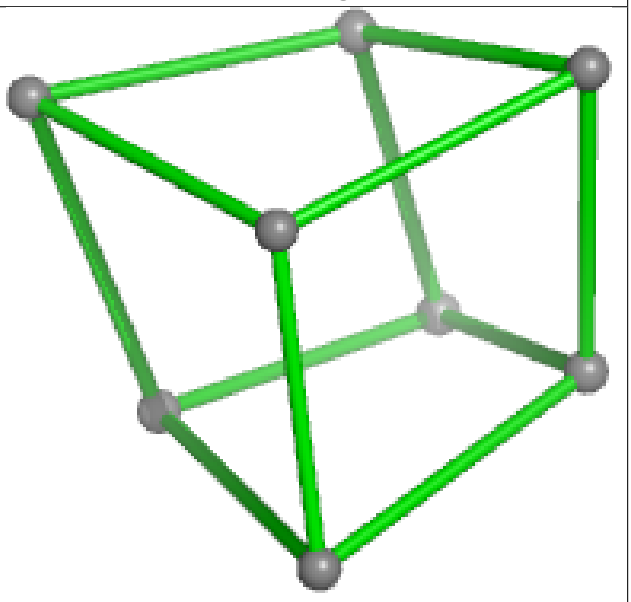
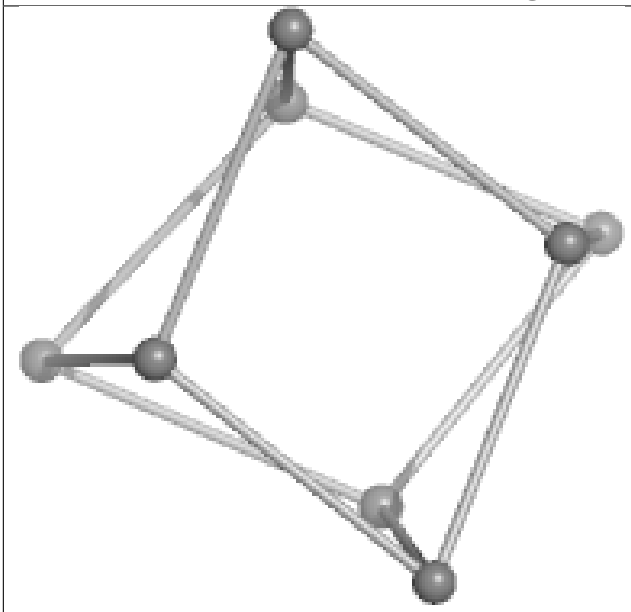


Rings

Ligand SF4 E 1102



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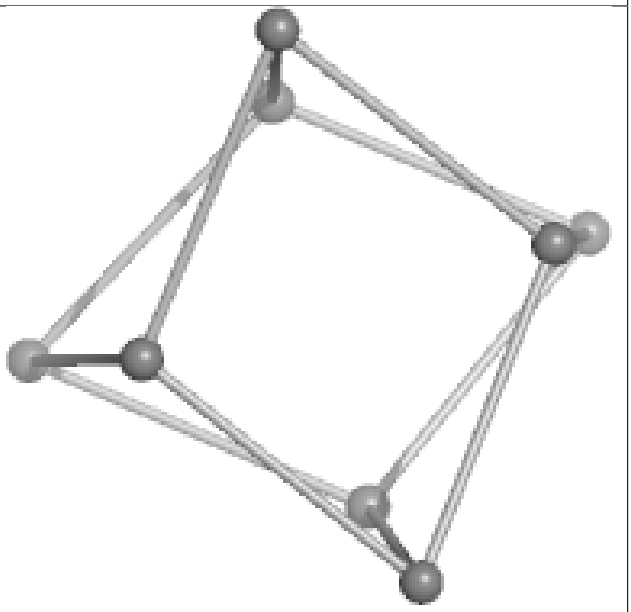

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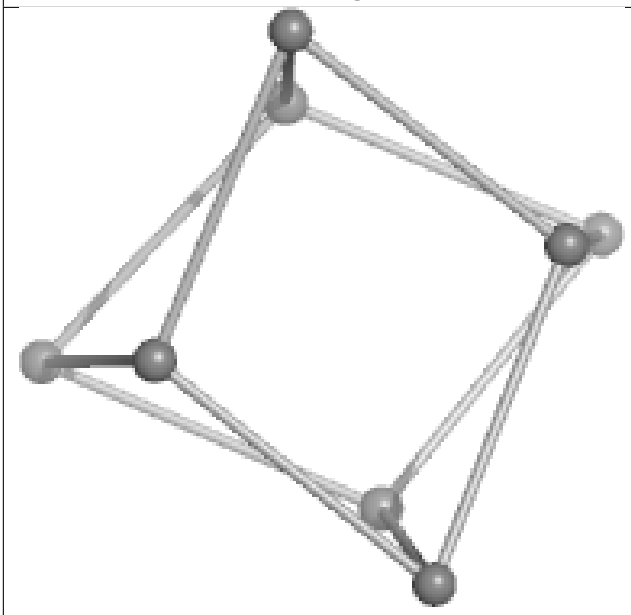

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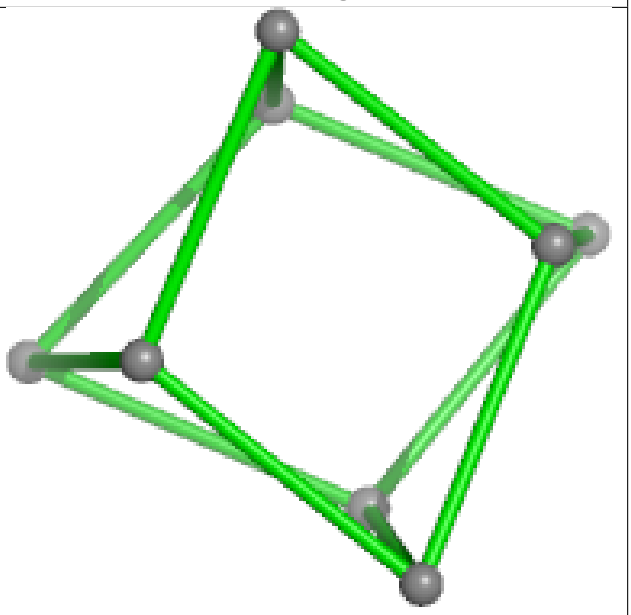
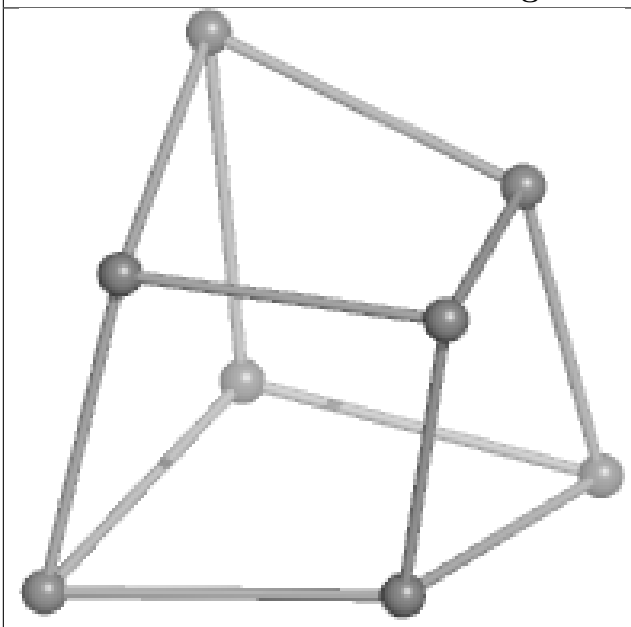


Rings

Ligand SF4 K 1102



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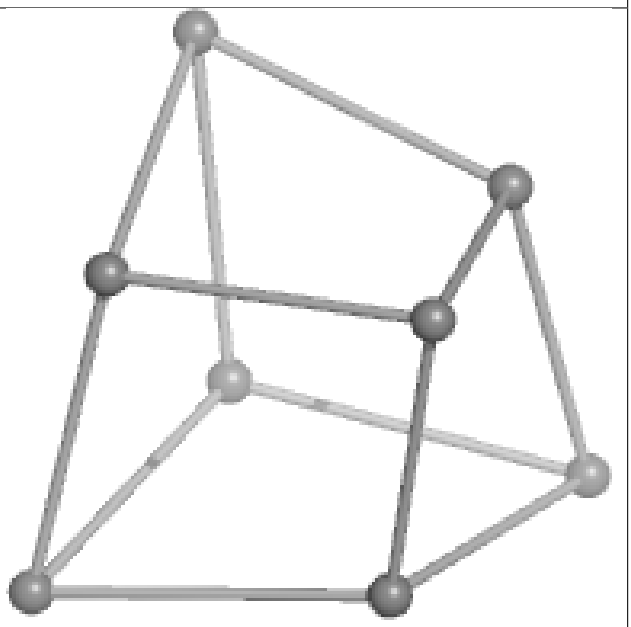
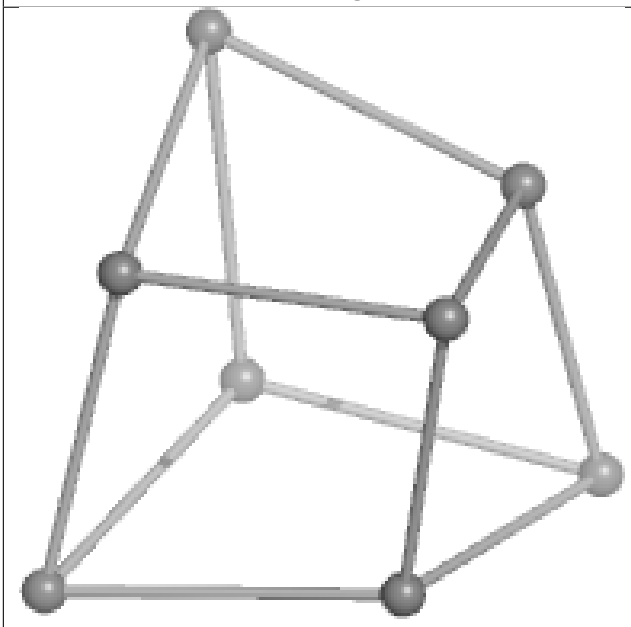


Bond angles



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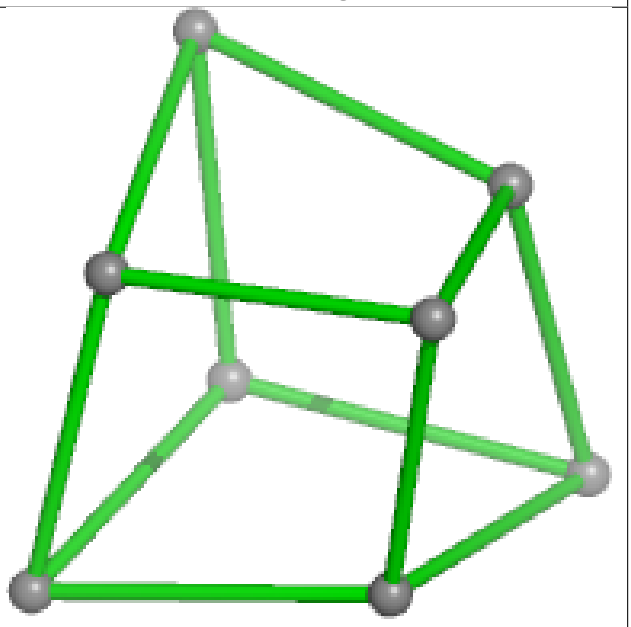
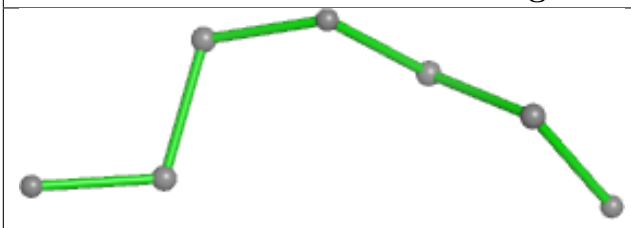


Rings

Ligand PE4 B 507



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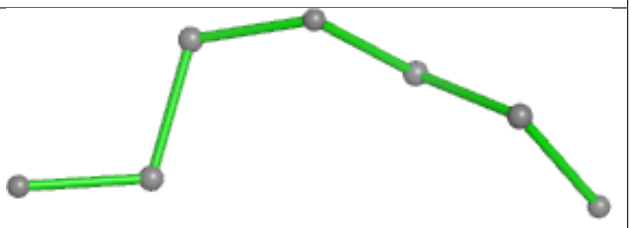
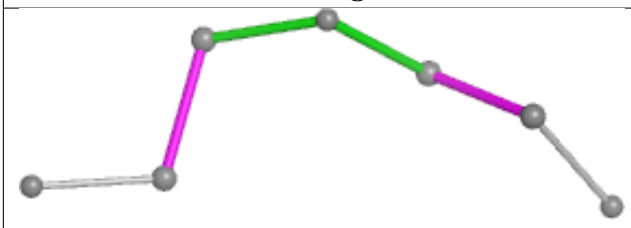
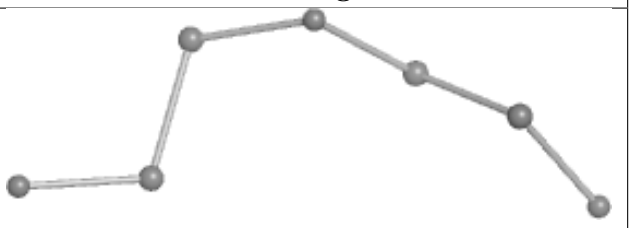


Bond angles

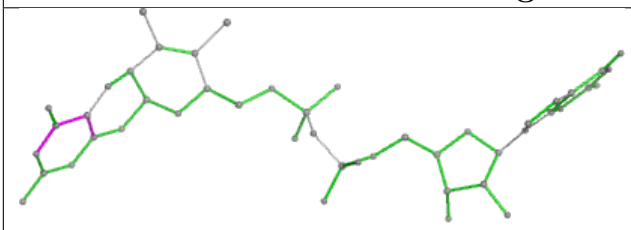


Torsions



Rings

Ligand MGD B 504



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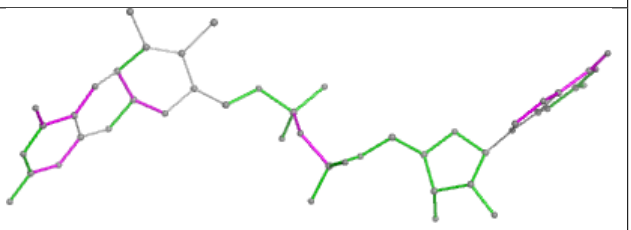

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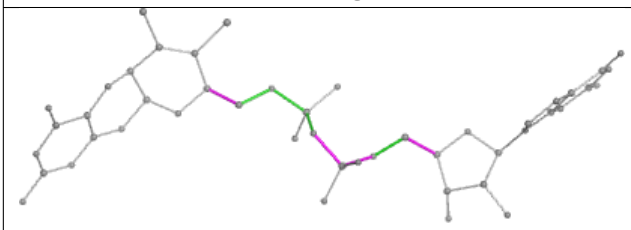

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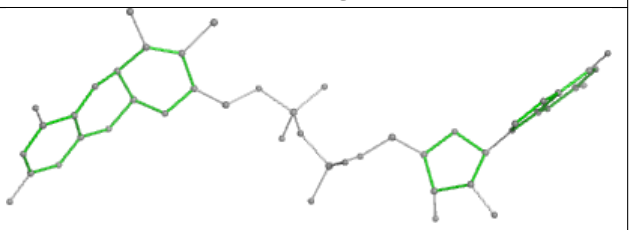
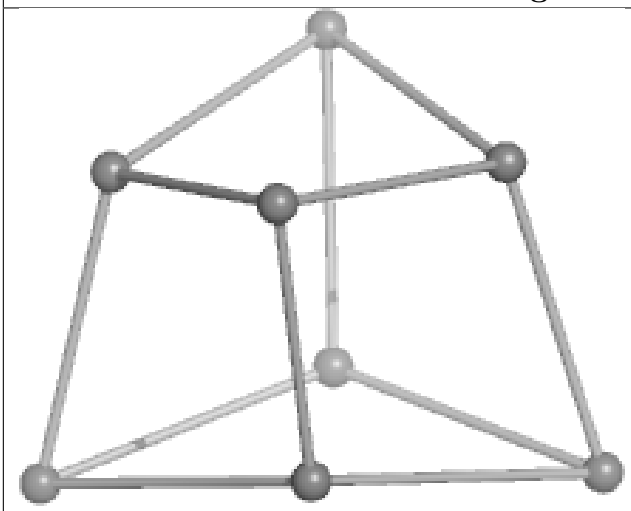


Rings

Ligand SF4 H 501



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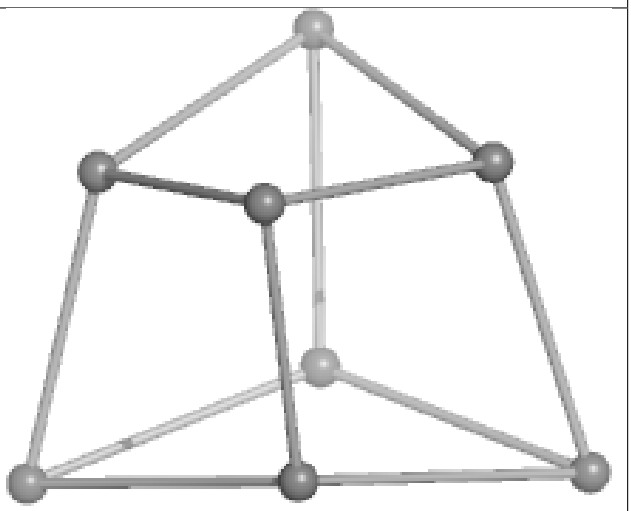
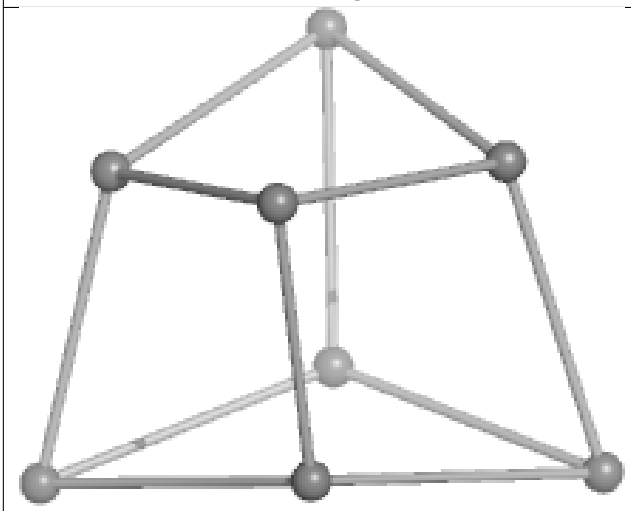


Bond angles



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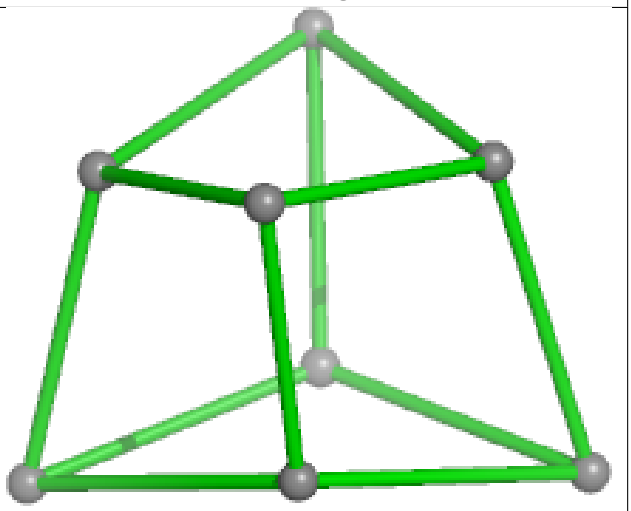
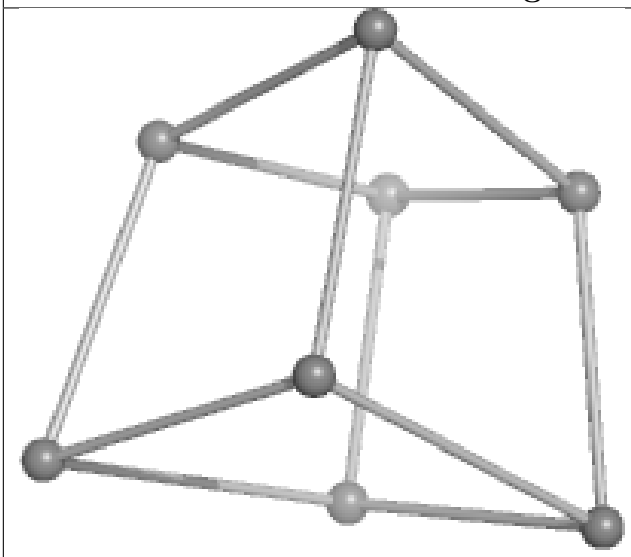
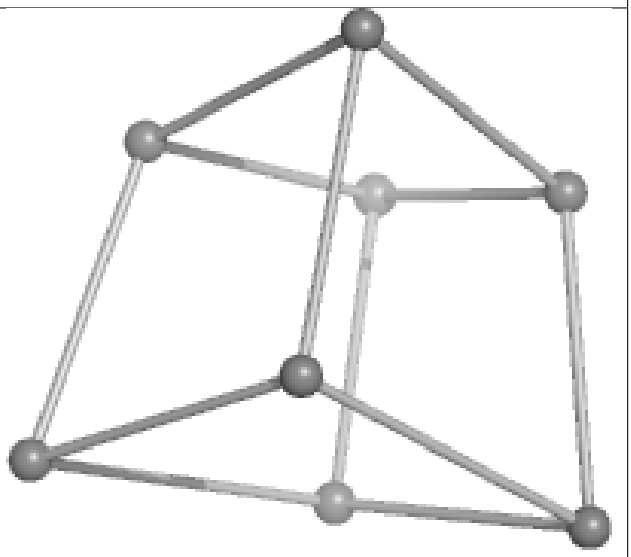


Rings

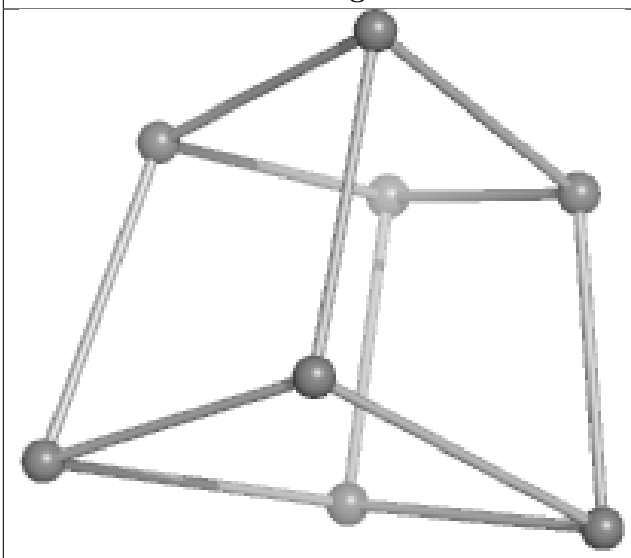
Ligand SF4 E 1101



Bond lengths



Bond angles



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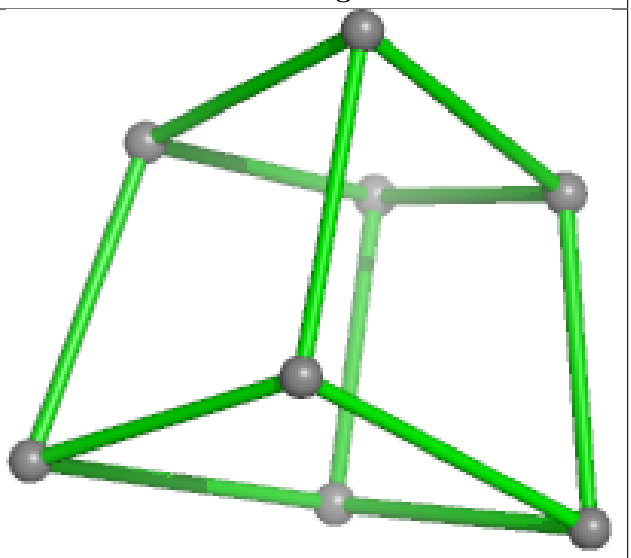
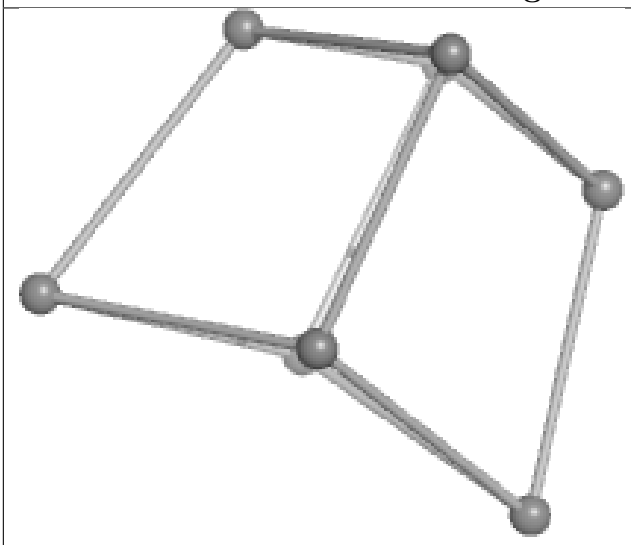
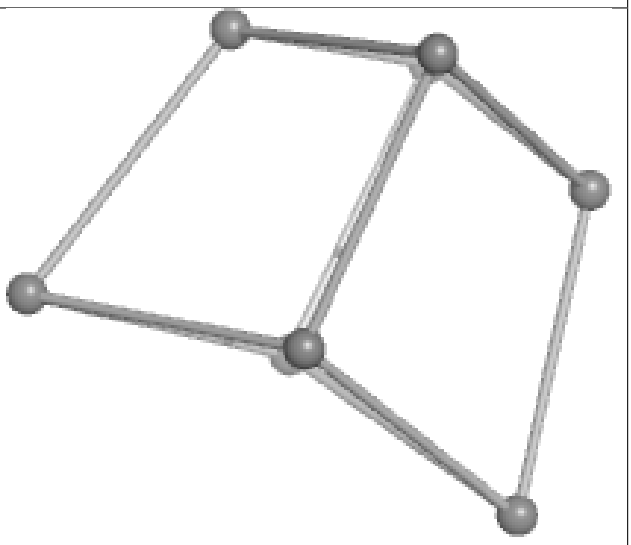


Rings

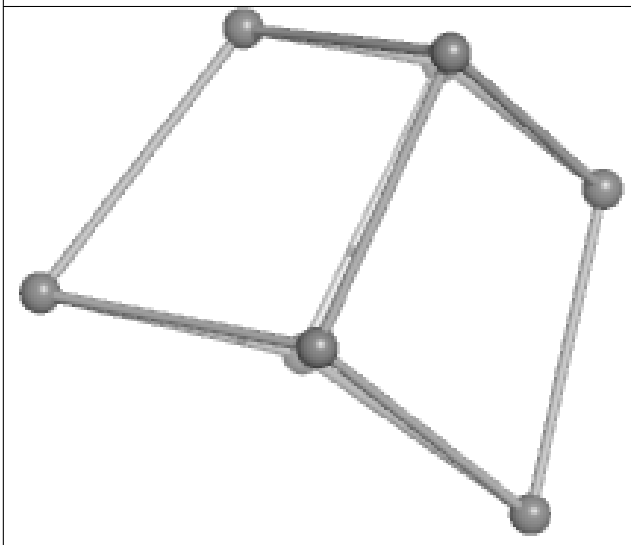
Ligand SF4 E 1104



Bond lengths



Bond angles



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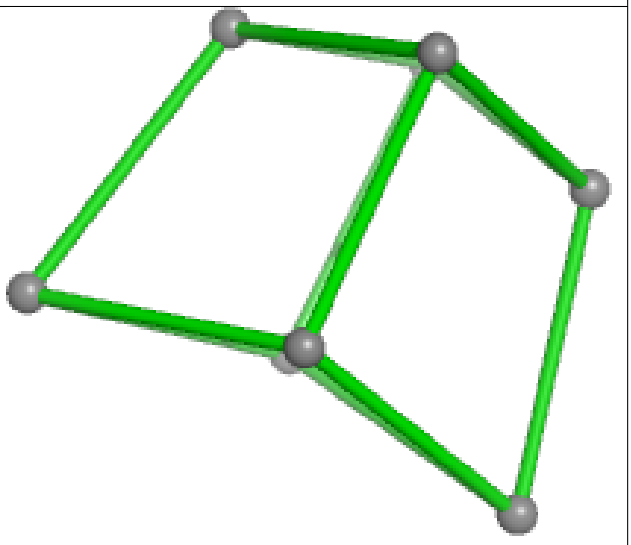
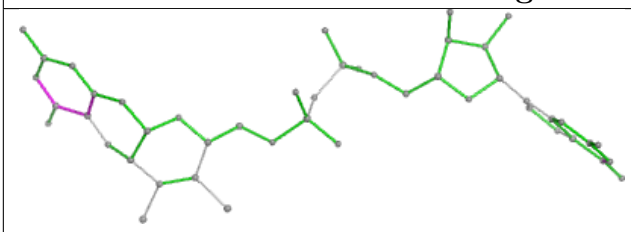


Rings

Ligand MGD H 504



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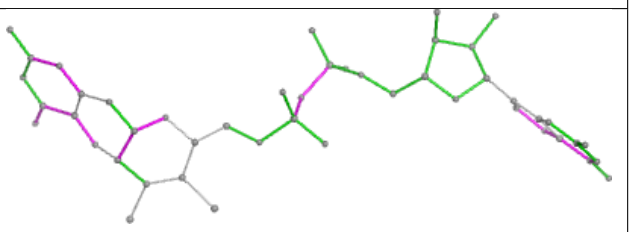
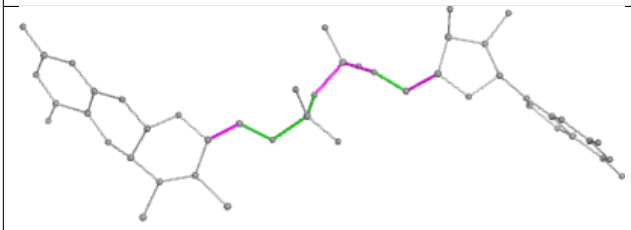


Bond angles



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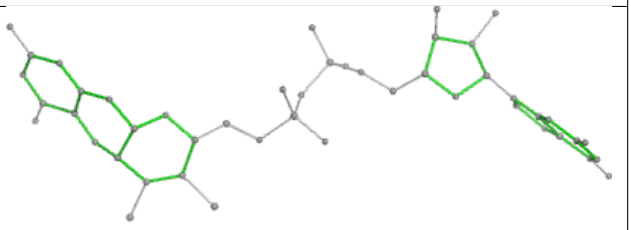
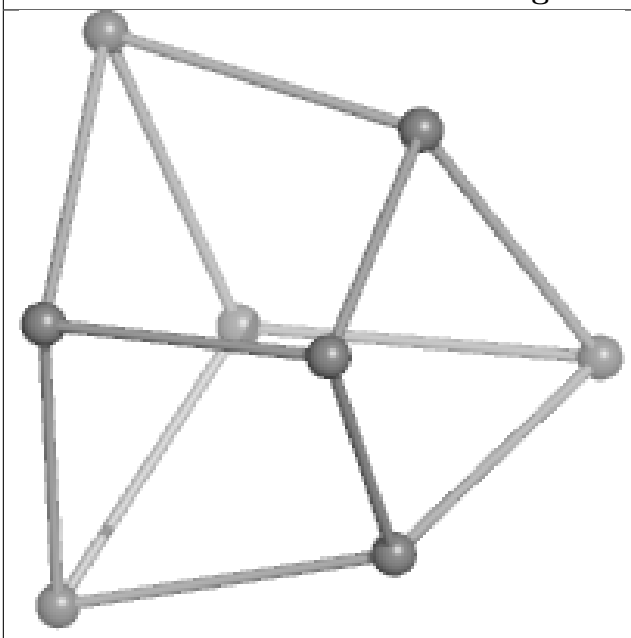
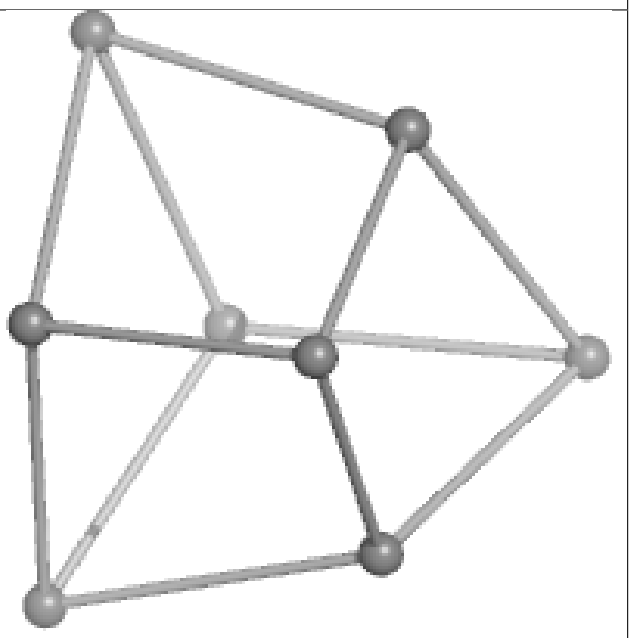


Rings

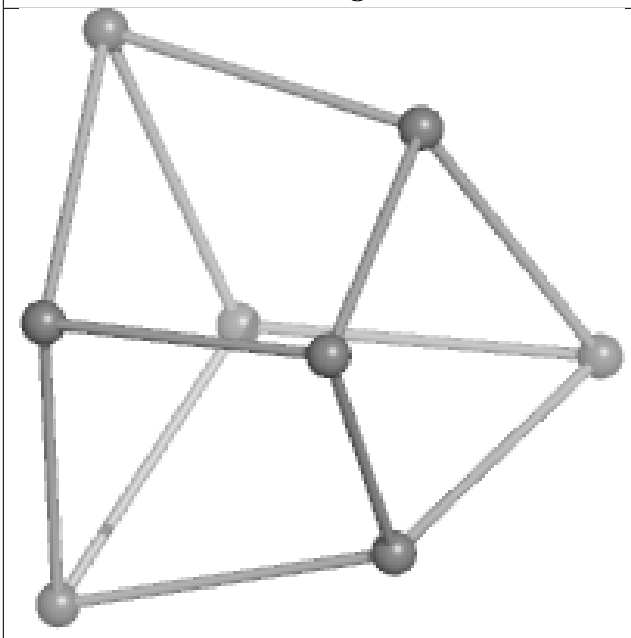
Ligand SF4 B 501



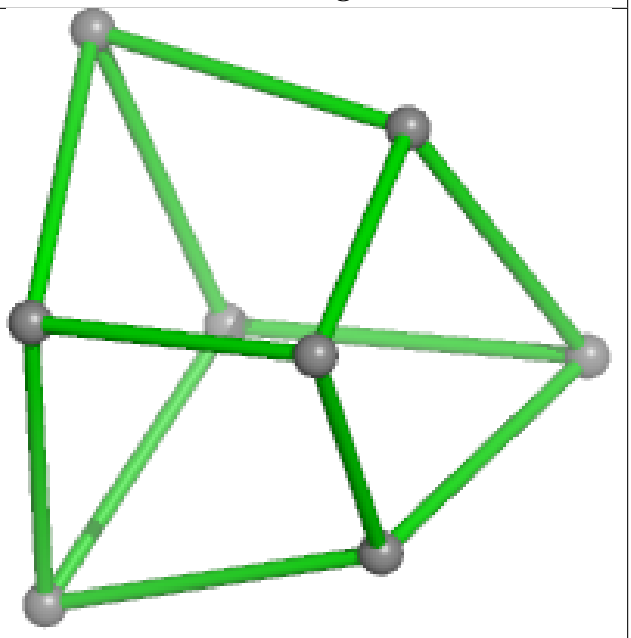
Bond lengths



Bond angles

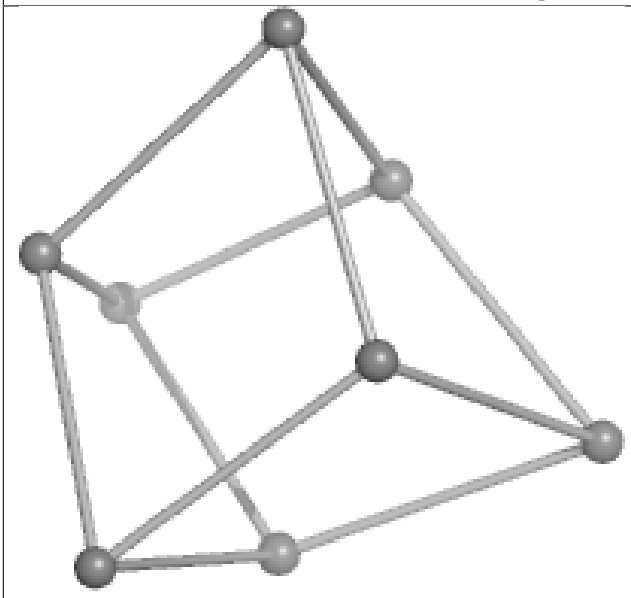


Torsions

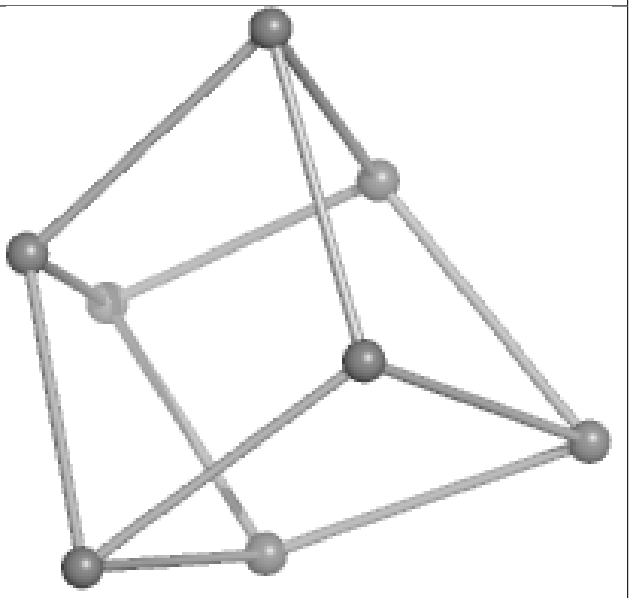


Rings

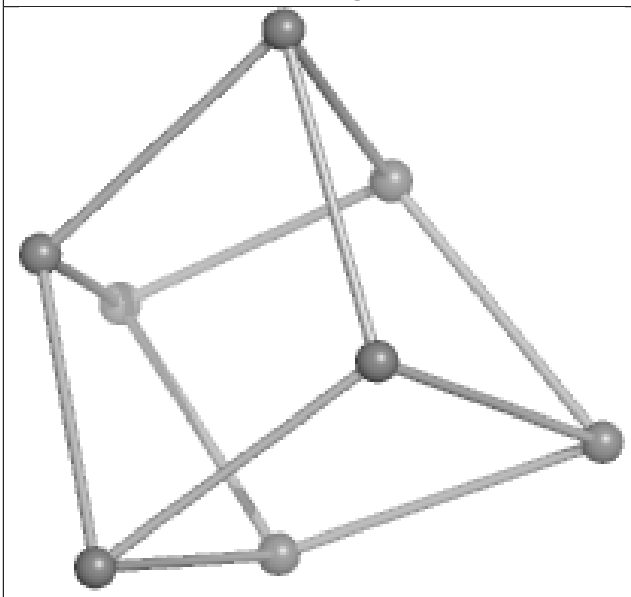
Ligand SF4 F 101



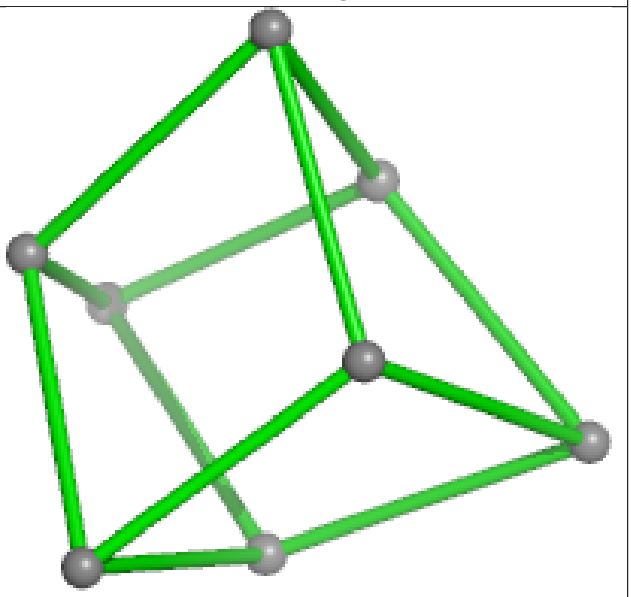
Bond lengths



Bond angles

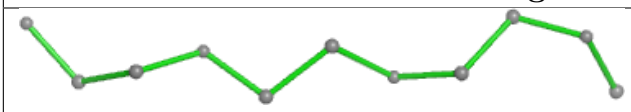


Torsions

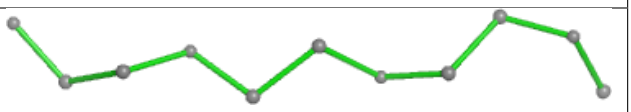


Rings

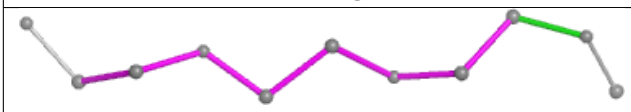
Ligand PE4 A 606



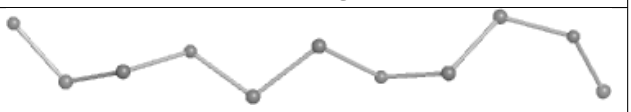
Bond lengths



Bond angles

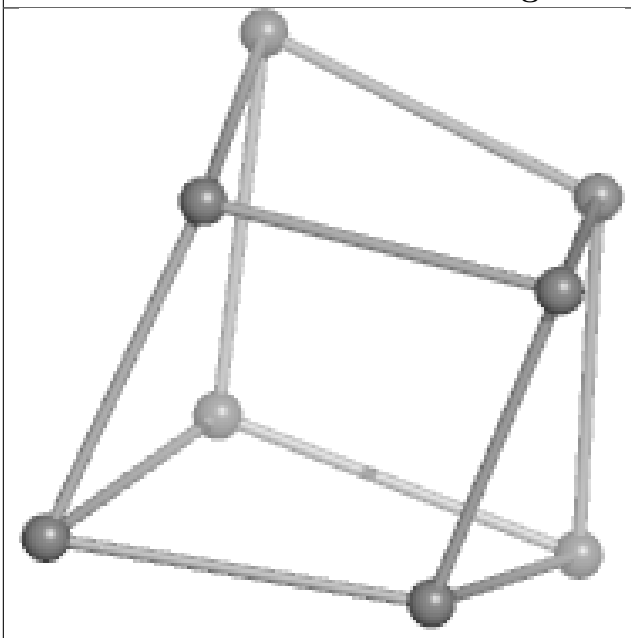


Torsions

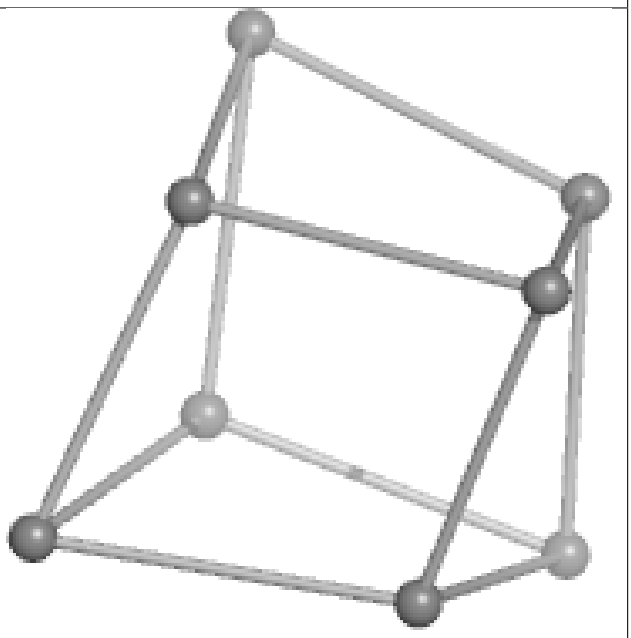


Rings

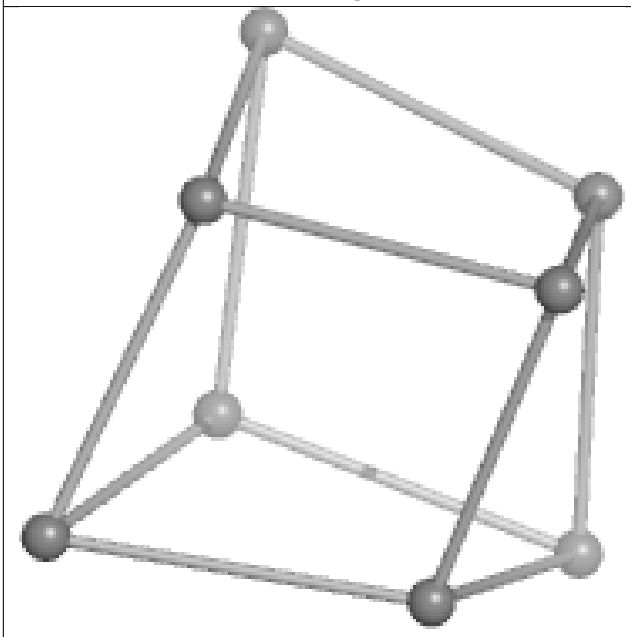
Ligand SF4 K 1101



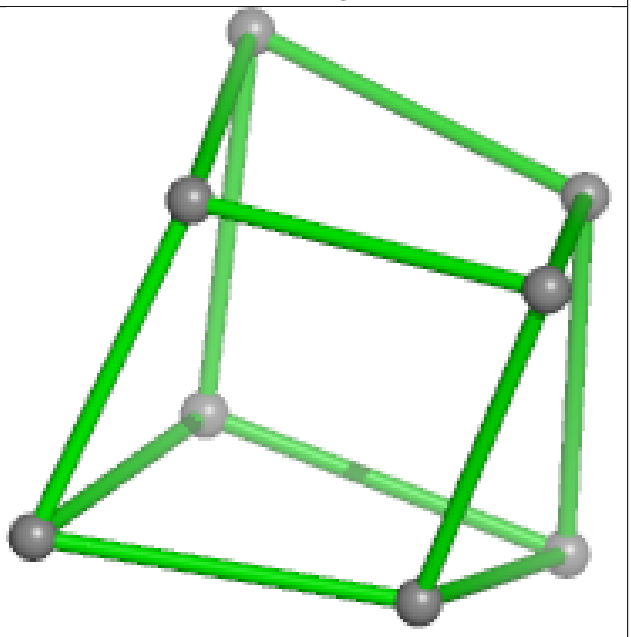
Bond lengths



Bond angles

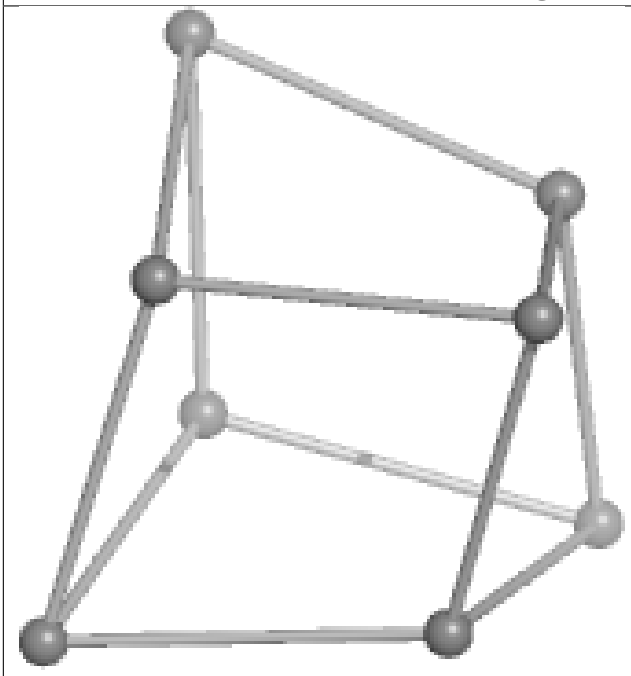


Torsions

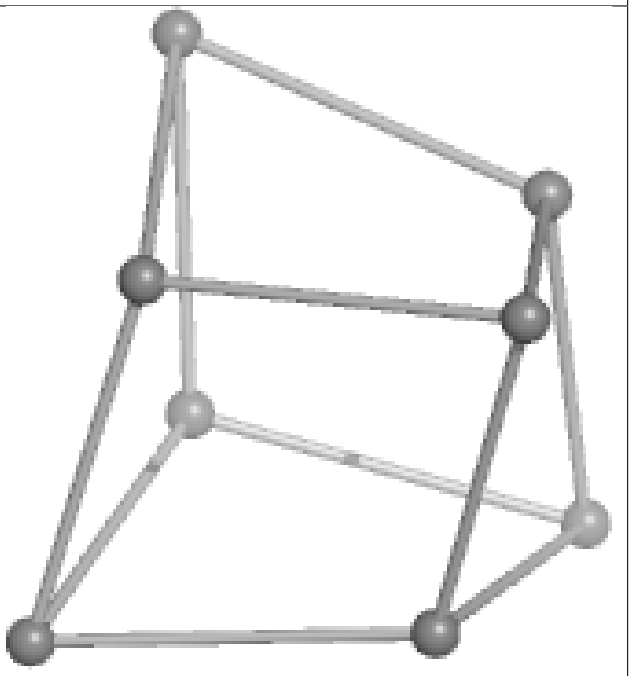


Rings

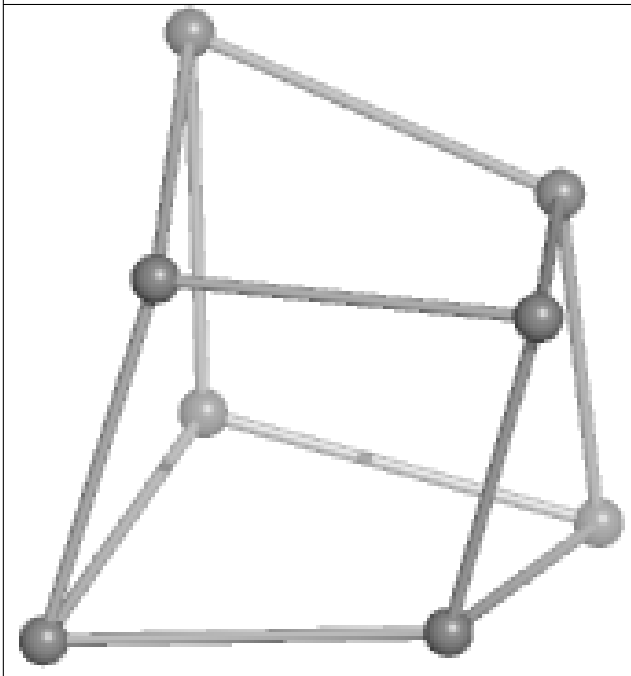
Ligand SF4 L 101



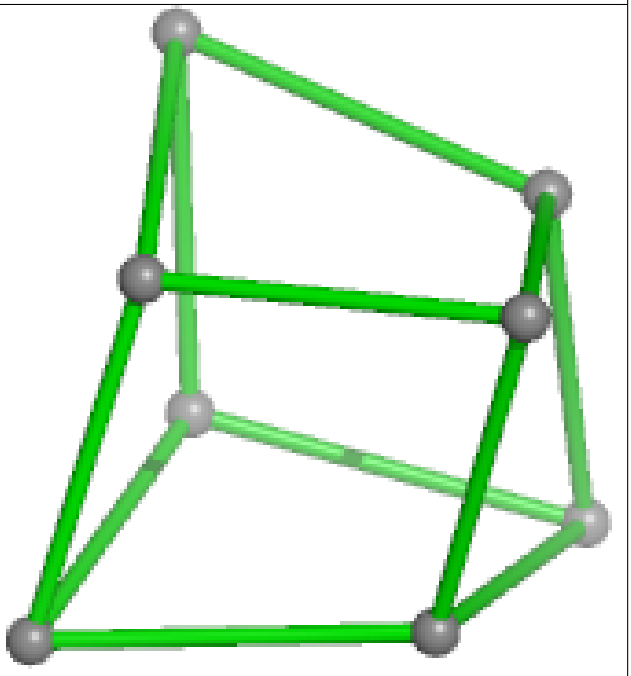
Bond lengths



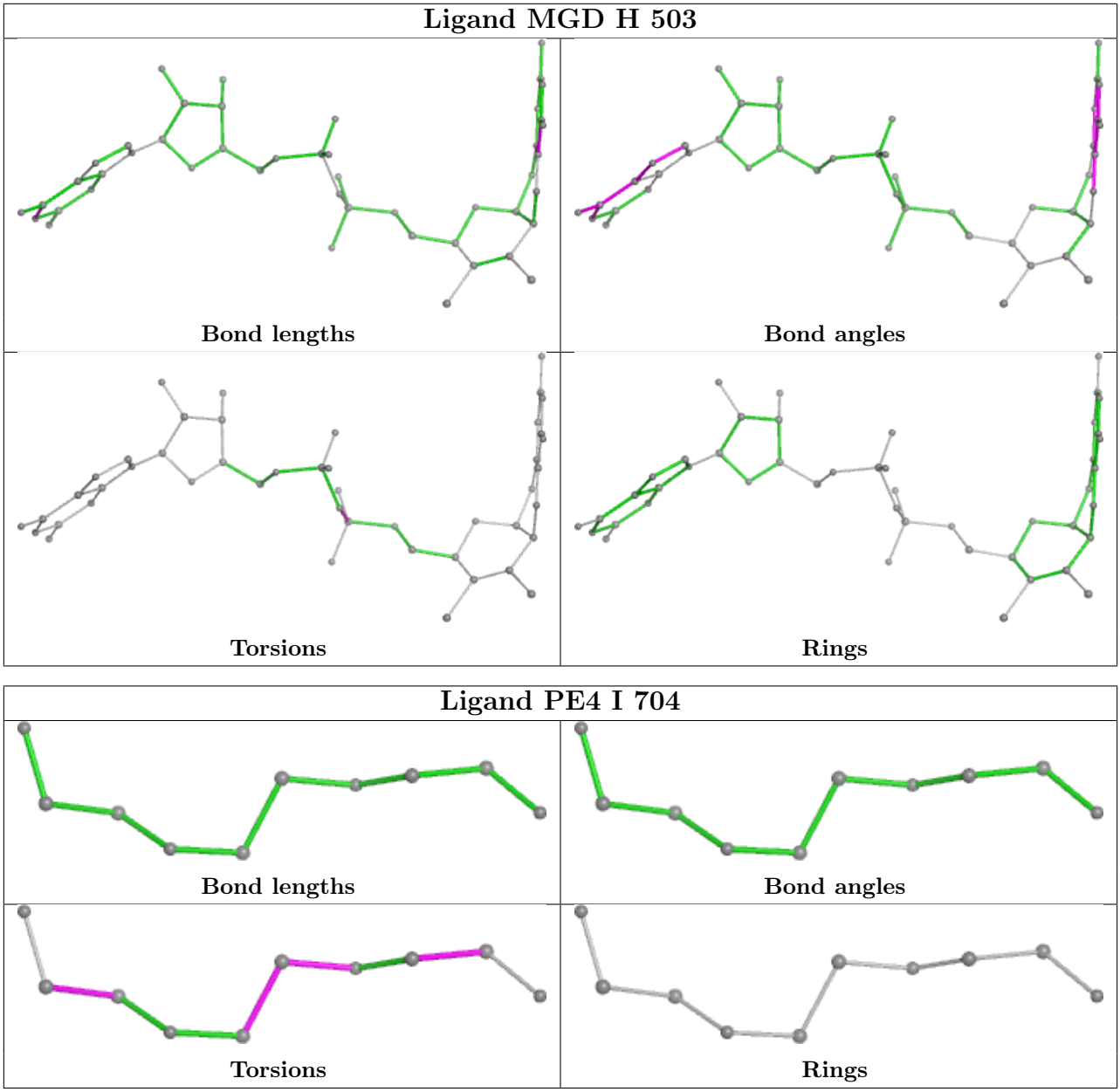
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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%)	-0.28	3 (0%) 87 91	11, 18, 31, 63	0
1	G	565/567 (99%)	-0.31	1 (0%) 92 94	10, 17, 29, 64	1 (0%)
2	B	429/430 (99%)	-0.24	1 (0%) 92 94	10, 18, 31, 61	0
2	H	429/430 (99%)	-0.16	2 (0%) 87 91	10, 18, 36, 66	1 (0%)
3	C	253/253 (100%)	0.24	11 (4%) 40 51	15, 26, 51, 78	0
3	I	253/253 (100%)	-0.18	3 (1%) 76 83	11, 19, 37, 75	0
4	D	124/126 (98%)	0.16	2 (1%) 70 78	14, 25, 41, 67	0
4	J	125/126 (99%)	-0.08	0 100 100	14, 23, 38, 74	0
5	E	351/359 (97%)	0.42	17 (4%) 36 47	18, 30, 55, 85	0
5	K	351/359 (97%)	1.18	63 (17%) 4 7	23, 41, 71, 100	0
6	F	77/85 (90%)	0.33	5 (6%) 26 37	17, 23, 51, 93	0
6	L	78/85 (91%)	0.14	4 (5%) 34 45	15, 24, 52, 75	0
All	All	3600/3640 (98%)	0.03	112 (3%) 51 62	10, 21, 50, 100	2 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	K	233	VAL	5.2
5	K	231	LEU	5.0
3	I	11	SER	4.5
5	K	351	ARG	4.5
5	K	259	ILE	4.4
5	K	228	LEU	4.2
6	F	5	MET	4.1
6	F	81	GLU	3.9
5	K	255	GLY	3.8
5	K	227	ILE	3.7
5	K	291	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
5	K	136	TYR	3.5
6	F	7	PHE	3.4
5	K	229	GLN	3.4
5	E	74	THR	3.4
5	K	245	LYS	3.4
5	K	256	GLU	3.3
3	C	233	SER	3.3
6	L	7	PHE	3.3
5	K	327	GLU	3.2
6	F	6	SER	3.2
5	K	258	LYS	3.2
5	K	252	LEU	3.2
5	K	235	ILE	3.2
6	L	5	MET	3.1
5	K	97	THR	3.1
5	K	44	ARG	3.0
5	K	349	LYS	3.0
5	K	341	ILE	3.0
5	E	349	LYS	2.9
5	K	260	ILE	2.9
4	D	42	ARG	2.9
1	G	567	ASN	2.9
5	E	326	ASP	2.9
5	K	265	LEU	2.9
5	K	324	THR	2.8
3	I	1	MET	2.8
5	K	262	HIS	2.8
3	C	11	SER	2.8
3	I	253	ALA	2.8
5	E	324	THR	2.7
5	K	39	LYS	2.7
1	A	567	ASN	2.7
5	K	253	LYS	2.7
5	E	235	ILE	2.6
5	E	321	GLU	2.6
5	E	348	ILE	2.6
5	K	305	GLU	2.6
5	K	114	LEU	2.6
4	D	43	ALA	2.6
5	K	269	VAL	2.6
5	E	234	ASP	2.6
3	C	231	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
5	E	325	VAL	2.6
6	L	81	GLU	2.6
3	C	1	MET	2.6
5	K	315	LEU	2.6
5	K	318	GLY	2.6
3	C	253	ALA	2.6
5	K	257	LYS	2.5
5	K	153	ALA	2.5
5	K	297	TRP	2.5
6	L	82	PRO	2.5
2	B	234	GLU	2.5
5	K	108	GLY	2.5
5	K	280	ASN	2.5
5	E	305	GLU	2.5
5	K	230	ASP	2.5
5	K	237	ASP	2.5
5	K	236	ALA	2.5
5	K	137	ASN	2.5
1	A	197	ARG	2.4
5	E	1	MET	2.4
5	K	346	THR	2.4
5	K	238	VAL	2.4
5	E	327	GLU	2.4
5	K	104	VAL	2.3
5	E	53	ARG	2.3
3	C	30	THR	2.3
2	H	57	SER	2.3
6	F	80	TYR	2.3
5	K	319	LEU	2.3
5	K	232	GLU	2.3
5	K	348	ILE	2.3
3	C	28	GLY	2.3
5	E	144	LYS	2.3
5	K	254	SER	2.3
5	K	317	LYS	2.2
5	K	248	LEU	2.2
5	K	333	ILE	2.2
5	K	328	LYS	2.2
5	K	37	GLU	2.2
2	H	172	ASP	2.2
3	C	31	VAL	2.2
5	E	351	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
5	K	325	VAL	2.2
3	C	230	ASP	2.2
5	K	147	ASP	2.2
1	A	8	ASN	2.2
5	E	315	LEU	2.2
5	K	330	LEU	2.2
5	K	98	TYR	2.2
5	E	331	LYS	2.1
5	K	10	GLU	2.1
3	C	232	VAL	2.1
3	C	229	LEU	2.1
5	K	261	PRO	2.0
5	K	31	GLN	2.0
5	K	74	THR	2.0
5	K	101	ILE	2.0
5	K	311	TYR	2.0
5	K	102	GLN	2.0

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, 95^{th} 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	0.91	0.09	11,14,26,27	0
1	KCX	A	180	12/13	0.93	0.09	11,14,28,31	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	0.53	0.18	55,56,56,63	0
12	EDO	E	1109	4/4	0.61	0.24	48,48,49,52	0
9	GOL	A	611	6/6	0.62	0.21	40,44,49,53	0
12	EDO	K	1105	4/4	0.67	0.26	46,46,47,56	0
12	EDO	H	510	4/4	0.69	0.19	49,52,52,52	0
8	PEG	A	603	7/7	0.72	0.15	28,33,40,40	0
12	EDO	B	508	4/4	0.73	0.17	34,34,37,45	0
12	EDO	G	605	4/4	0.73	0.17	35,40,41,52	0
10	ACT	A	605	4/4	0.74	0.14	33,37,41,45	0
12	EDO	A	610	4/4	0.75	0.18	33,35,36,55	0
12	EDO	G	606	4/4	0.75	0.18	34,36,38,41	0
9	GOL	H	505	6/6	0.76	0.19	33,39,41,45	0
10	ACT	B	506	4/4	0.78	0.15	33,35,36,38	0
10	ACT	I	705	4/4	0.78	0.11	24,29,38,40	0
11	PE4	B	507	7/24	0.79	0.15	26,30,40,51	0
10	ACT	H	507	4/4	0.79	0.17	30,32,37,44	0
9	GOL	I	703	6/6	0.79	0.20	34,38,39,40	0
12	EDO	E	1107	4/4	0.80	0.19	33,38,43,44	0
9	GOL	H	509	6/6	0.81	0.18	36,37,38,38	0
9	GOL	I	701	6/6	0.81	0.13	36,38,42,44	0
12	EDO	A	609	4/4	0.81	0.13	32,33,36,36	0
20	PG4	I	702	10/13	0.81	0.16	32,48,57,65	0
11	PE4	I	704	10/24	0.82	0.13	29,33,36,39	0
11	PE4	A	606	11/24	0.82	0.12	29,32,41,43	0
12	EDO	G	607	4/4	0.83	0.13	25,31,36,36	0
19	NA	H	511	1/1	0.83	0.14	47,47,47,47	0
12	EDO	G	604	4/4	0.83	0.12	31,31,33,35	0
12	EDO	K	1106	4/4	0.84	0.13	43,45,45,48	0
19	NA	E	1110	1/1	0.85	0.11	47,47,47,47	0
9	GOL	E	1105	6/6	0.85	0.13	27,37,41,43	0
13	CL	A	612	1/1	0.85	0.11	61,61,61,61	0
9	GOL	A	608	6/6	0.86	0.13	27,30,32,40	0
12	EDO	E	1106	4/4	0.87	0.10	30,32,34,35	0
19	NA	K	1107	1/1	0.88	0.11	46,46,46,46	0
10	ACT	A	607	4/4	0.90	0.12	32,32,34,36	0
9	GOL	A	604	6/6	0.90	0.14	30,33,35,37	0
9	GOL	H	508	6/6	0.91	0.10	27,31,34,37	0
17	H2S	B	505	1/1	0.91	0.11	24,24,24,24	0
18	FAD	K	1103	53/53	0.93	0.09	25,32,39,42	0
13	CL	C	301	1/1	0.94	0.10	62,62,62,62	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

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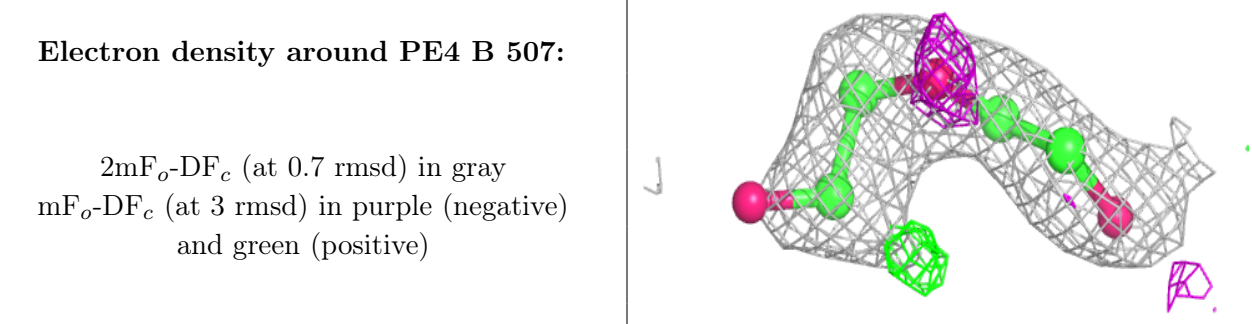
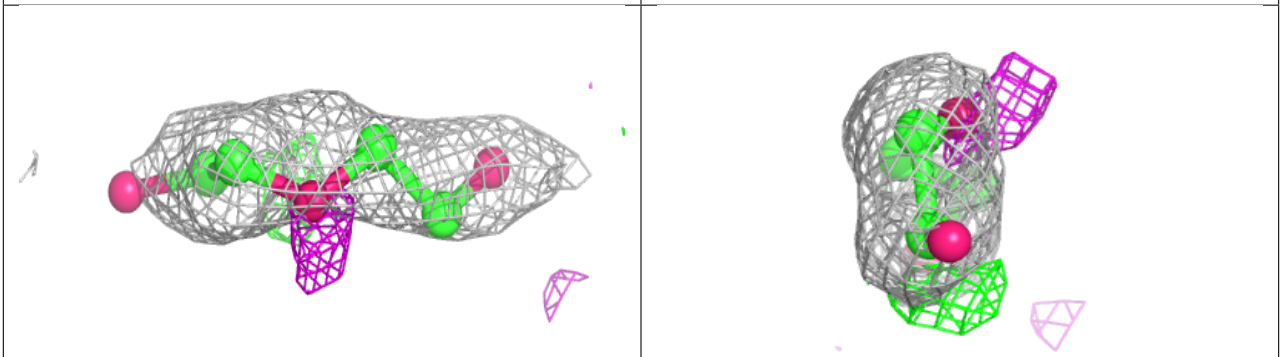
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	MGD	H	504	47/47	0.97	0.06	11,15,19,26	0
13	CL	F	103	1/1	0.97	0.06	31,31,31,31	0
13	CL	L	103	1/1	0.97	0.04	26,26,26,26	0
16	MGD	H	503	47/47	0.98	0.05	8,15,19,20	0
7	ZN	G	601	1/1	0.98	0.09	42,42,42,42	0
14	SF4	B	501	8/8	0.98	0.03	8,11,12,14	0
14	SF4	E	1101	8/8	0.98	0.04	21,23,24,28	0
14	SF4	E	1104	8/8	0.98	0.04	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
14	SF4	L	101	8/8	0.98	0.03	12,15,17,17	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
14	SF4	K	1104	8/8	0.99	0.03	17,19,22,22	0
7	ZN	G	602	1/1	0.99	0.04	33,33,33,33	0
14	SF4	L	102	8/8	0.99	0.03	14,19,21,24	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
14	SF4	E	1102	8/8	0.99	0.03	13,15,16,17	0
14	SF4	K	1102	8/8	0.99	0.03	16,17,22,23	0
15	W	H	502	1/1	1.00	0.03	15,15,15,15	0
15	W	B	502	1/1	1.00	0.03	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 B 507:

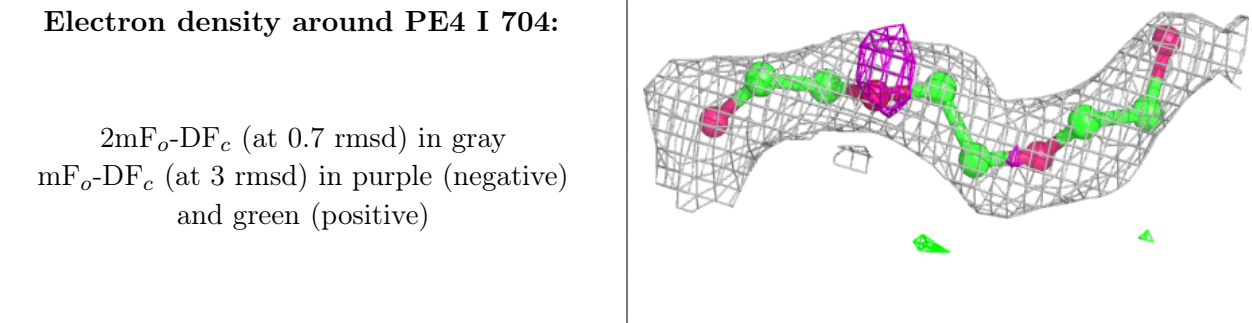
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

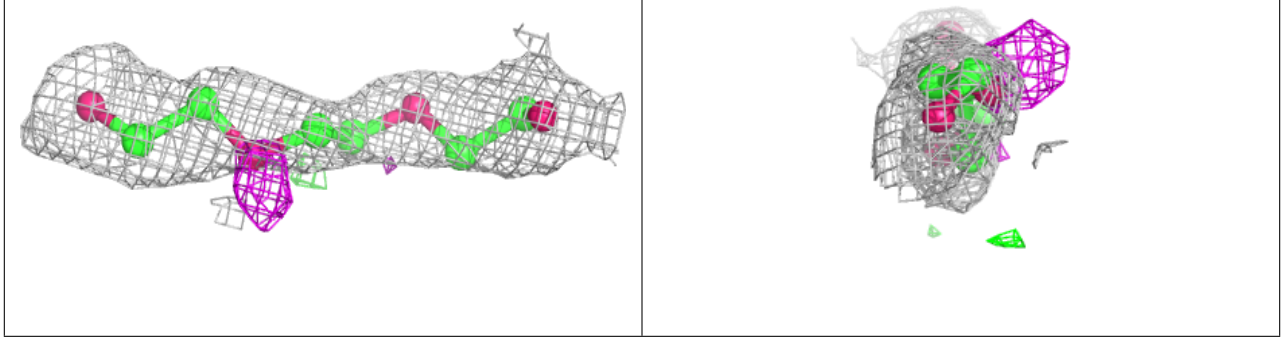




Electron density around PE4 I 704:

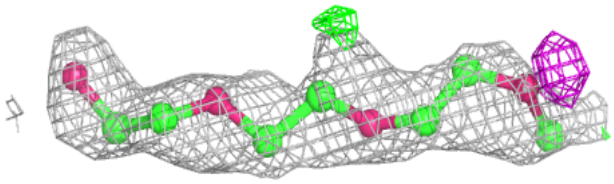
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

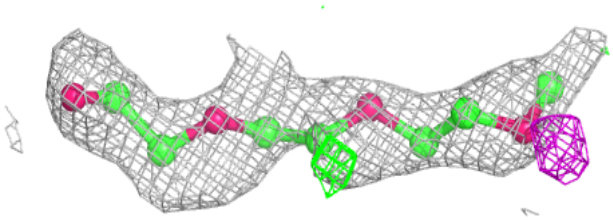


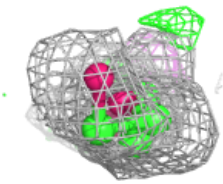


Electron density around PE4 A 606:

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

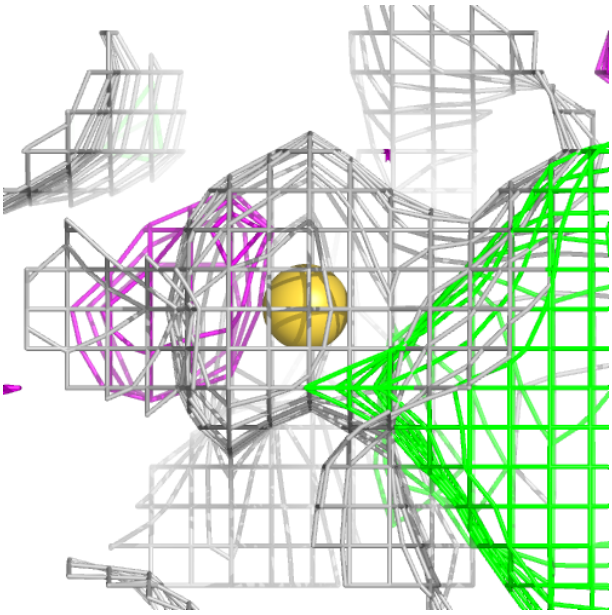


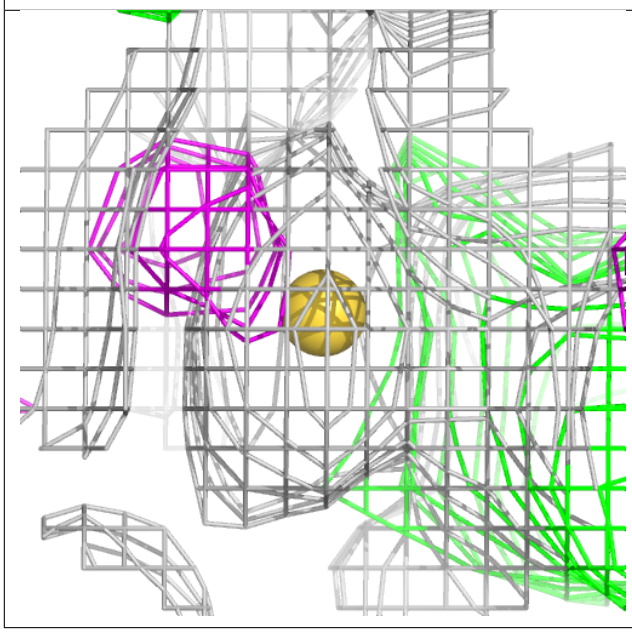


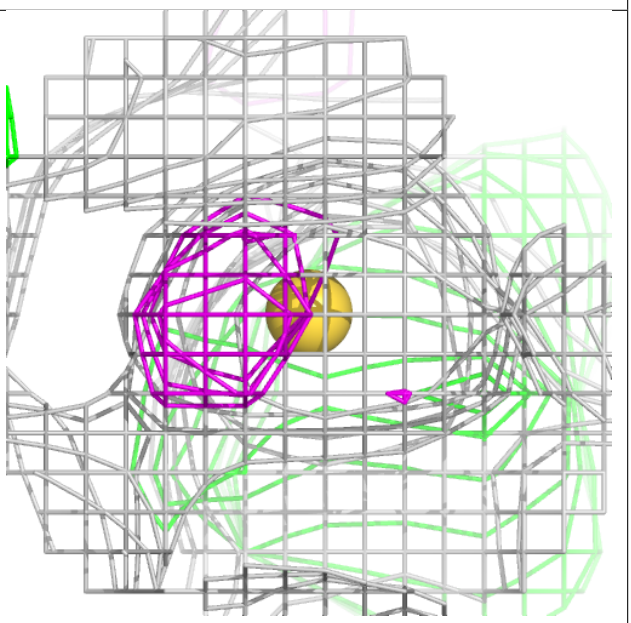


Electron density around H2S B 505:

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

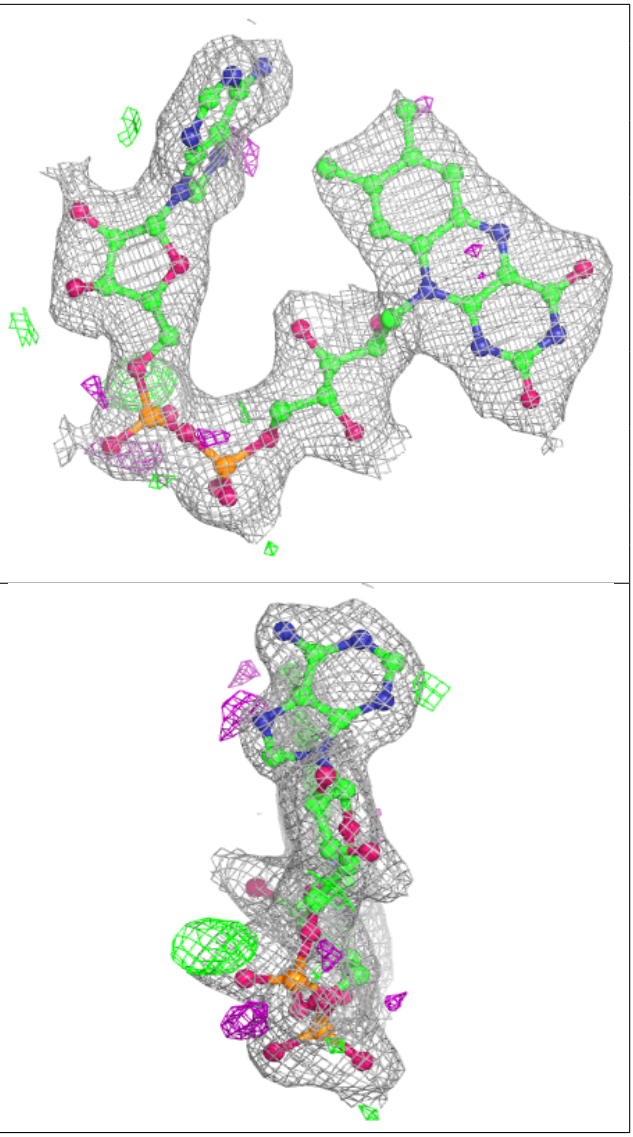


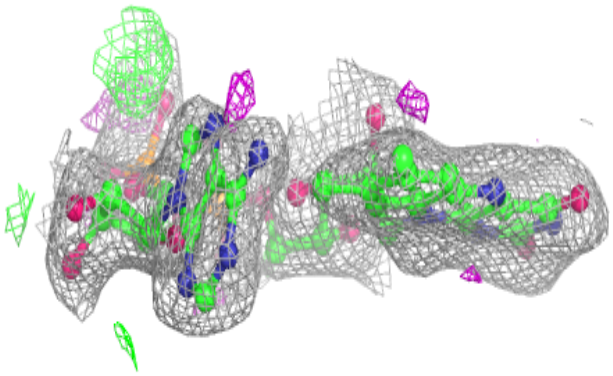




Electron density around FAD K 1103:

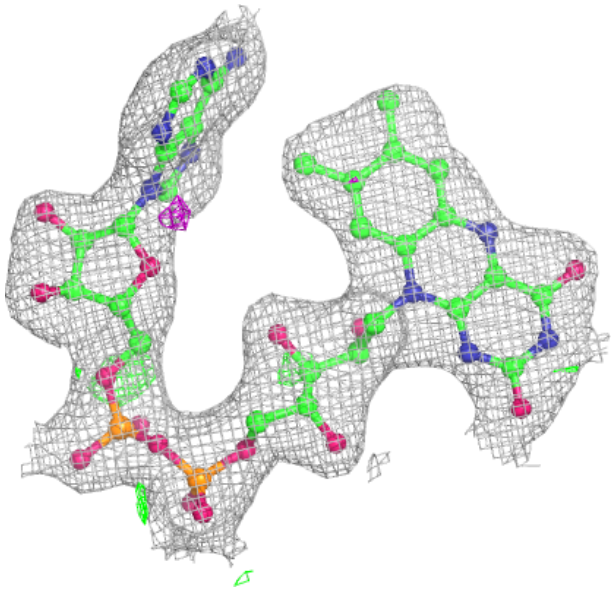
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

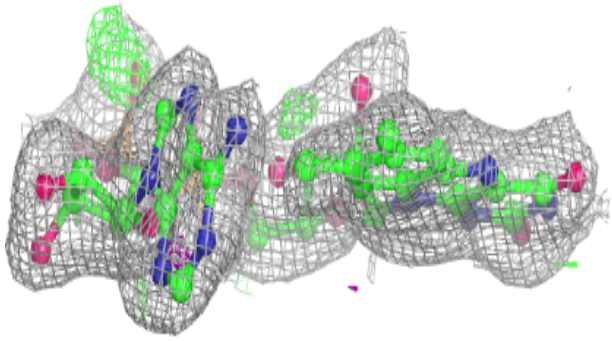


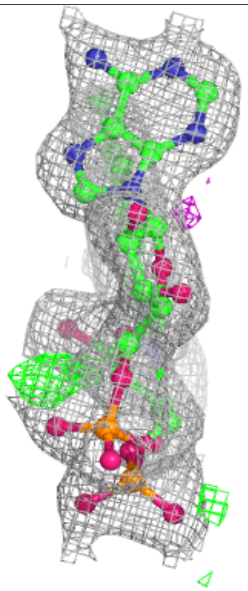


Electron density around FAD E 1103:

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

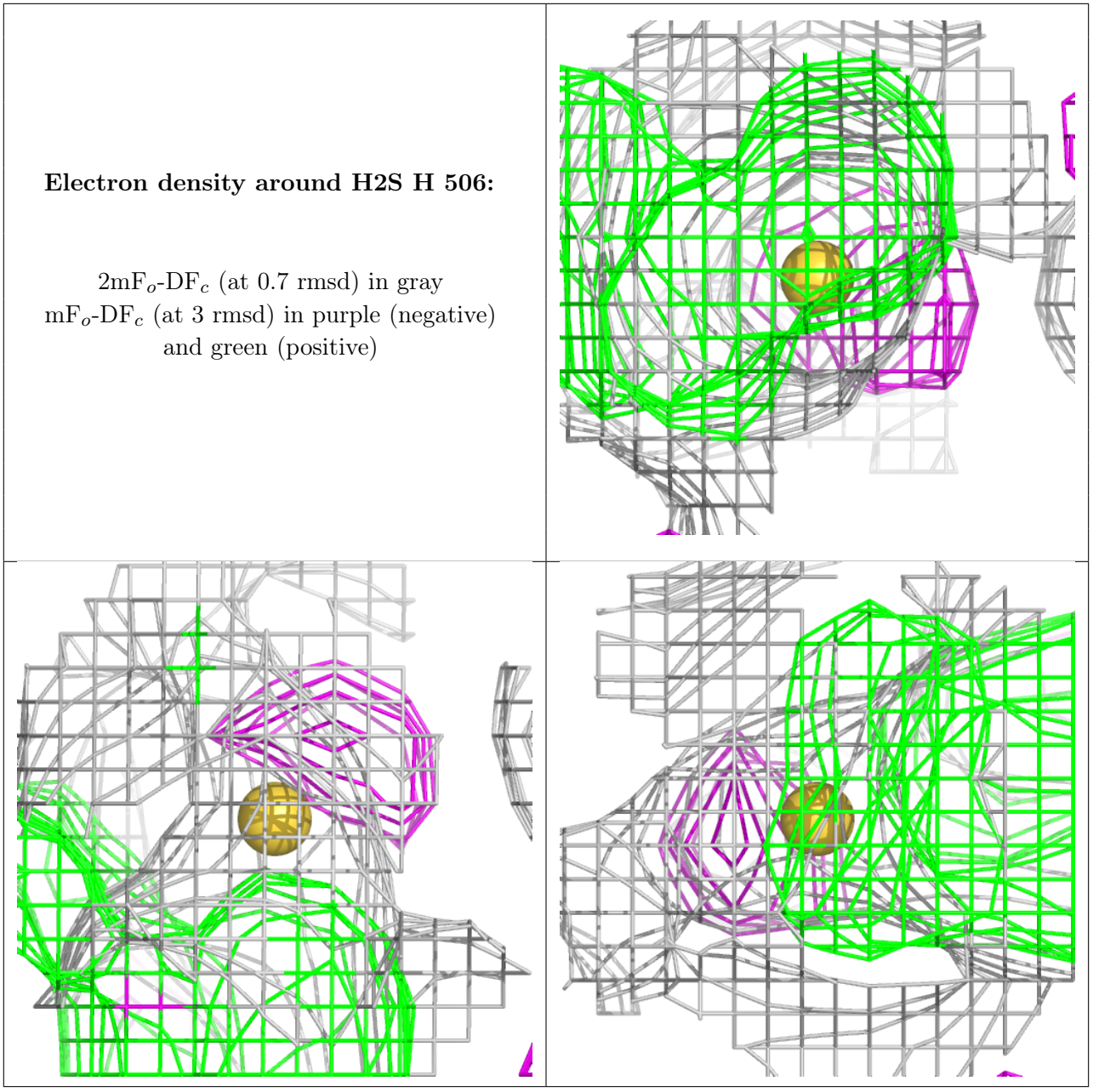






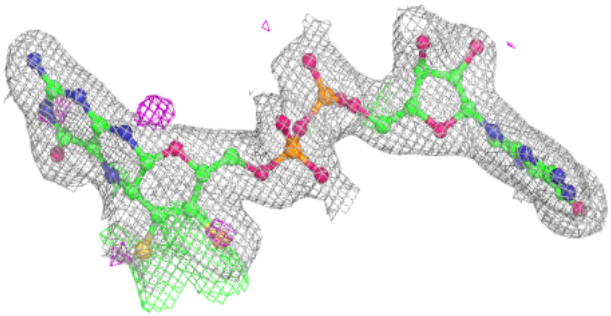
Electron density around H2S H 506:

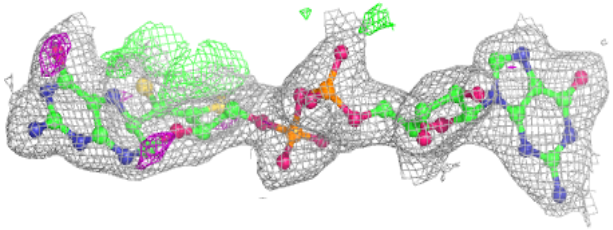
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

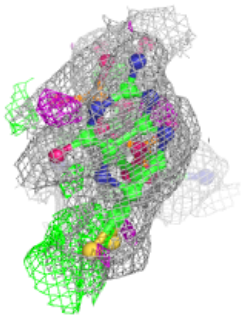


Electron density around MGD H 504:

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

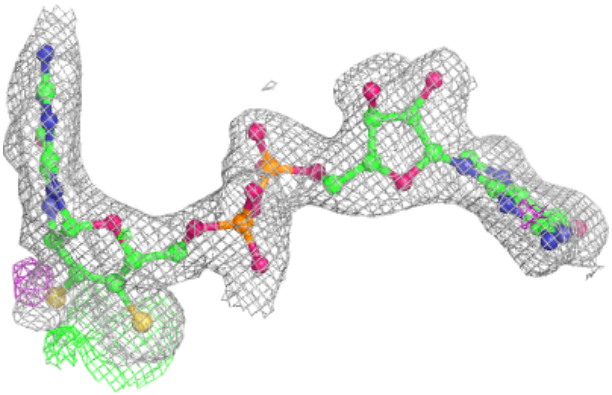


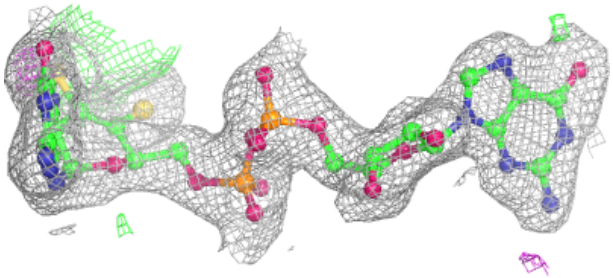


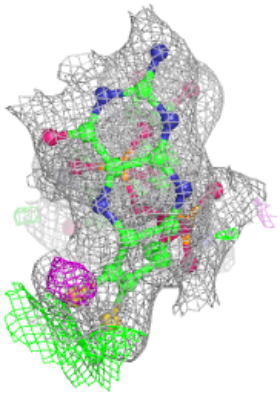


Electron density around MGD H 503:

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

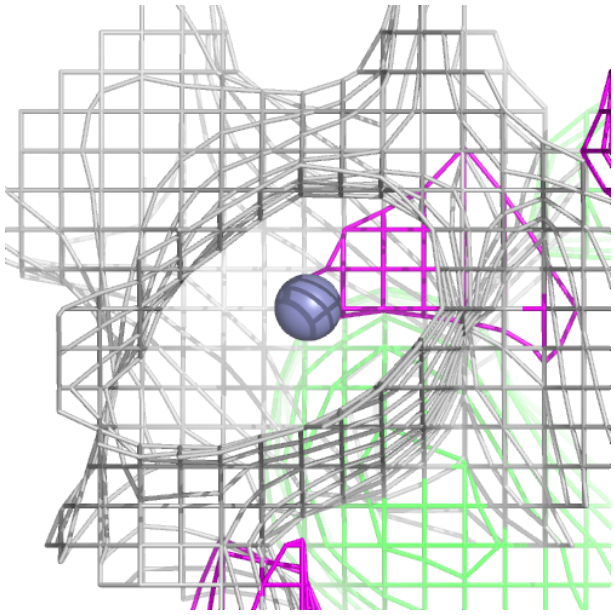


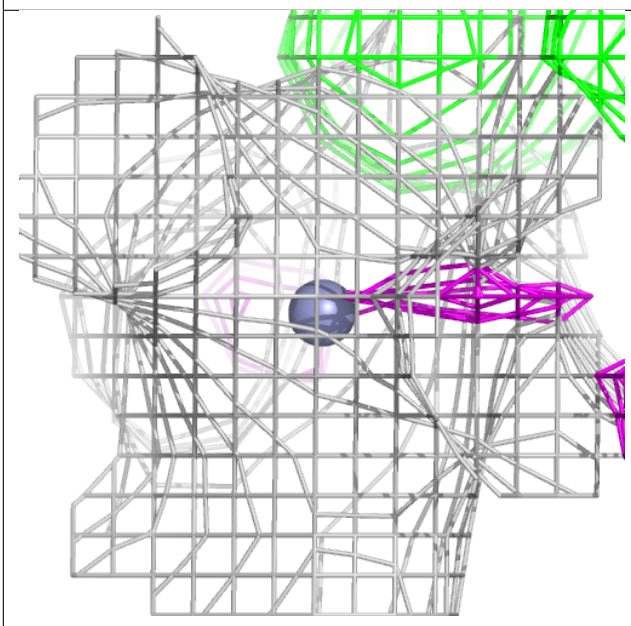


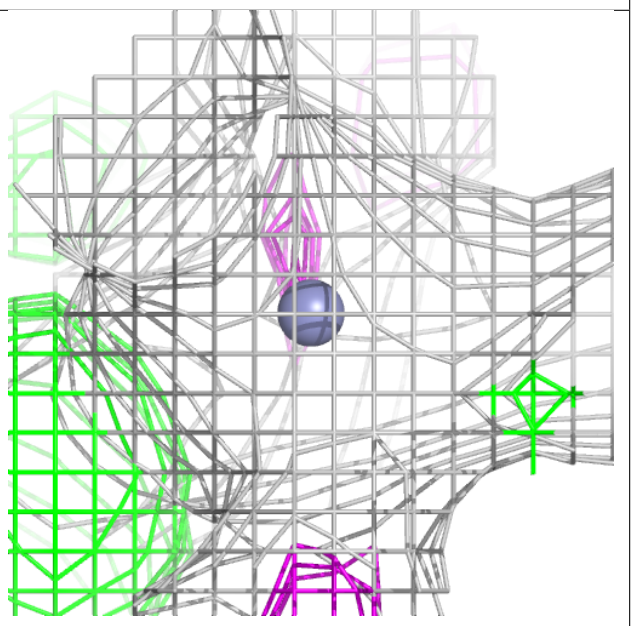


Electron density around ZN G 601:

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

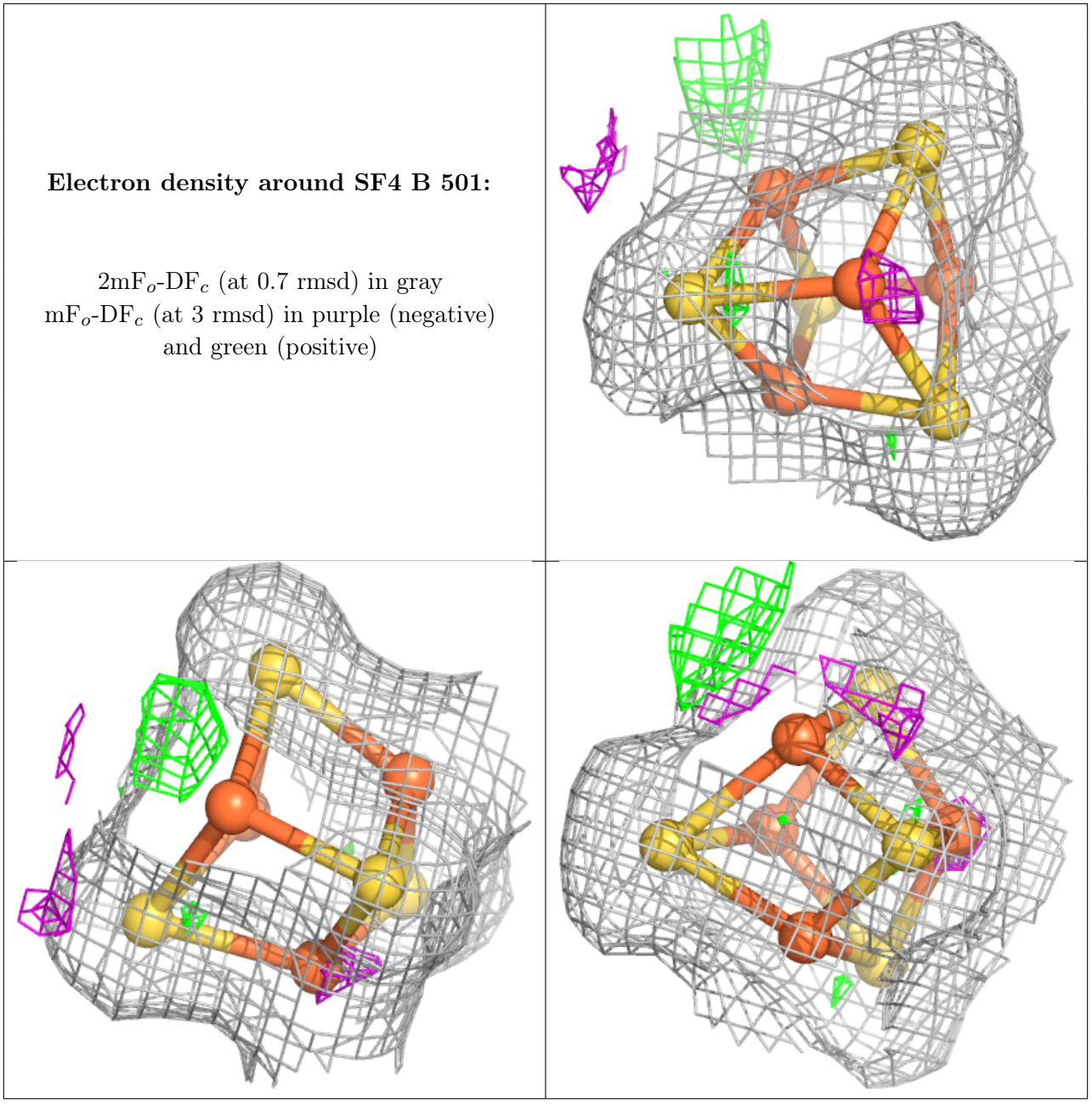






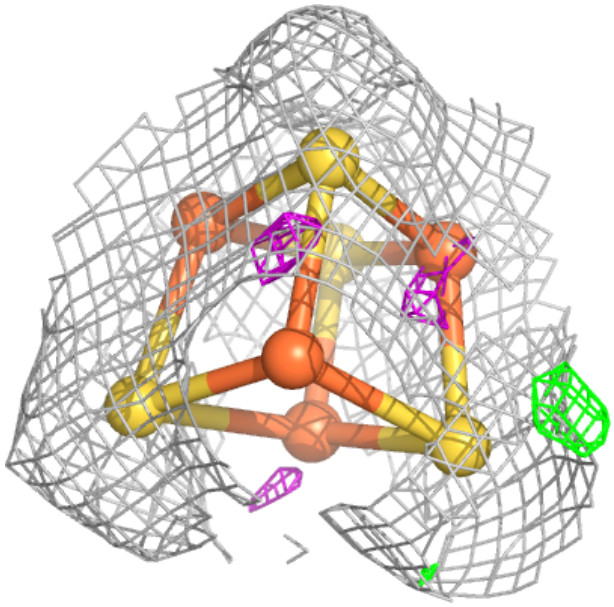
Electron density around SF4 B 501:

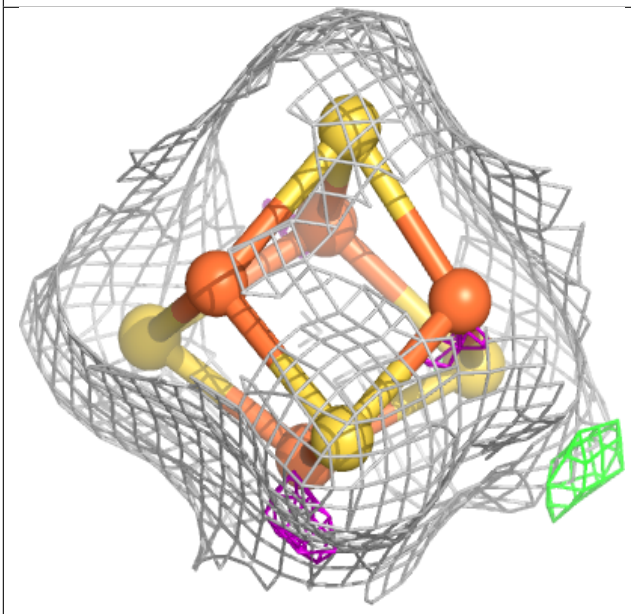
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

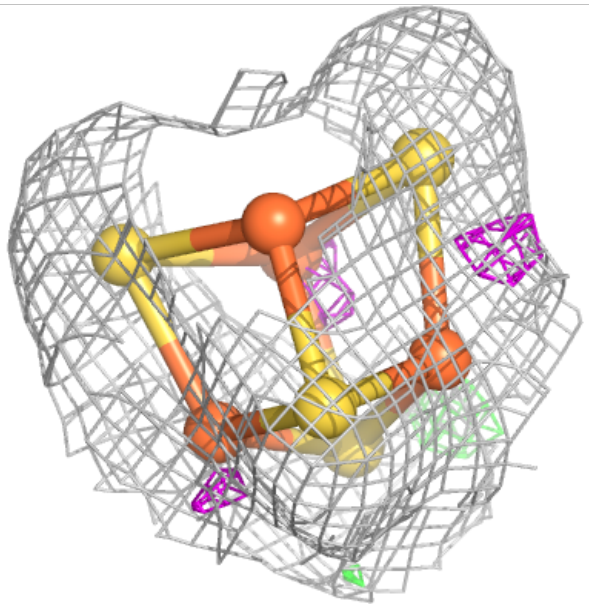


Electron density around SF4 E 1101:

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

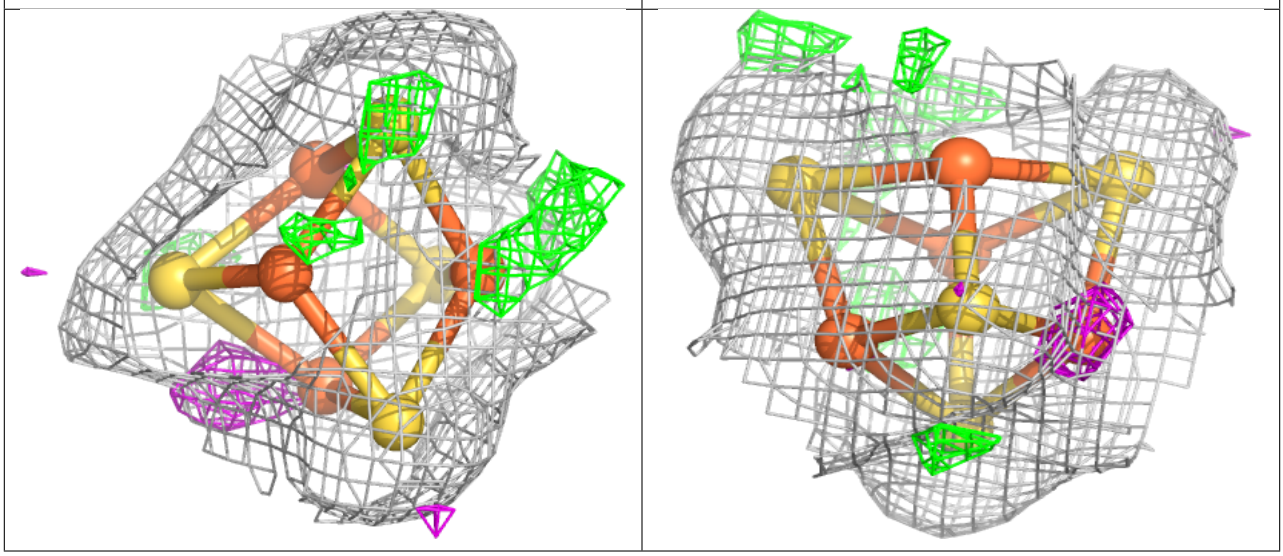






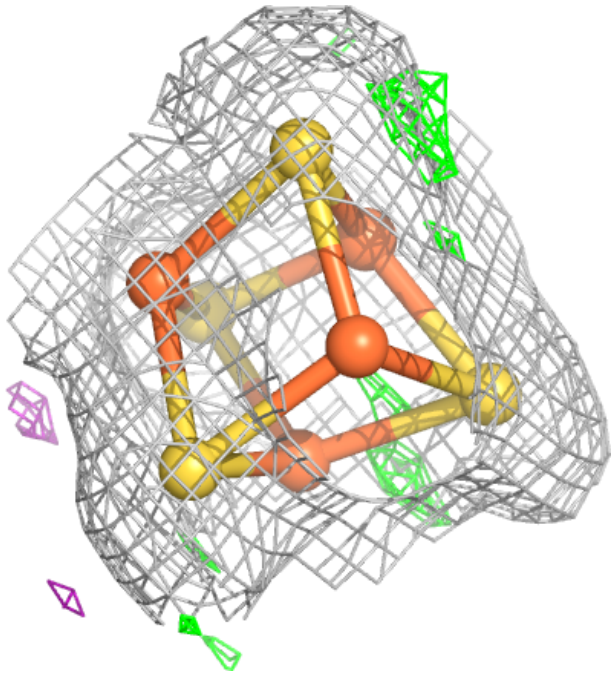
Electron density around SF4 E 1104:

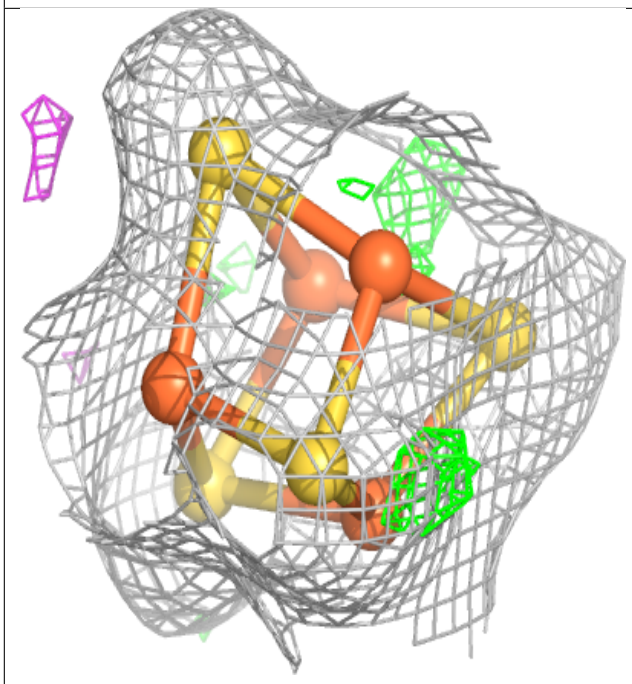
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

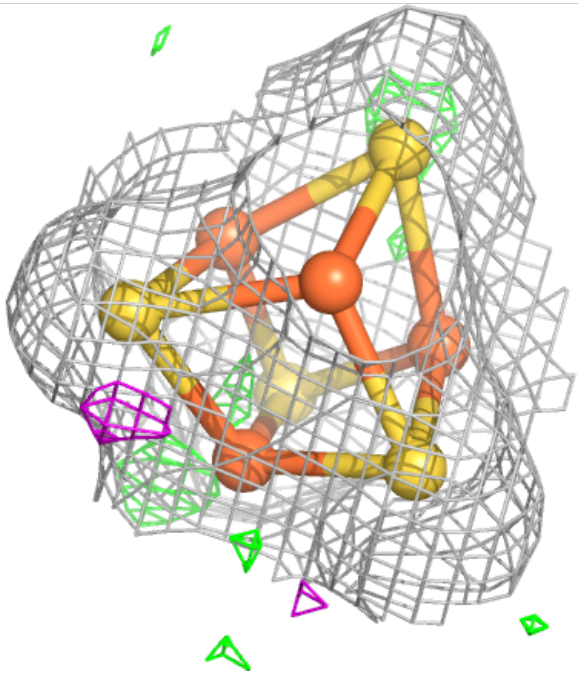


Electron density around SF4 F 101:

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

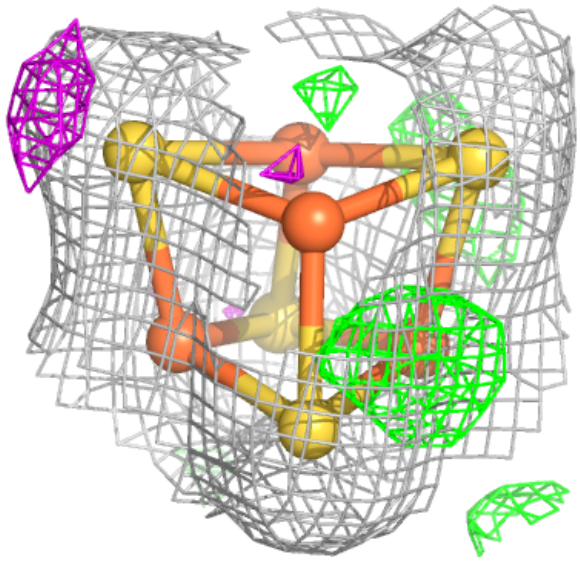


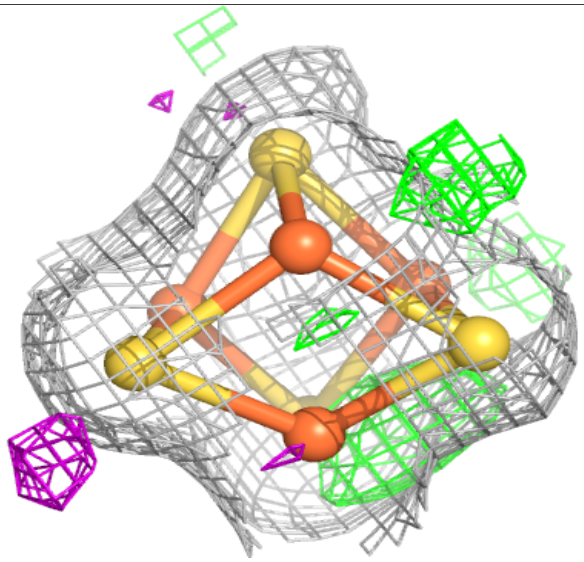


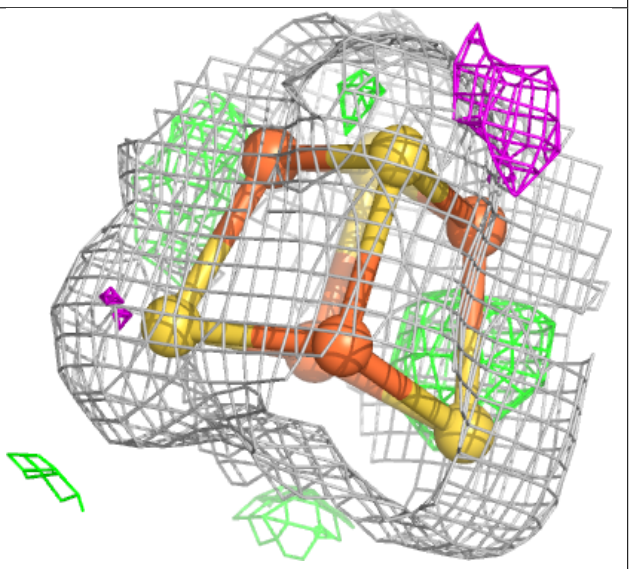


Electron density around SF4 H 501:

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

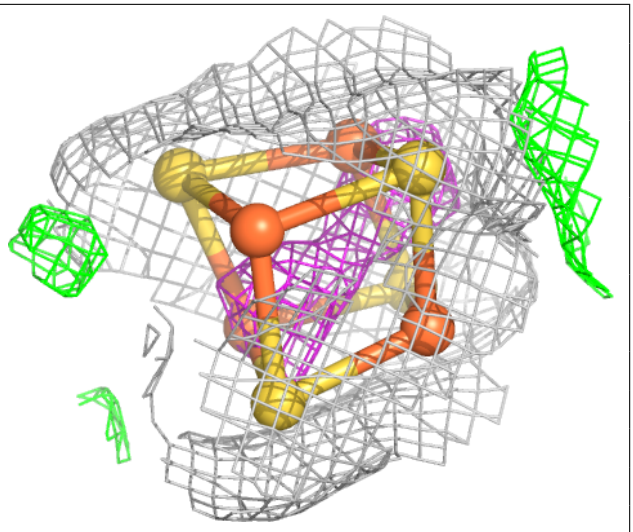


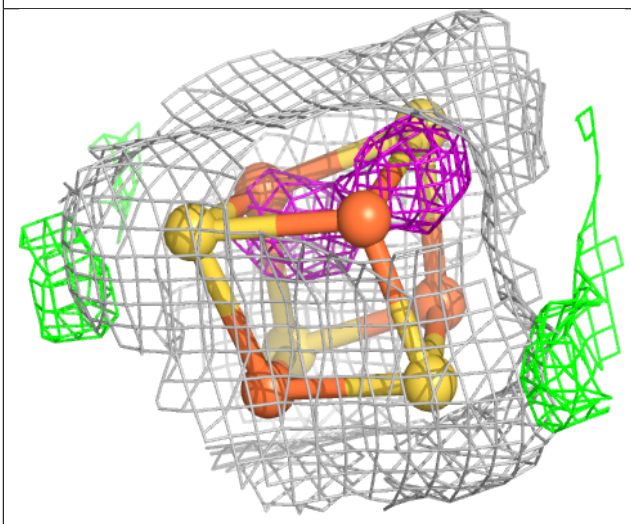


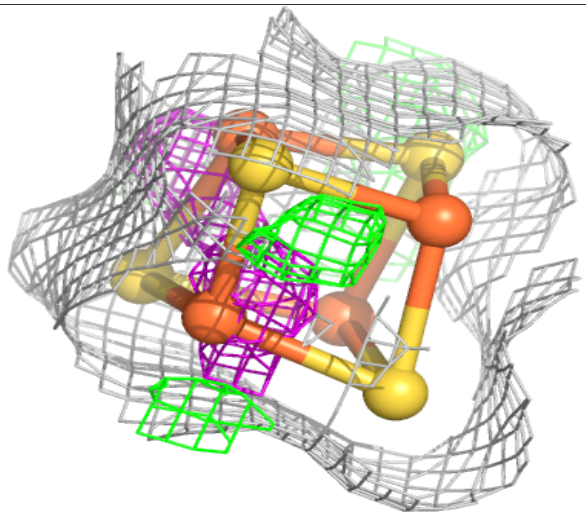


Electron density around SF4 K 1101:

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

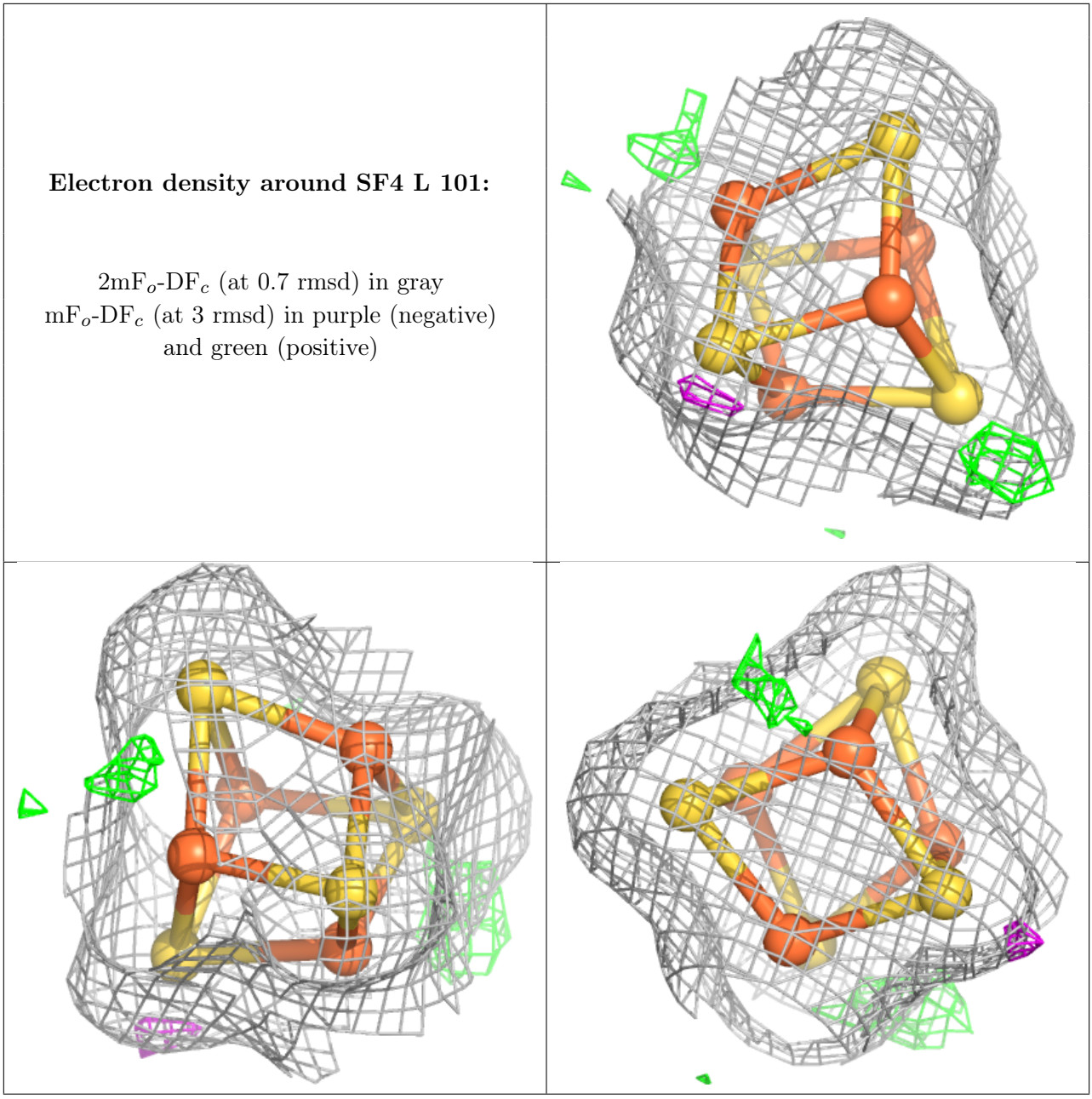






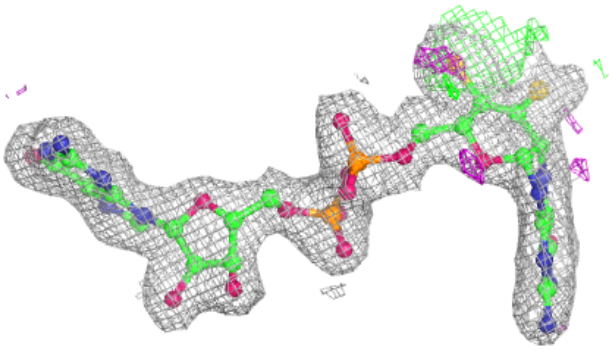
Electron density around SF4 L 101:

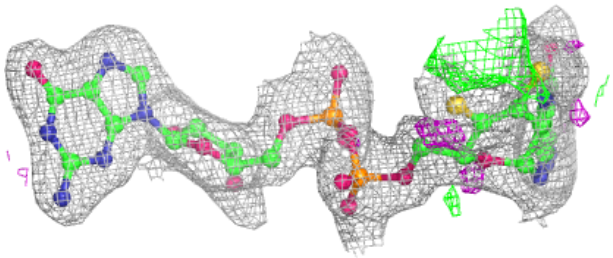
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

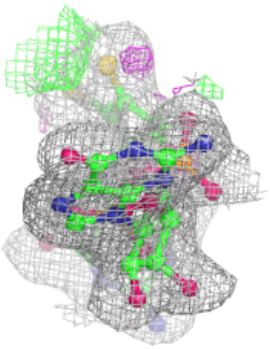


Electron density around MGD B 503:

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

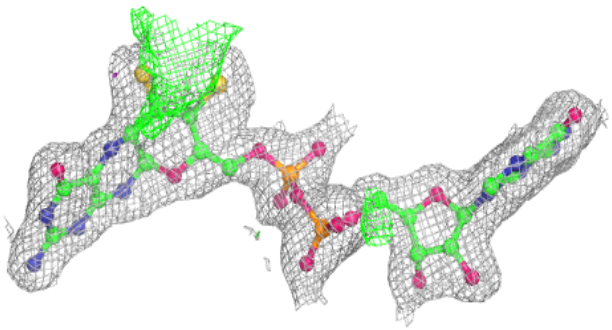


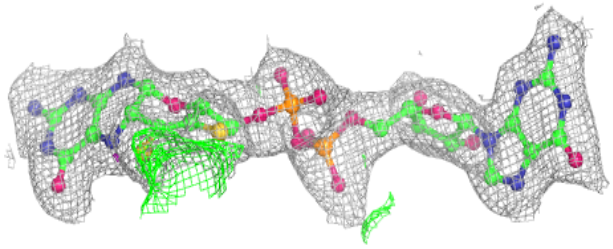


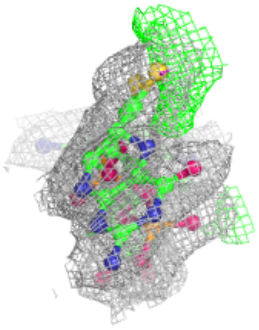


Electron density around MGD B 504:

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

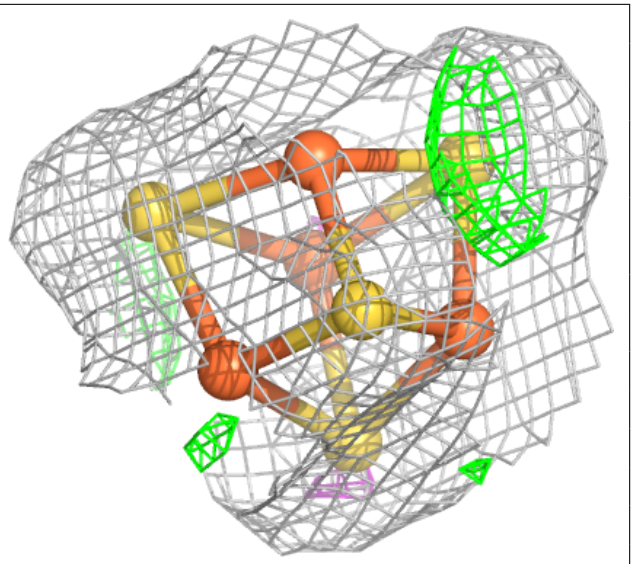


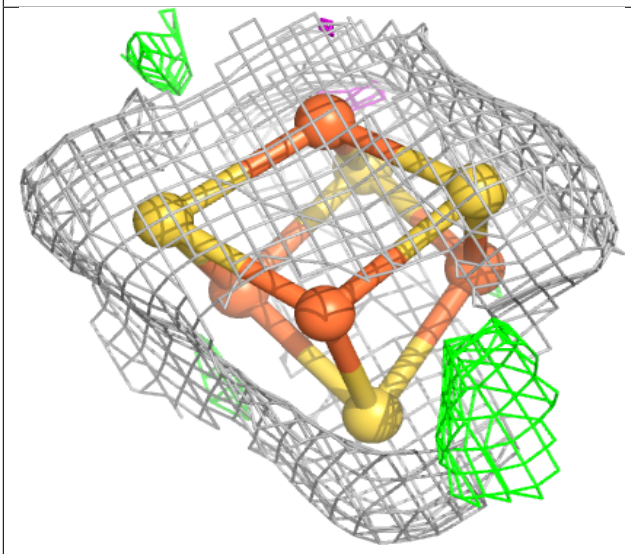


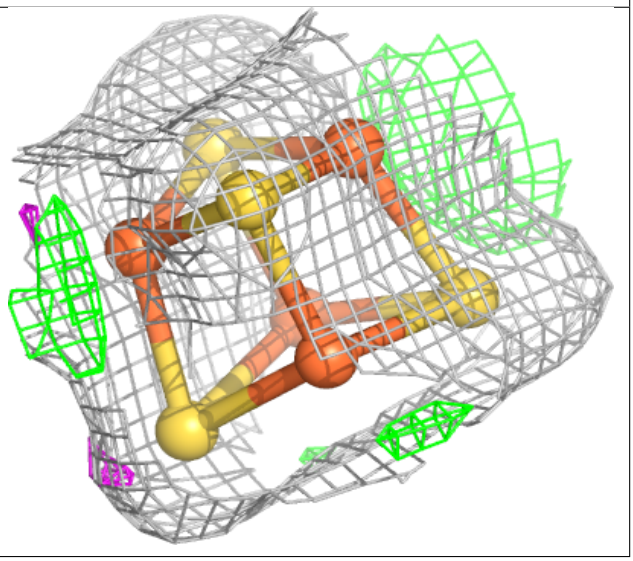


Electron density around SF4 K 1104:

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

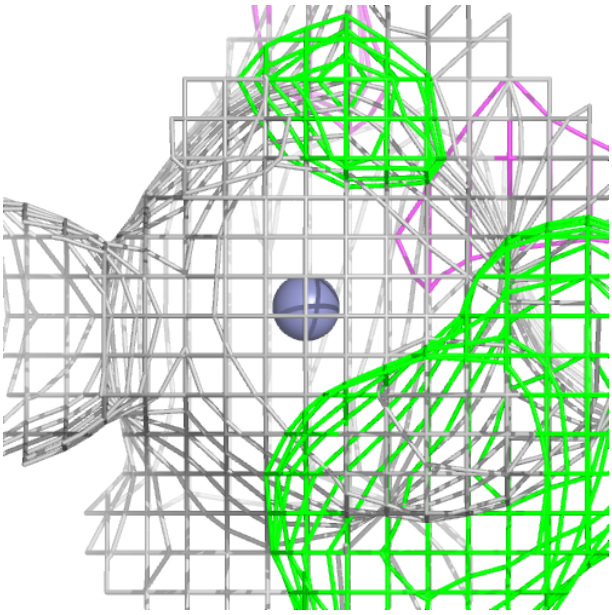


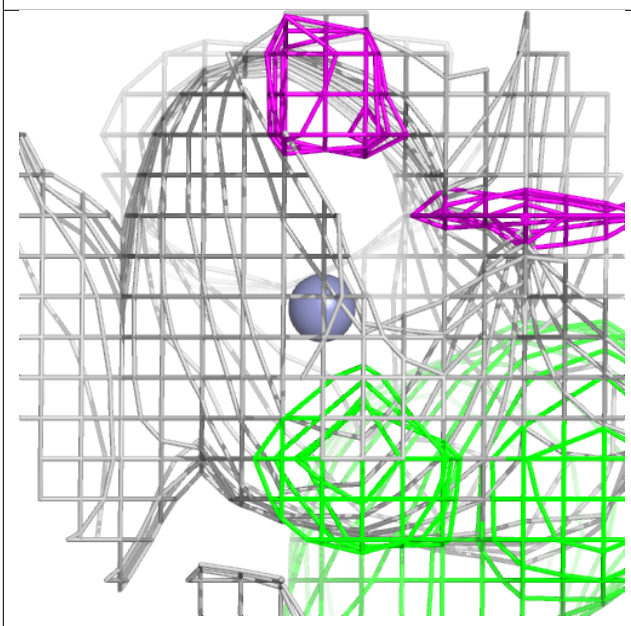


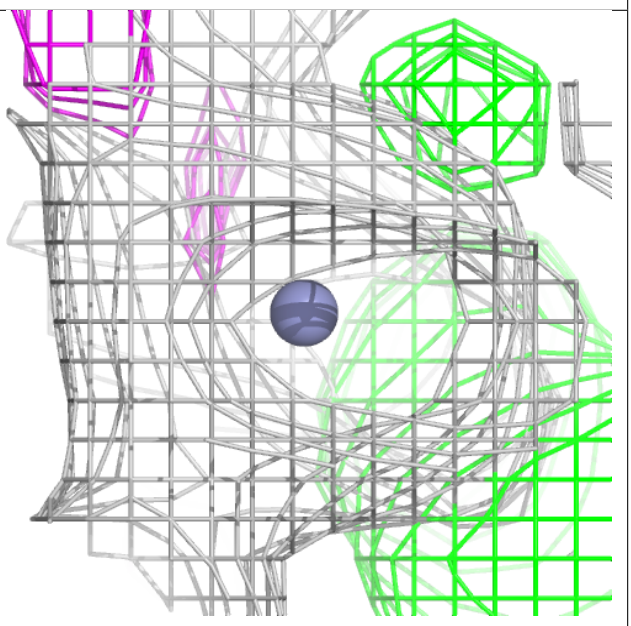


Electron density around ZN G 602:

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

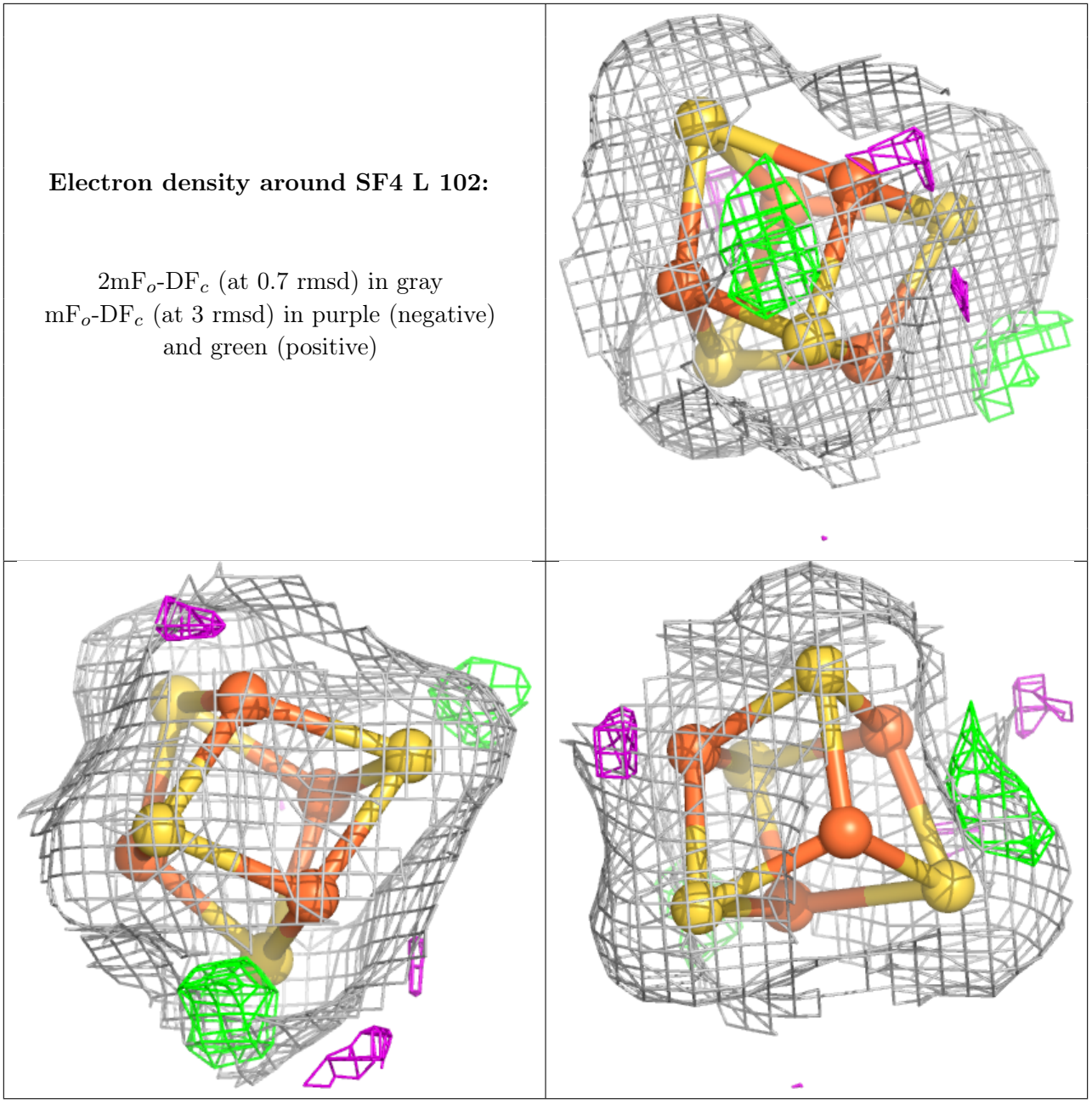






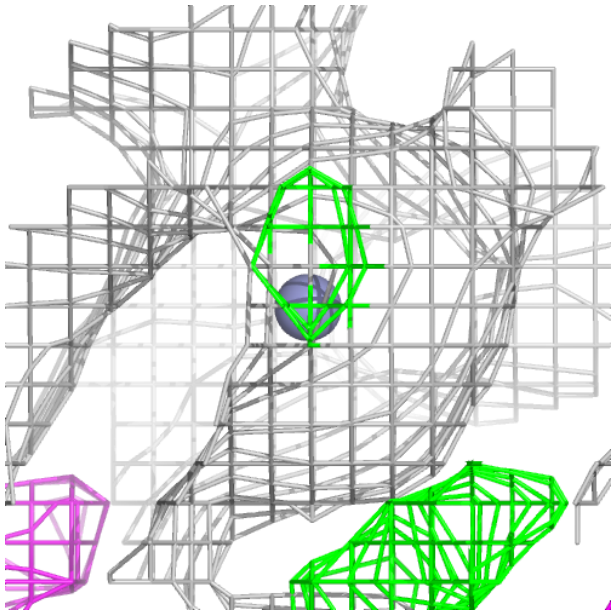
Electron density around SF4 L 102:

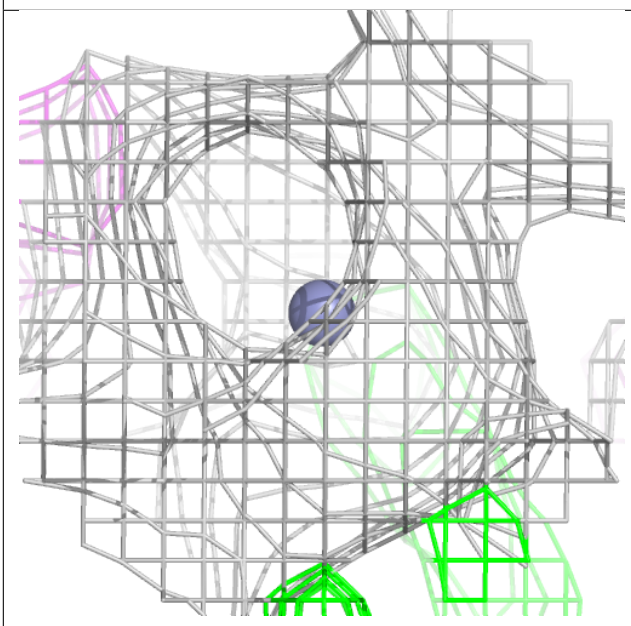
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

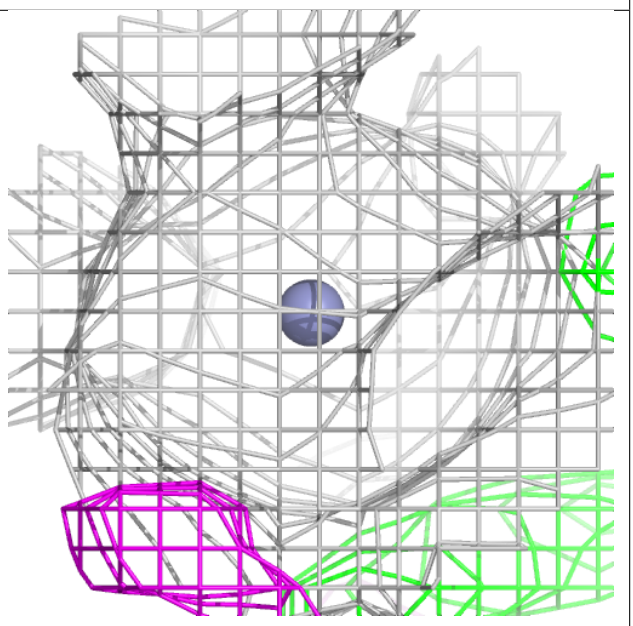


Electron density around ZN A 602:

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

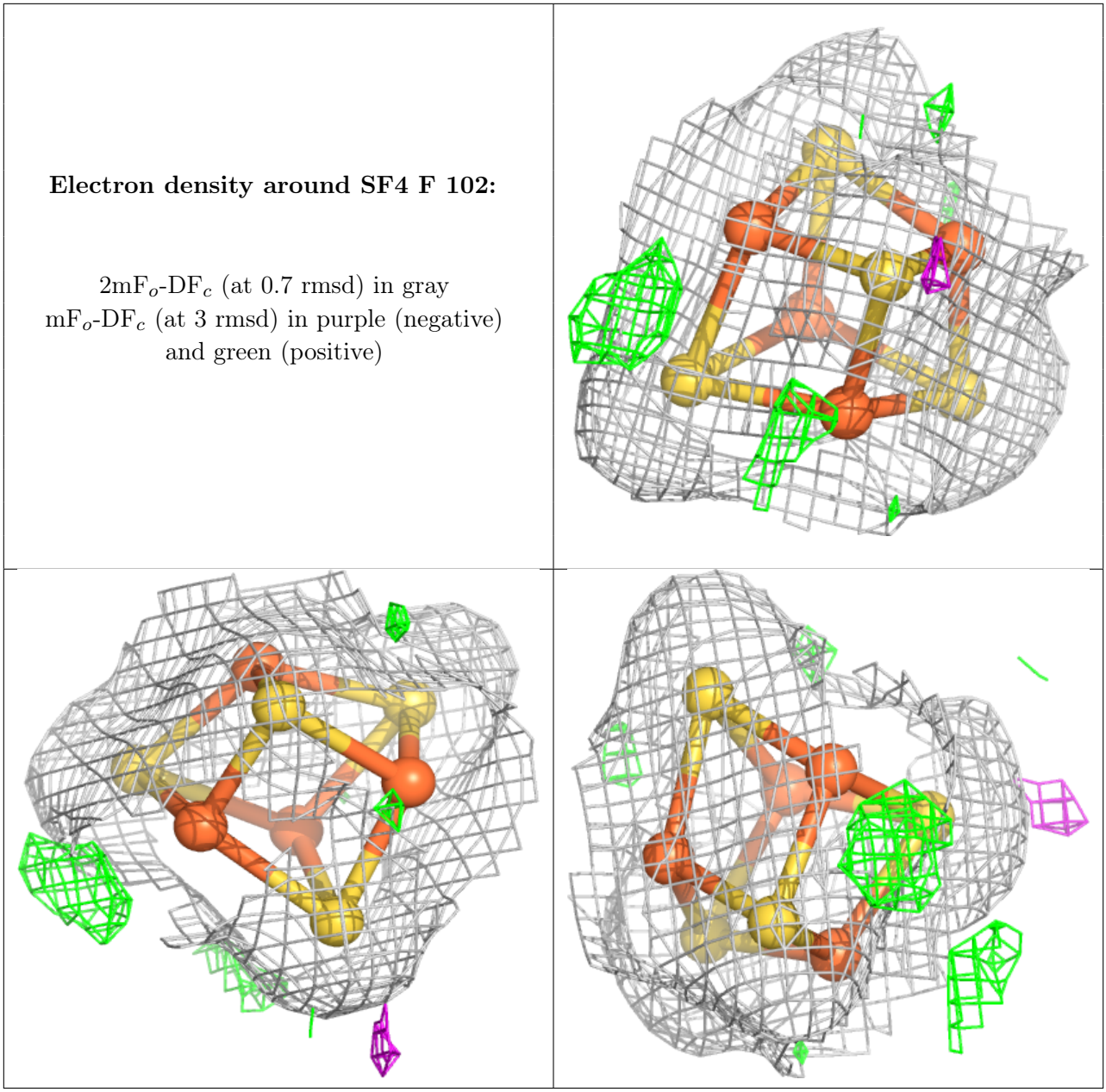






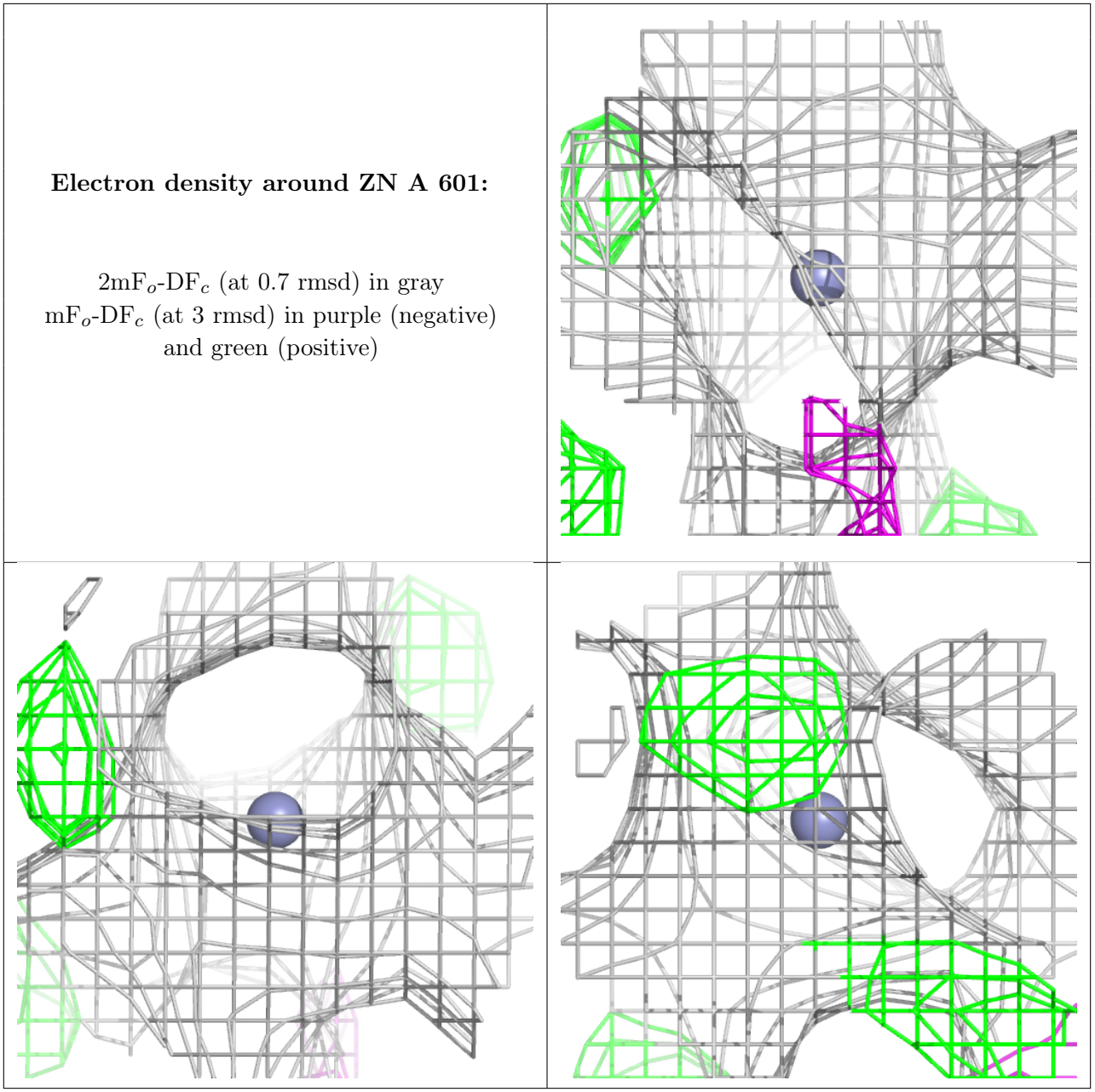
Electron density around SF4 F 102:

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



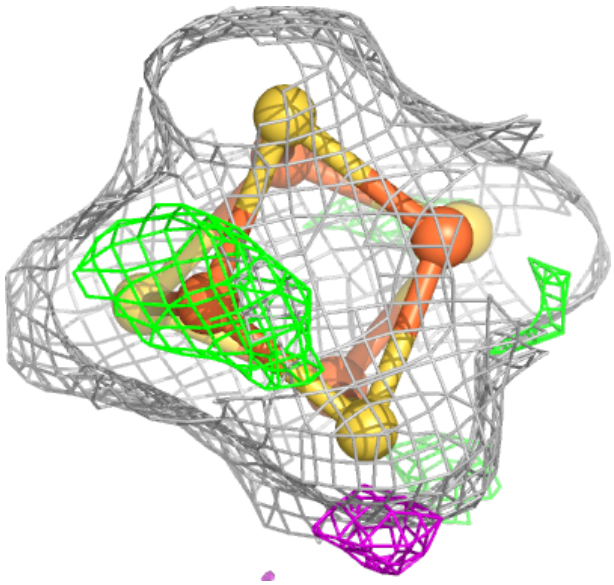
Electron density around ZN A 601:

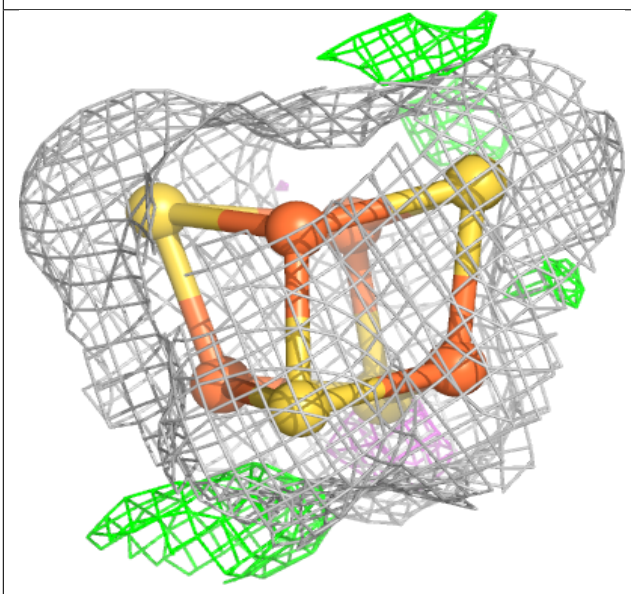
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

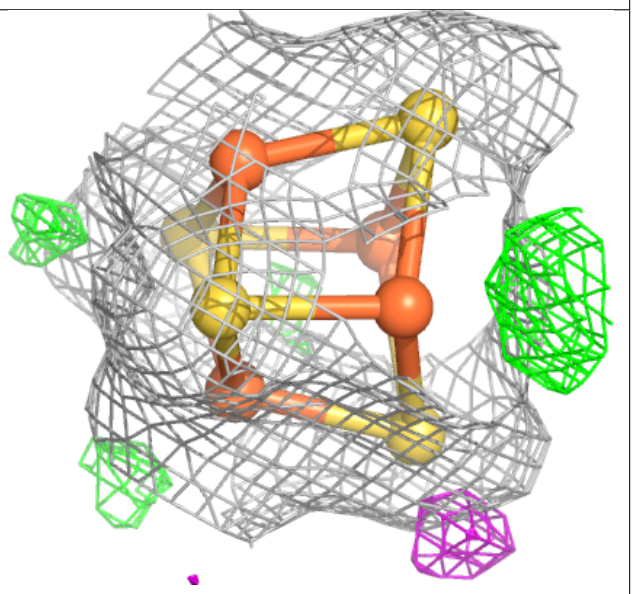


Electron density around SF4 E 1102:

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

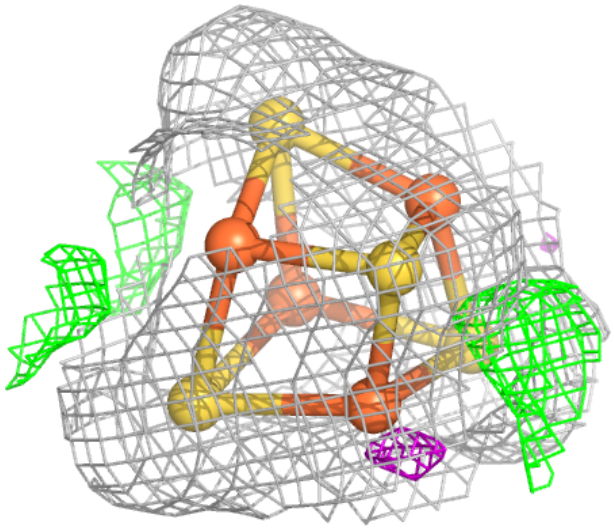


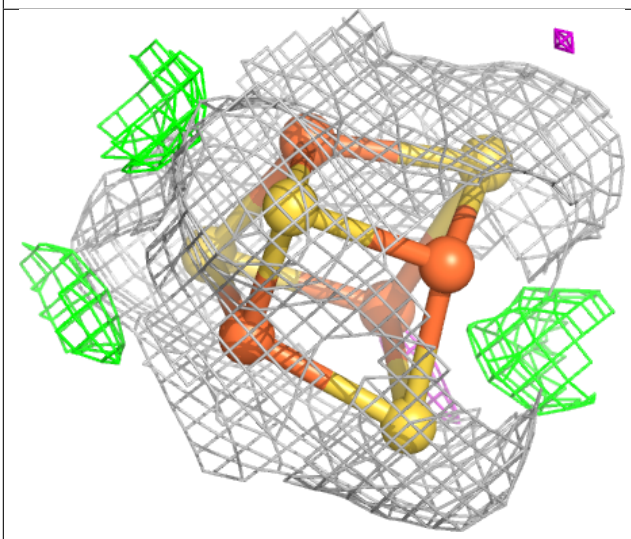


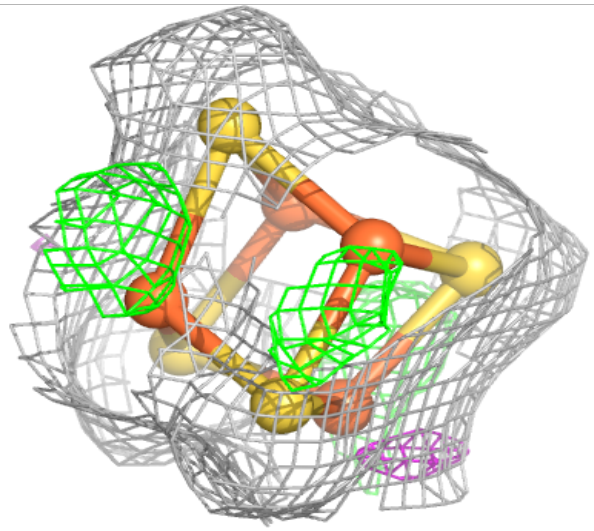


Electron density around SF4 K 1102:

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

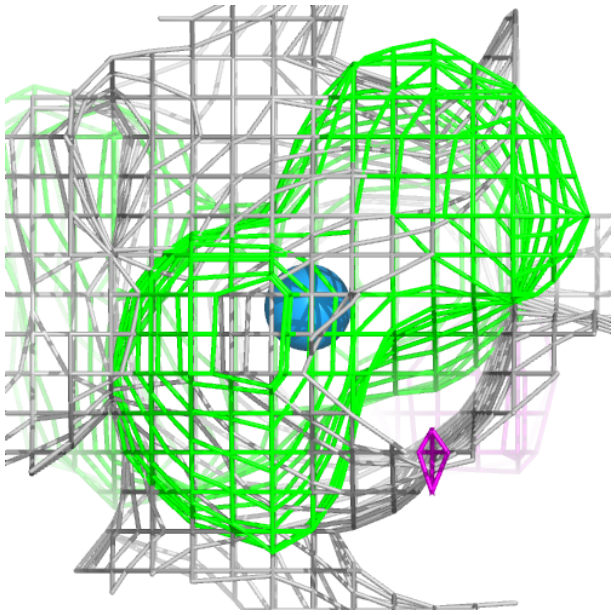


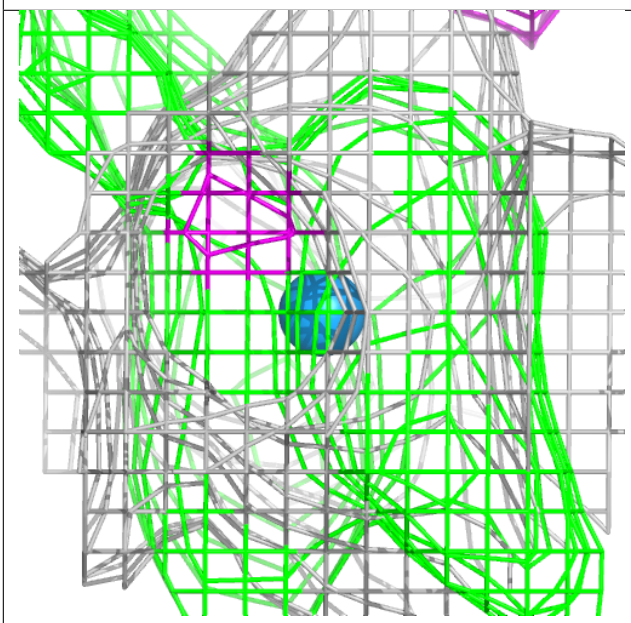


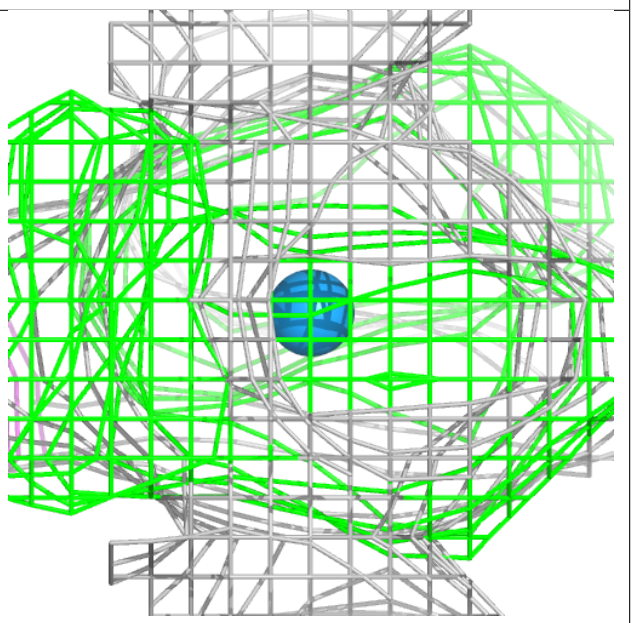


Electron density around W H 502:

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

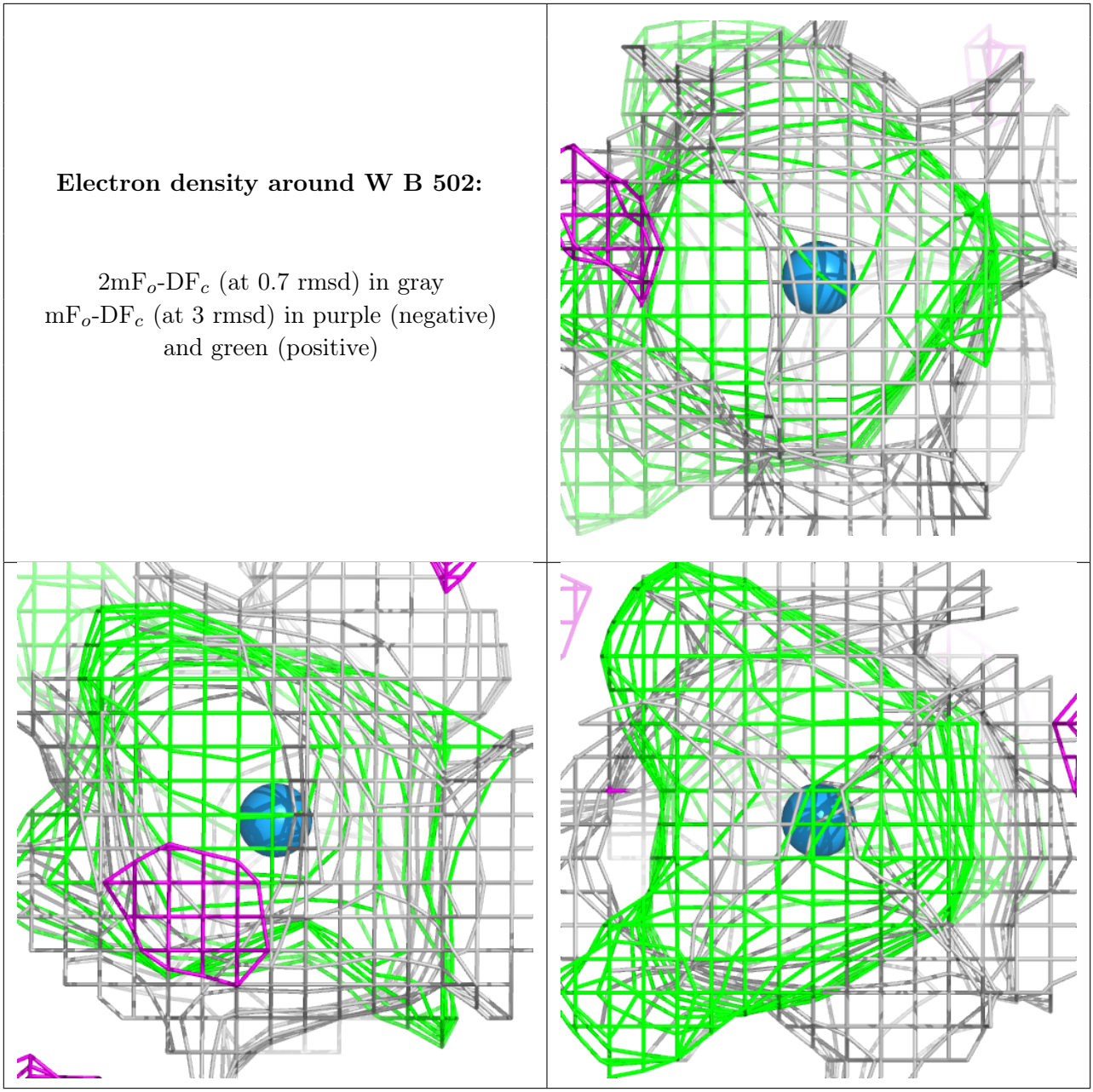






Electron density around W B 502:

$2mF_o$-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 (i)

There are no such residues in this entry.