wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 04:29 AM EDT

PDB ID	:	7M31
Title	:	Dihydropyrimidine Dehydrogenase (DPD) C671S Mutant Soaked with Thymine and NADPH Anaerobically
Authors	:	Butrin, A.; Beaupre, B.; Forouzesh, D.; Liu, D.; Moran, G.
Deposited on	:	2021-03-18
Resolution	:	1.69 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

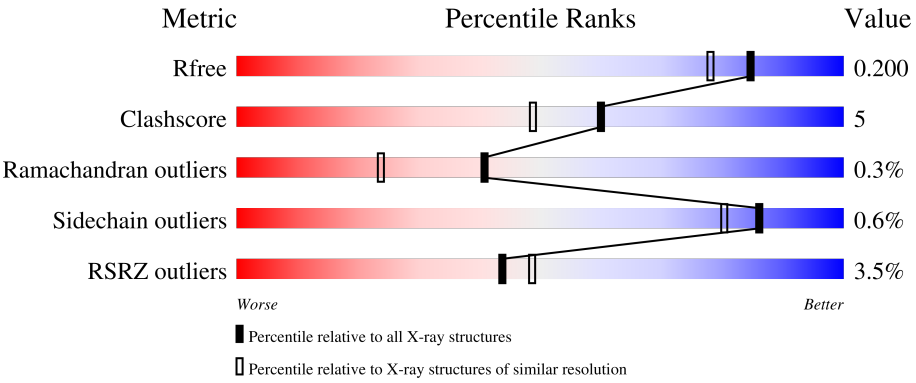
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.69 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	1025	3% 89% 9% .
1	B	1025	4% 90% 8% ..
1	C	1025	3% 88% 9% .
1	D	1025	4% 90% 9% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	TDR	A	1108	-	X	-	-
6	TDR	B	1107	-	X	-	-
6	TDR	C	1108	-	X	-	-
6	TDR	D	1107	-	X	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 35847 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.

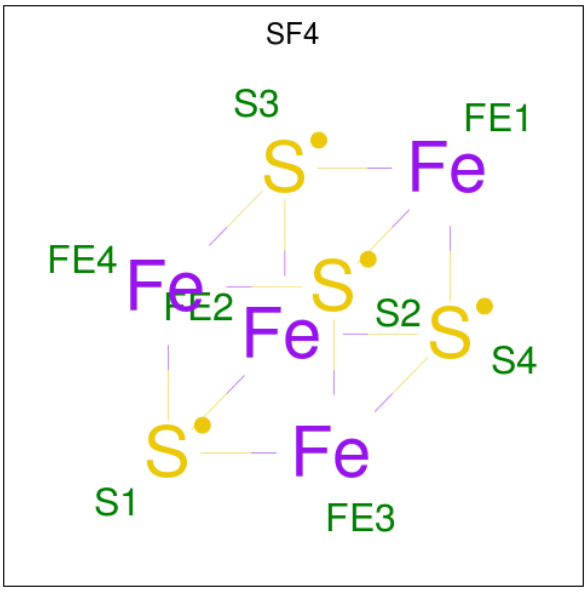
- Molecule 1 is a protein called Dihydropyrimidine dehydrogenase [NADP(+)].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	42	4	0
			7705	4886	1306	1459	54			
1	B	1011	Total	C	N	O	S	34	3	0
			7734	4905	1309	1466	54			
1	C	1007	Total	C	N	O	S	0	2	0
			7671	4869	1297	1452	53			
1	D	1017	Total	C	N	O	S	43	1	0
			7740	4910	1313	1462	55			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLY	conflict	UNP Q28943
A	671	SER	CYS	engineered mutation	UNP Q28943
B	60	ASP	GLY	conflict	UNP Q28943
B	671	SER	CYS	engineered mutation	UNP Q28943
C	60	ASP	GLY	conflict	UNP Q28943
C	671	SER	CYS	engineered mutation	UNP Q28943
D	60	ASP	GLY	conflict	UNP Q28943
D	671	SER	CYS	engineered mutation	UNP Q28943

- Molecule 2 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
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	C	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0

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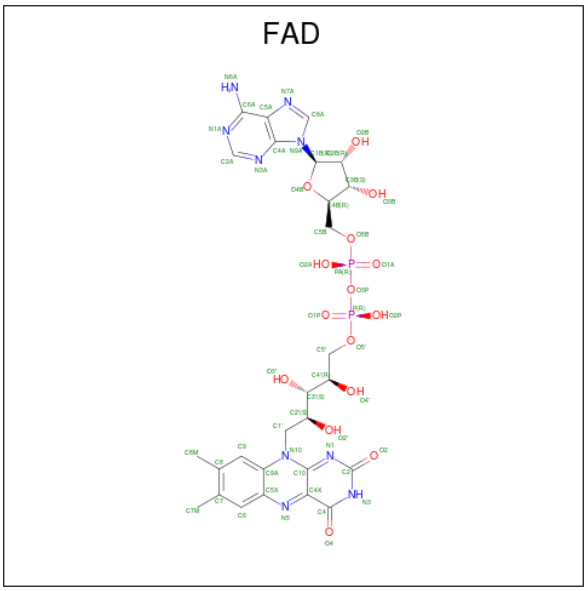
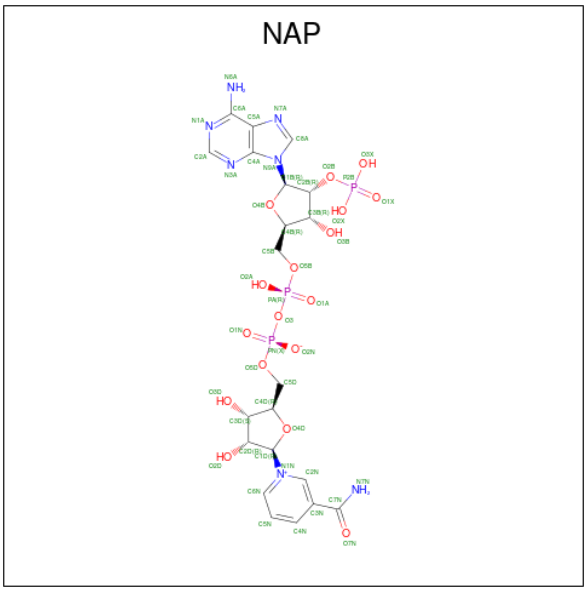
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0

- Molecule 3 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).



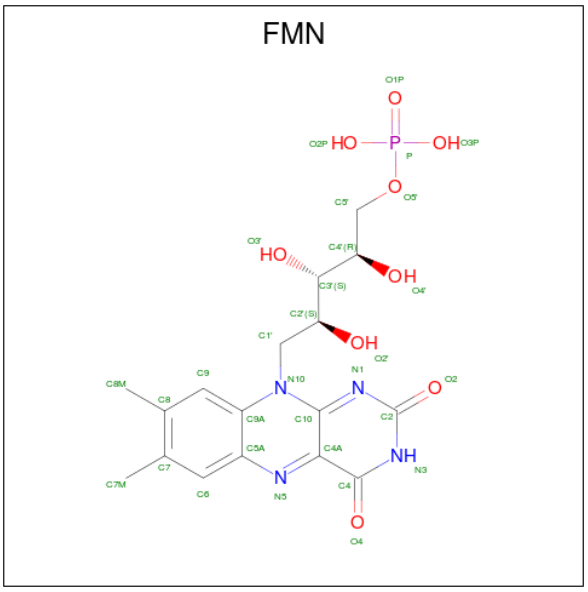
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 53 27 9 15 2	0	0
3	B	1	Total C N O P 53 27 9 15 2	0	0
3	C	1	Total C N O P 53 27 9 15 2	0	0
3	D	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



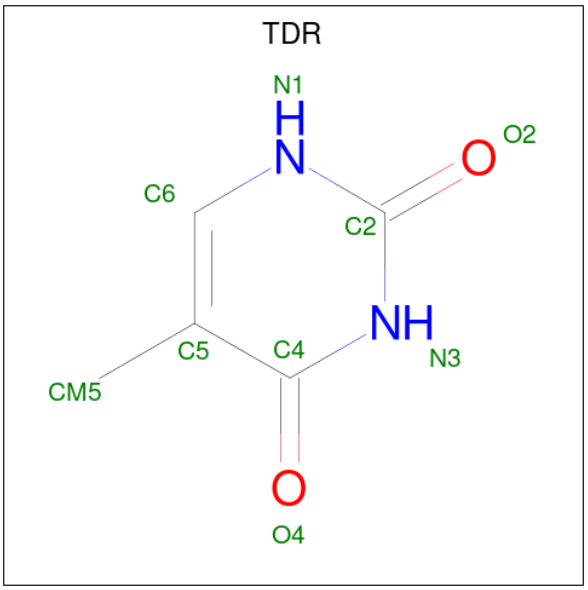
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	D	1	Total	C	N	O	P	0	0
			40	15	6	16	3		

- Molecule 5 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



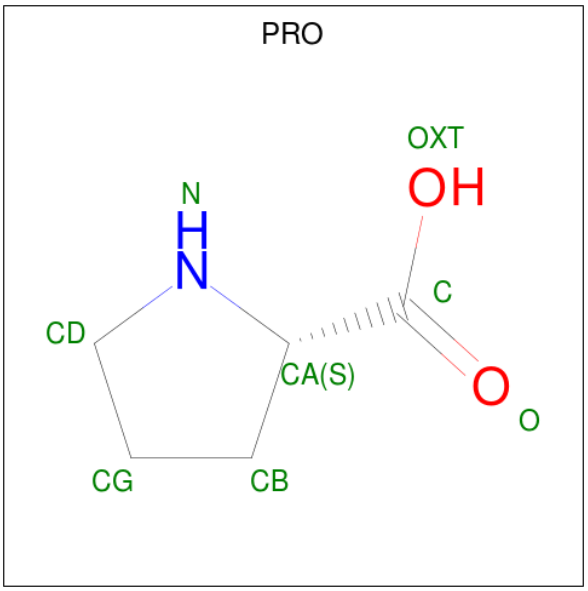
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 31 17 4 9 1	0	0
5	B	1	Total C N O P 31 17 4 9 1	0	0
5	C	1	Total C N O P 31 17 4 9 1	0	0
5	D	1	Total C N O P 31 17 4 9 1	0	0

- Molecule 6 is THYMINE (three-letter code: TDR) (formula: $C_5H_6N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 9 5 2 2	0	0
6	B	1	Total C N O 9 5 2 2	0	0
6	C	1	Total C N O 9 5 2 2	0	0
6	D	1	Total C N O 9 5 2 2	0	0

- Molecule 7 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C N O 7 5 1 1	0	0

- Molecule 8 is water.

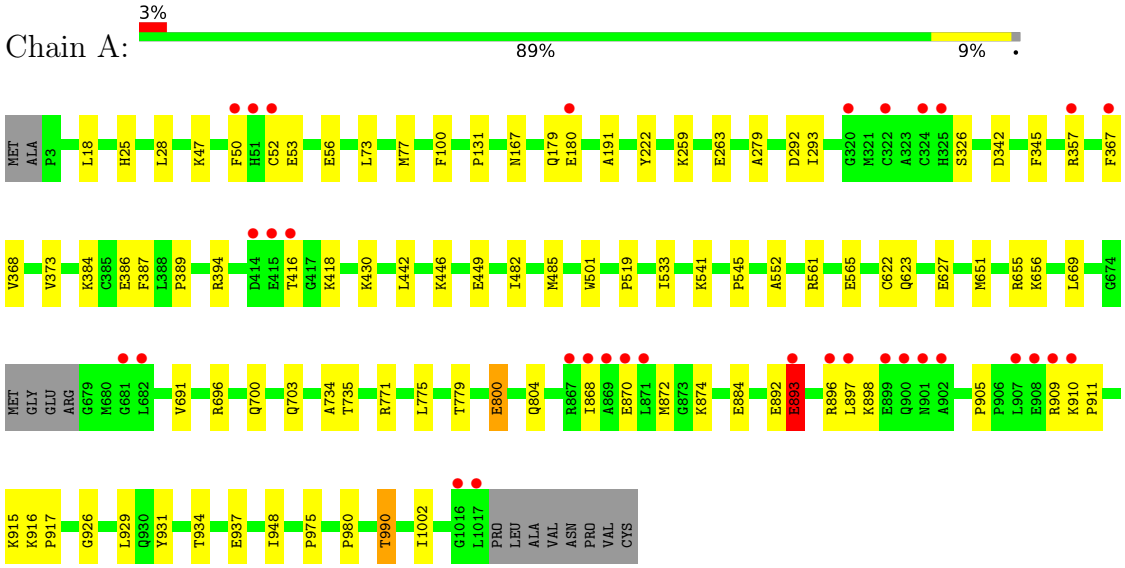
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1072	Total O 1072 1072	0	0
8	B	1004	Total O 1004 1004	0	0
8	C	1103	Total O 1103 1103	0	0
8	D	1127	Total O 1127 1127	0	0

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.

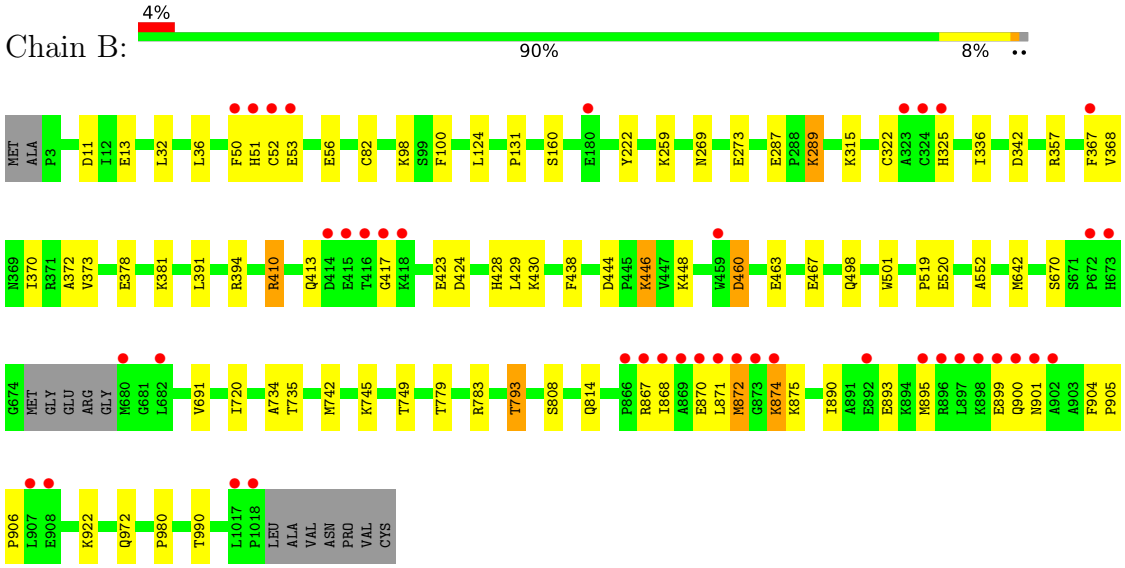
• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]

Chain A:



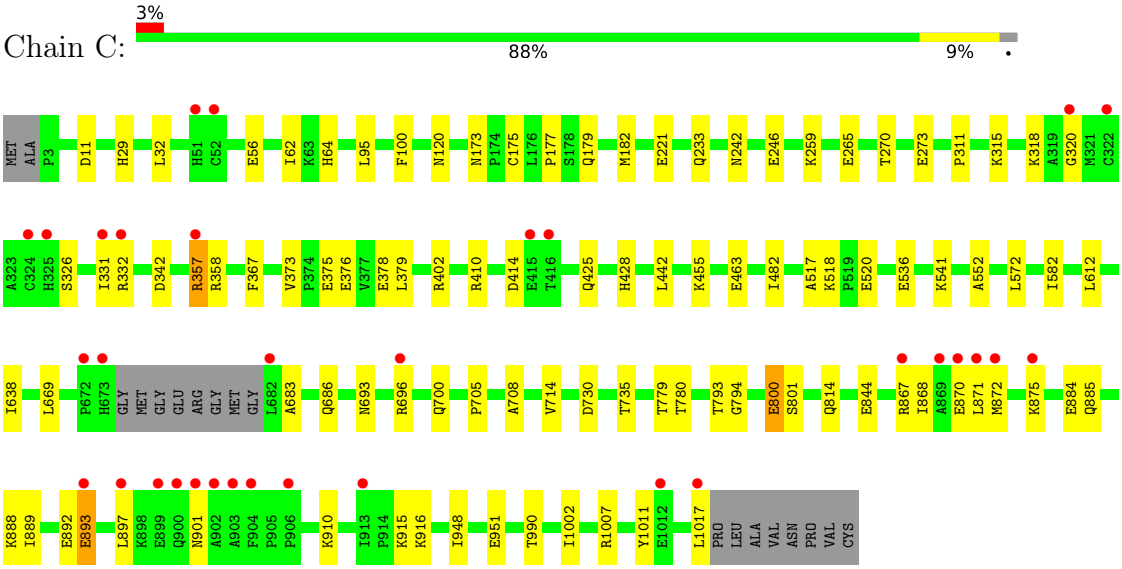
• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]

Chain B:



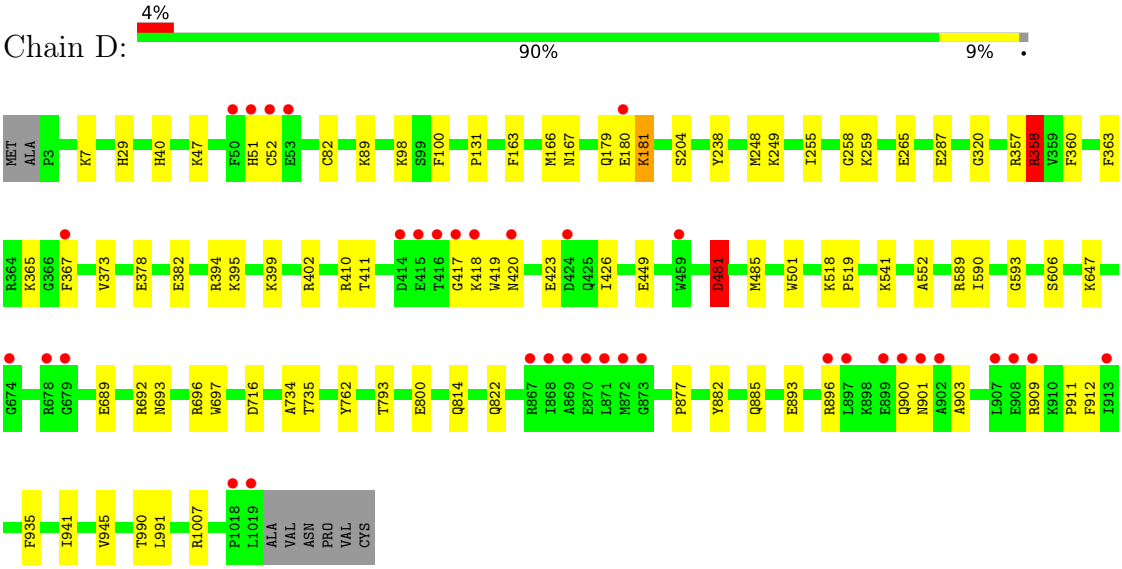
• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]

Chain C:



• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.04Å 159.56Å 162.95Å 90.00° 95.75° 90.00°	Depositor
Resolution (Å)	36.15 – 1.69 45.35 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.0 (36.15-1.69) 99.0 (45.35-1.69)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 1.69Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.177 , 0.200 0.177 , 0.200	Depositor DCC
R_{free} test set	22720 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	35847	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: FMN, FAD, NAP, SF4, TDR

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	0.31	0/7865	0.57	2/10665 (0.0%)
1	B	0.32	0/7895	0.57	1/10701 (0.0%)
1	C	0.32	0/7829	0.86	7/10616 (0.1%)
1	D	0.31	0/7902	0.63	8/10714 (0.1%)
All	All	0.31	0/31491	0.67	18/42696 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	520	GLU	OE1-CD-OE2	-39.23	76.22	123.30
1	C	893	GLU	OE1-CD-OE2	-34.84	81.49	123.30
1	C	893	GLU	CG-CD-OE1	21.13	160.56	118.30
1	C	520	GLU	CG-CD-OE1	19.86	158.01	118.30
1	C	893	GLU	CG-CD-OE2	-19.35	79.60	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	50	PHE	Peptide
1	C	402	ARG	Sidechain
1	D	358	ARG	Sidechain
1	D	481	ASP	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7705	0	7690	72	0
1	B	7734	0	7754	79	1
1	C	7671	0	7668	71	0
1	D	7740	0	7746	71	1
2	A	32	0	0	0	0
2	B	32	0	0	0	0
2	C	32	0	0	0	0
2	D	32	0	0	0	0
3	A	53	0	31	1	0
3	B	53	0	31	1	0
3	C	53	0	31	1	0
3	D	53	0	31	0	0
4	A	48	0	25	5	0
4	B	48	0	25	5	0
4	C	48	0	25	4	0
4	D	40	0	19	1	0
5	A	31	0	19	1	0
5	B	31	0	19	1	0
5	C	31	0	19	1	0
5	D	31	0	19	1	0
6	A	9	0	6	0	0
6	B	9	0	6	0	0
6	C	9	0	6	0	0
6	D	9	0	6	0	0
7	C	7	0	7	0	0
8	A	1072	0	0	27	2
8	B	1004	0	0	24	4
8	C	1103	0	0	23	6
8	D	1127	0	0	25	6
All	All	35847	0	31183	285	11

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 5.

The worst 5 of 285 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:MET:SD	8:D:2247:HOH:O	2.19	1.01
1:A:884:GLU:OE1	8:A:1201:HOH:O	1.83	0.96
1:B:315:LYS:NZ	8:B:1204:HOH:O	1.97	0.95
1:A:541:LYS:NZ	8:A:1207:HOH:O	2.02	0.93
1:B:793[B]:THR:HG22	1:B:814:GLN:HB2	1.49	0.93

The worst 5 of 11 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1986:HOH:O	8:D:2013:HOH:O[2_646]	1.61	0.59
8:B:2039:HOH:O	8:C:2227:HOH:O[2_645]	1.85	0.35
8:A:2018:HOH:O	8:C:2268:HOH:O[1_556]	1.95	0.25
8:C:1931:HOH:O	8:D:1724:HOH:O[2_555]	1.97	0.23
1:B:460:ASP:OD2	1:D:395:LYS:NZ[1_656]	1.98	0.22

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	1011/1025 (99%)	970 (96%)	39 (4%)	2 (0%)	47	30
1	B	1010/1025 (98%)	970 (96%)	36 (4%)	4 (0%)	34	18
1	C	1005/1025 (98%)	971 (97%)	30 (3%)	4 (0%)	34	18
1	D	1016/1025 (99%)	976 (96%)	37 (4%)	3 (0%)	41	24
All	All	4042/4100 (99%)	3887 (96%)	142 (4%)	13 (0%)	41	24

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	905	PRO
1	B	900	GLN
1	B	905	PRO
1	C	326	SER
1	C	683	ALA

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	836/854 (98%)	834 (100%)	2 (0%)	93	90
1	B	846/854 (99%)	836 (99%)	10 (1%)	71	59
1	C	832/854 (97%)	829 (100%)	3 (0%)	91	87
1	D	841/854 (98%)	834 (99%)	7 (1%)	81	74
All	All	3355/3416 (98%)	3333 (99%)	22 (1%)	86	77

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	800	GLU
1	D	100	PHE
1	D	51	HIS
1	D	181	LYS
1	B	410	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	847	GLN
1	C	885	GLN
1	C	64	HIS
1	B	885	GLN
1	C	179	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

33 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAP	A	1106	-	45,52,52	2.79	11 (24%)	56,80,80	1.96	14 (25%)
6	TDR	D	1107	-	9,9,9	4.00	6 (66%)	12,12,12	2.84	7 (58%)
2	SF4	D	1102	1	0,12,12	-	-	-		
2	SF4	C	1103	1	0,12,12	-	-	-		
5	FMN	D	1108	-	33,33,33	3.60	14 (42%)	48,50,50	1.45	12 (25%)
3	FAD	B	1105	-	53,58,58	0.47	0	68,89,89	0.47	1 (1%)
3	FAD	C	1106	-	53,58,58	0.47	0	68,89,89	0.48	1 (1%)
2	SF4	B	1103	1	0,12,12	-	-	-		
4	NAP	D	1106	-	36,43,52	2.35	6 (16%)	44,67,80	1.72	10 (22%)
2	SF4	C	1104	1	0,12,12	-	-	-		
2	SF4	D	1101	1	0,12,12	-	-	-		
2	SF4	D	1104	1	0,12,12	-	-	-		
4	NAP	B	1106	-	45,52,52	2.75	13 (28%)	56,80,80	1.93	13 (23%)
5	FMN	B	1108	-	33,33,33	3.61	15 (45%)	48,50,50	1.42	10 (20%)
5	FMN	C	1109	-	33,33,33	3.56	13 (39%)	48,50,50	1.50	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SF4	B	1101	1	0,12,12	-	-	-		
2	SF4	B	1104	1	0,12,12	-	-	-		
2	SF4	A	1103	1	0,12,12	-	-	-		
2	SF4	B	1102	1	0,12,12	-	-	-		
2	SF4	A	1101	1	0,12,12	-	-	-		
2	SF4	A	1102	1	0,12,12	-	-	-		
2	SF4	C	1105	1	0,12,12	-	-	-		
6	TDR	C	1108	-	9,9,9	4.06	5 (55%)	12,12,12	2.92	7 (58%)
2	SF4	D	1103	1	0,12,12	-	-	-		
5	FMN	A	1107	-	33,33,33	3.63	14 (42%)	48,50,50	1.43	10 (20%)
6	TDR	A	1108	-	9,9,9	4.11	5 (55%)	12,12,12	2.93	8 (66%)
4	NAP	C	1107	-	45,52,52	2.59	12 (26%)	56,80,80	1.90	14 (25%)
2	SF4	A	1104	1	0,12,12	-	-	-		
3	FAD	D	1105	-	53,58,58	0.45	0	68,89,89	0.49	1 (1%)
7	PRO	C	1101	-	5,7,8	0.51	0	7,8,10	1.27	0
3	FAD	A	1105	-	53,58,58	0.46	0	68,89,89	0.46	1 (1%)
6	TDR	B	1107	-	9,9,9	4.07	6 (66%)	12,12,12	2.96	7 (58%)
2	SF4	C	1102	1	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	A	1106	-	-	2/31/67/67	0/5/5/5
6	TDR	D	1107	-	-	-	0/1/1/1
2	SF4	D	1102	1	-	-	0/6/5/5
2	SF4	C	1103	1	-	-	0/6/5/5
5	FMN	D	1108	-	-	1/18/18/18	0/3/3/3
3	FAD	B	1105	-	-	2/30/50/50	0/6/6/6
3	FAD	C	1106	-	-	2/30/50/50	0/6/6/6
2	SF4	B	1103	1	-	-	0/6/5/5
4	NAP	D	1106	-	-	6/23/59/67	0/4/4/5
2	SF4	C	1104	1	-	-	0/6/5/5
2	SF4	D	1101	1	-	-	0/6/5/5
2	SF4	D	1104	1	-	-	0/6/5/5
4	NAP	B	1106	-	-	2/31/67/67	0/5/5/5
5	FMN	B	1108	-	-	1/18/18/18	0/3/3/3
5	FMN	C	1109	-	-	1/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	B	1101	1	-	-	0/6/5/5
2	SF4	B	1104	1	-	-	0/6/5/5
2	SF4	A	1103	1	-	-	0/6/5/5
2	SF4	B	1102	1	-	-	0/6/5/5
2	SF4	A	1101	1	-	-	0/6/5/5
2	SF4	A	1102	1	-	-	0/6/5/5
2	SF4	C	1105	1	-	-	0/6/5/5
6	TDR	C	1108	-	-	-	0/1/1/1
2	SF4	D	1103	1	-	-	0/6/5/5
5	FMN	A	1107	-	-	1/18/18/18	0/3/3/3
6	TDR	A	1108	-	-	-	0/1/1/1
4	NAP	C	1107	-	-	1/31/67/67	0/5/5/5
2	SF4	A	1104	1	-	-	0/6/5/5
3	FAD	D	1105	-	-	2/30/50/50	0/6/6/6
7	PRO	C	1101	-	-	0/0/9/11	0/1/1/1
3	FAD	A	1105	-	-	2/30/50/50	0/6/6/6
6	TDR	B	1107	-	-	-	0/1/1/1
2	SF4	C	1102	1	-	-	0/6/5/5

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1106	NAP	P2B-O2B	12.69	1.83	1.59
4	B	1106	NAP	P2B-O2B	12.14	1.82	1.59
4	C	1107	NAP	P2B-O2B	11.92	1.81	1.59
4	D	1106	NAP	P2B-O2B	11.65	1.81	1.59
5	B	1108	FMN	O4-C4	8.85	1.40	1.23

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1106	NAP	C5N-C4N-C3N	-6.99	112.07	120.34
4	C	1107	NAP	C5N-C4N-C3N	-6.74	112.37	120.34
4	A	1106	NAP	C5N-C4N-C3N	-6.68	112.44	120.34
4	A	1106	NAP	PN-O3-PA	-5.75	113.10	132.83
4	B	1106	NAP	PN-O3-PA	-5.57	113.72	132.83

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1105	FAD	PA-O3P-P-O5'
4	A	1106	NAP	C2B-O2B-P2B-O3X
4	D	1106	NAP	O4D-C4D-C5D-O5D
4	D	1106	NAP	C3D-C4D-C5D-O5D
5	B	1108	FMN	C4'-C5'-O5'-P

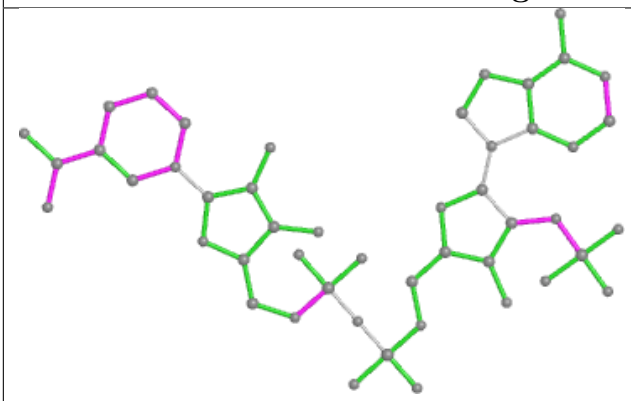
There are no ring outliers.

11 monomers are involved in 19 short contacts:

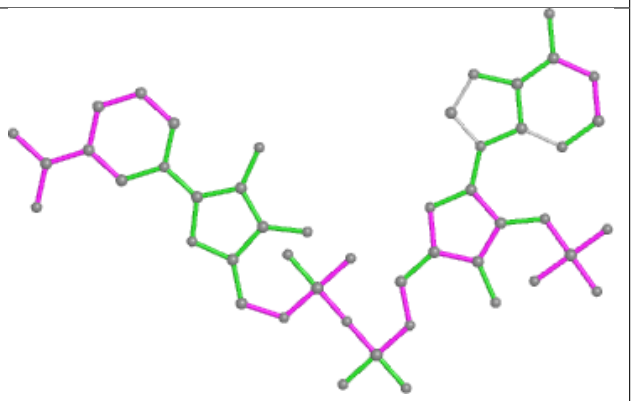
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1106	NAP	5	0
5	D	1108	FMN	1	0
3	B	1105	FAD	1	0
3	C	1106	FAD	1	0
4	D	1106	NAP	1	0
4	B	1106	NAP	5	0
5	B	1108	FMN	1	0
5	C	1109	FMN	1	0
5	A	1107	FMN	1	0
4	C	1107	NAP	4	0
3	A	1105	FAD	1	0

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

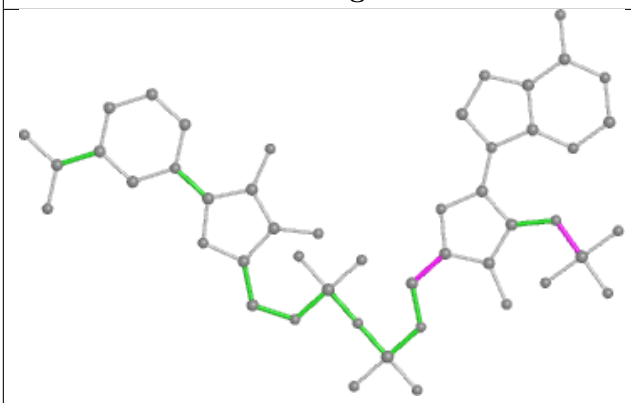
Ligand NAP A 1106



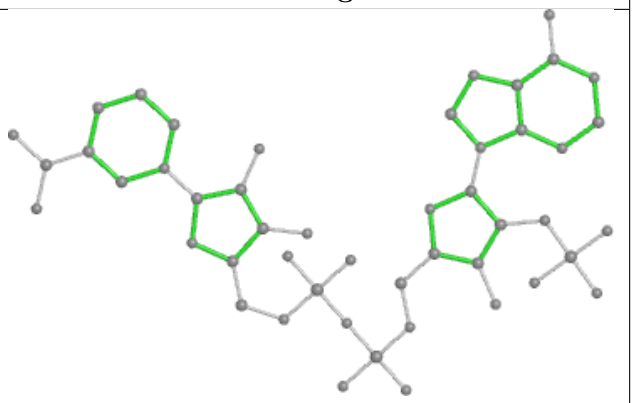
Bond lengths



Bond angles

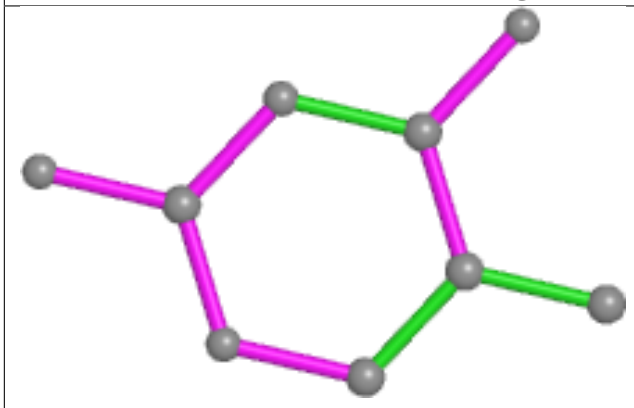


Torsions

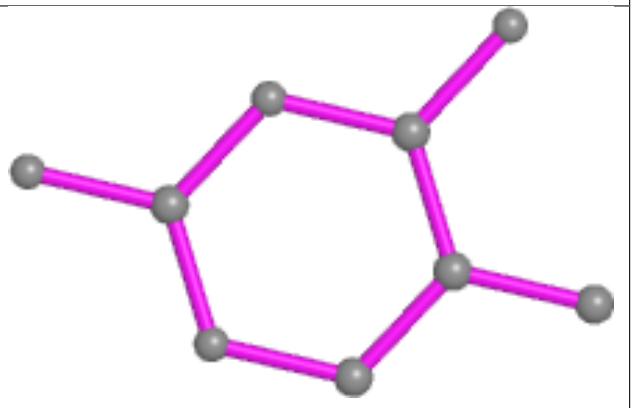


Rings

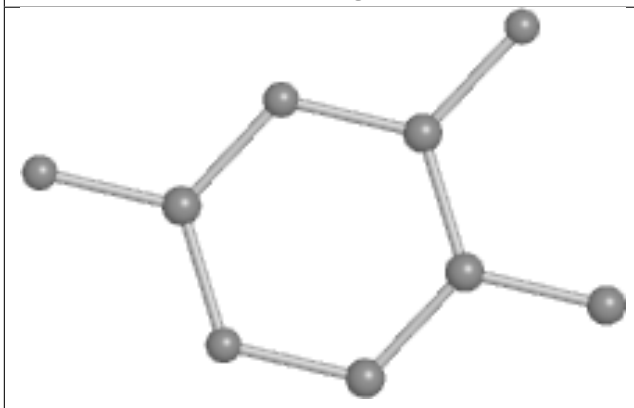
Ligand TDR D 1107



Bond lengths



Bond angles



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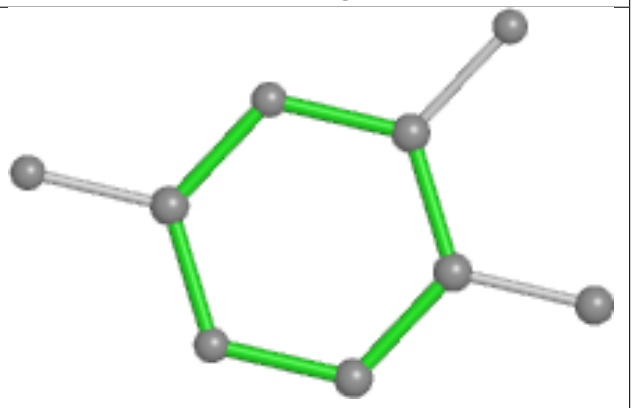
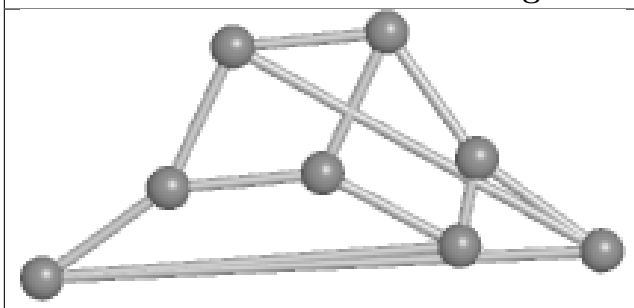
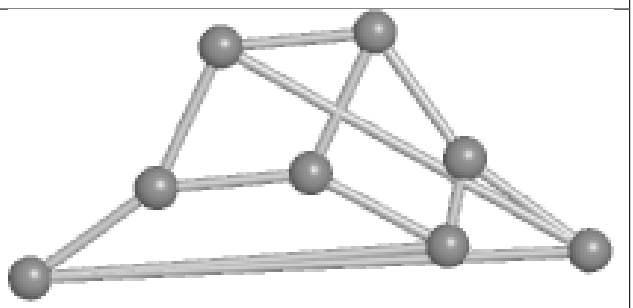


Rings

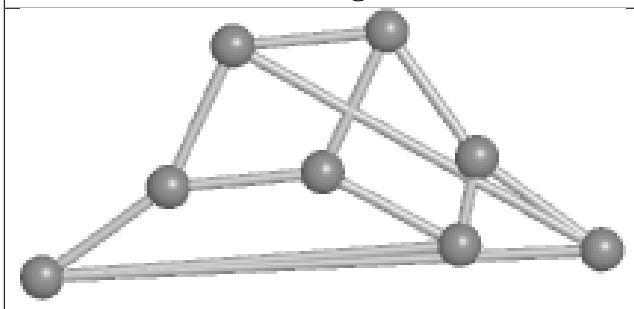
Ligand SF4 D 1102



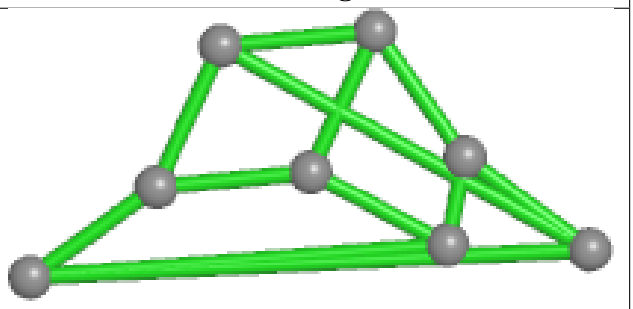
Bond lengths



Bond angles

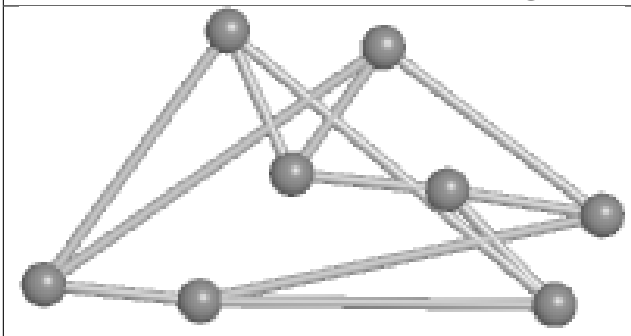


Torsions

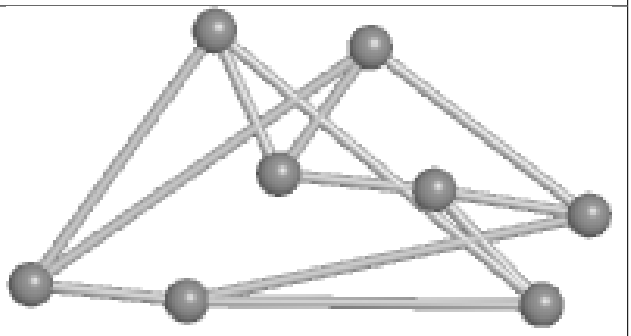


Rings

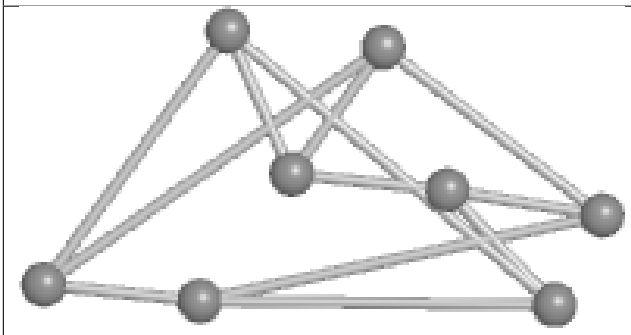
Ligand SF4 C 1103



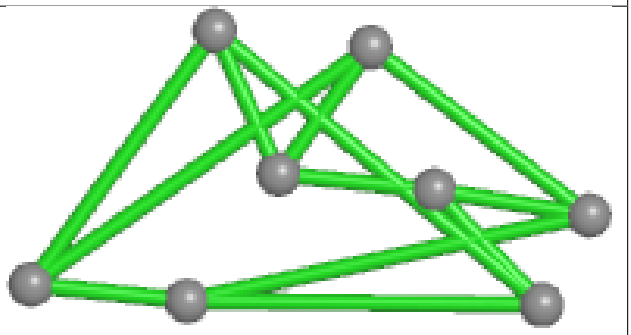
Bond lengths



Bond angles

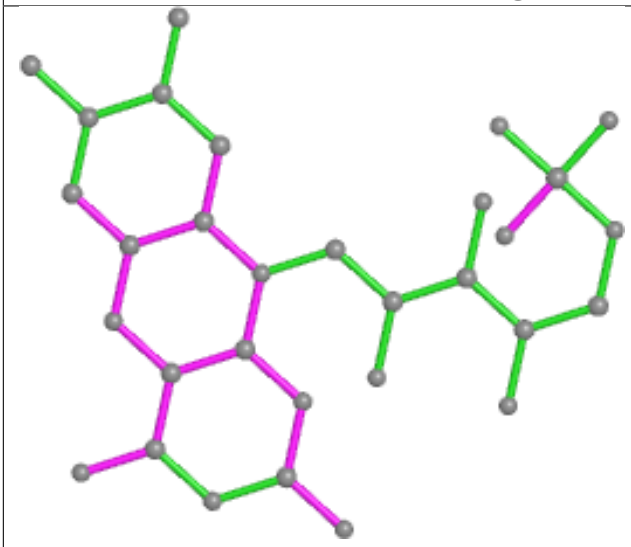


Torsions

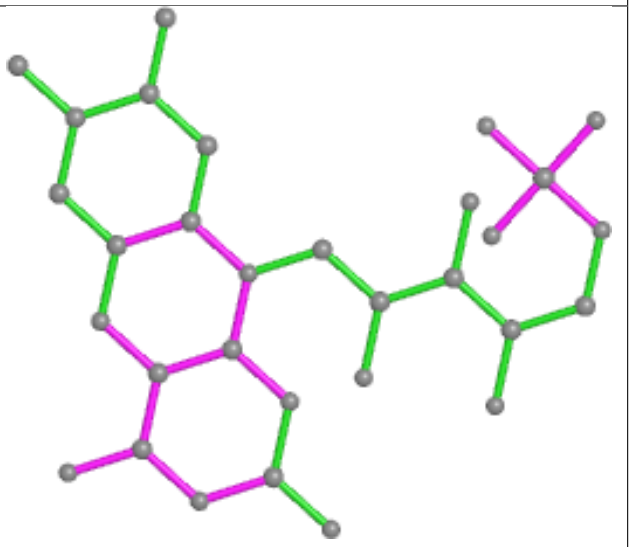


Rings

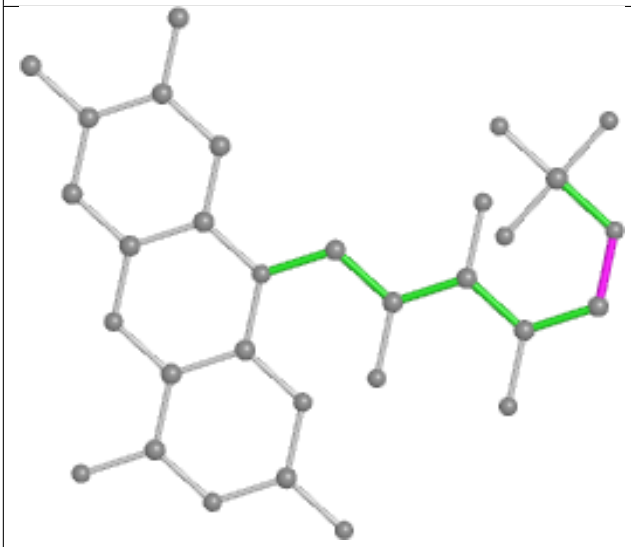
Ligand FMN D 1108



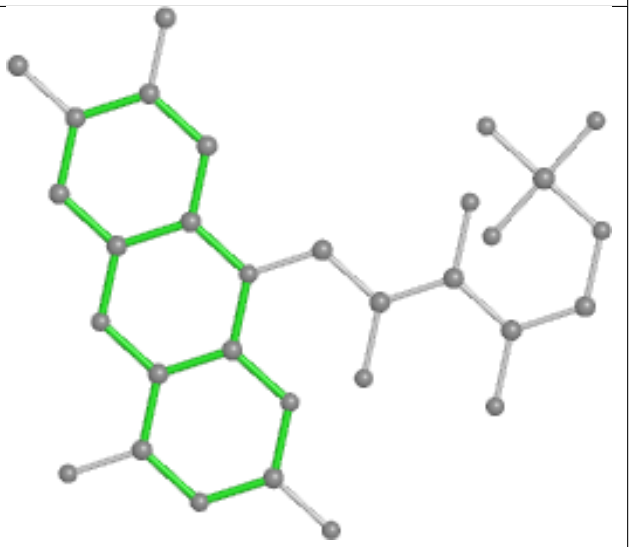
Bond lengths



Bond angles

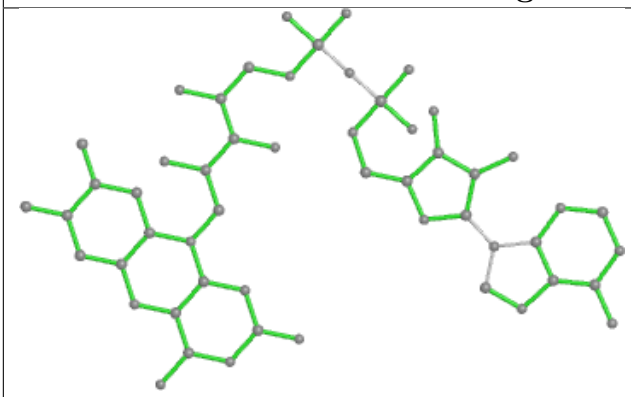


Torsions

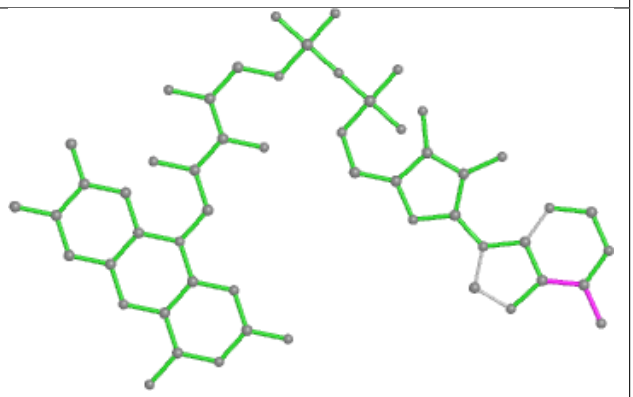


Rings

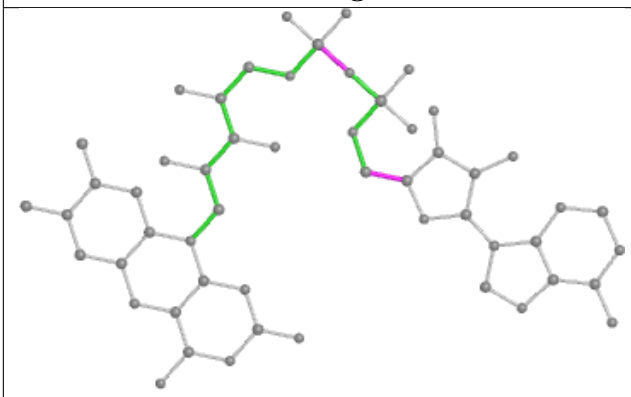
Ligand FAD B 1105



Bond lengths



Bond angles



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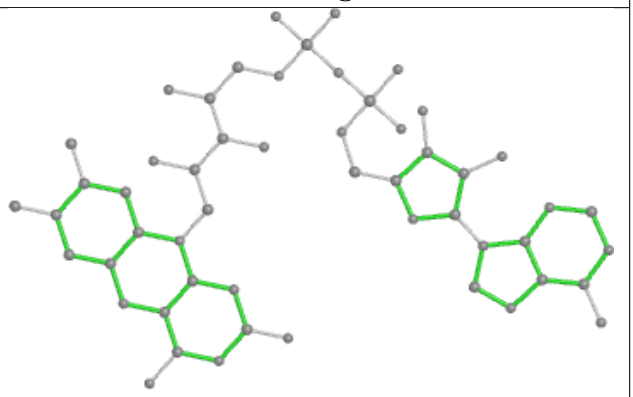
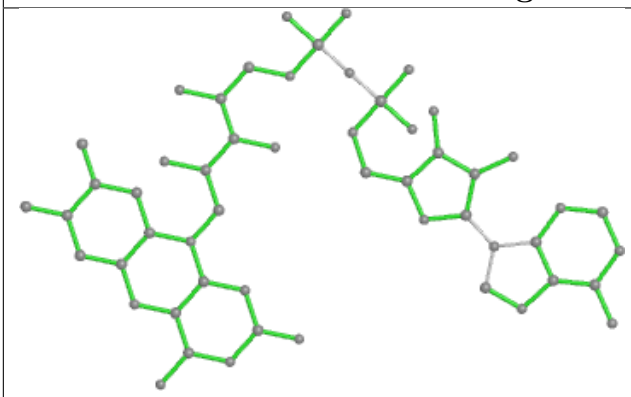
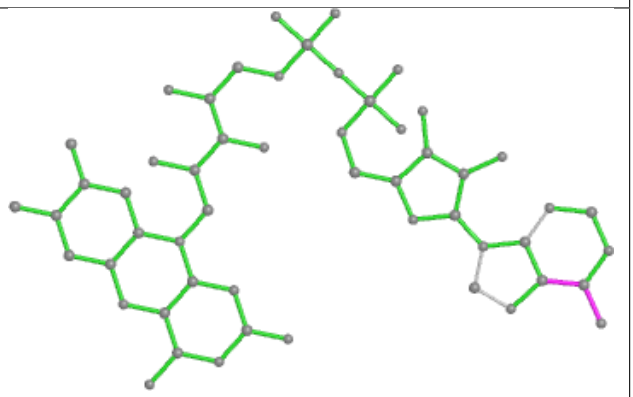


Rings

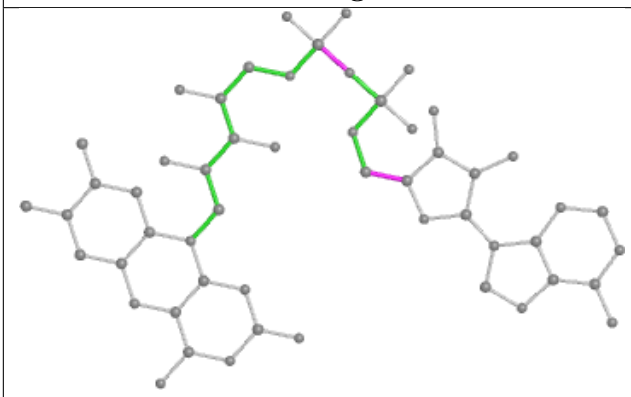
Ligand FAD C 1106



Bond lengths



Bond angles



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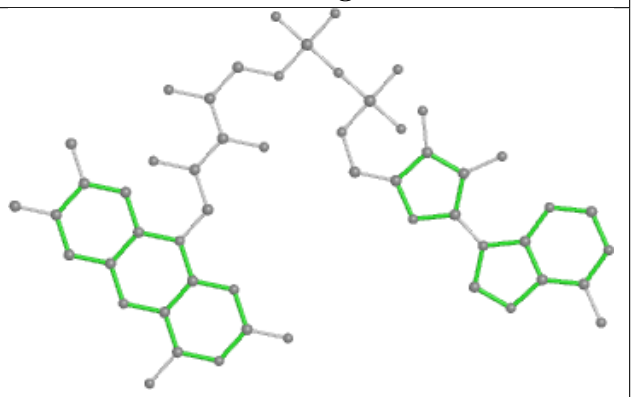
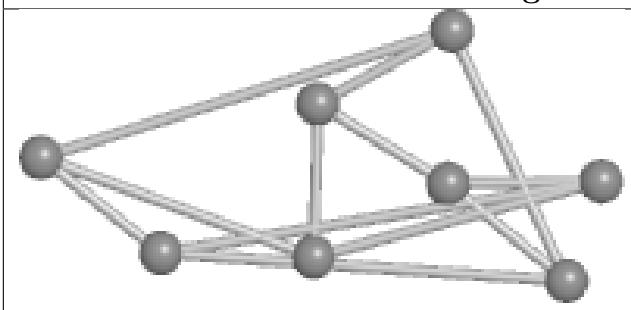


Rings

Ligand SF4 B 1103



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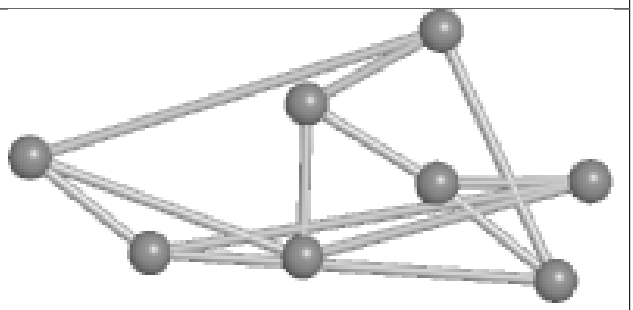

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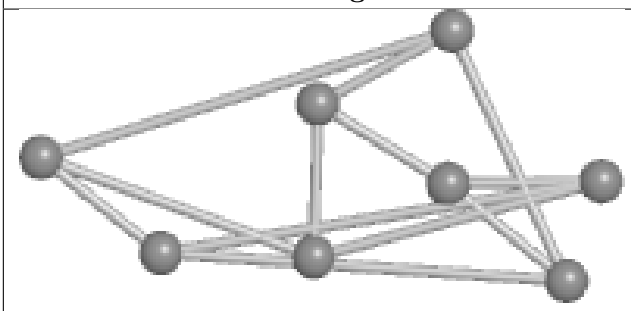

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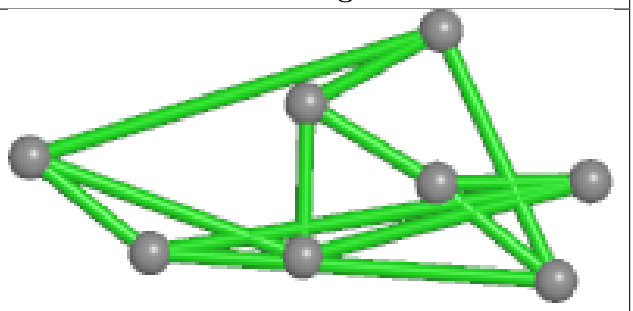
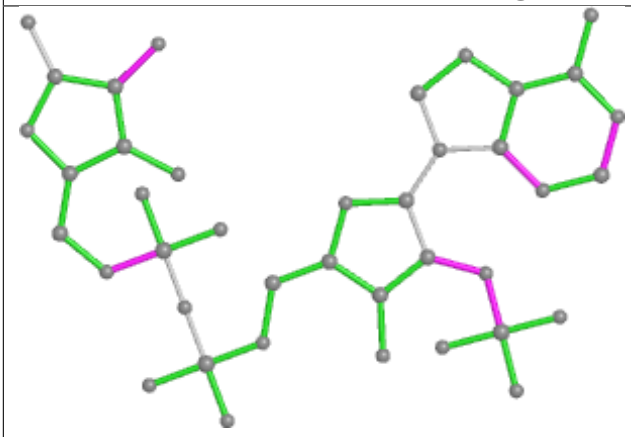
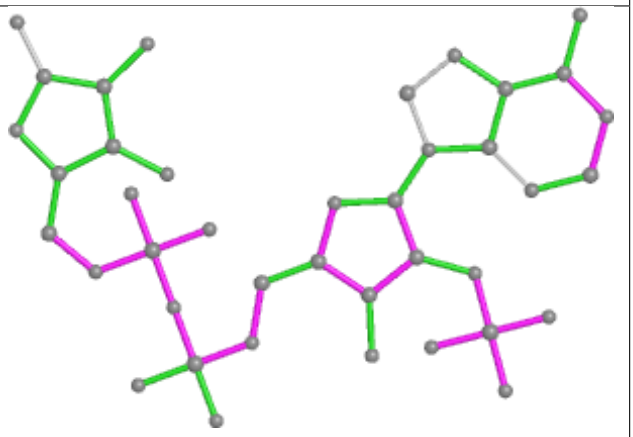


Rings

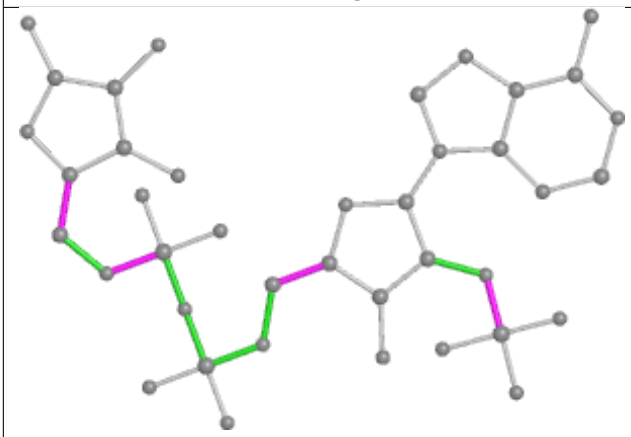
Ligand NAP D 1106



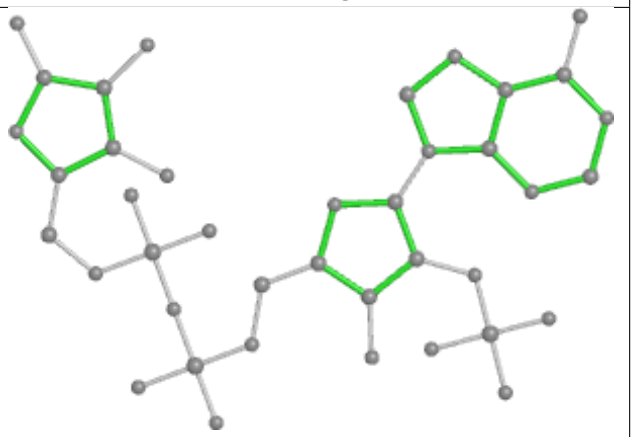
Bond lengths



Bond angles

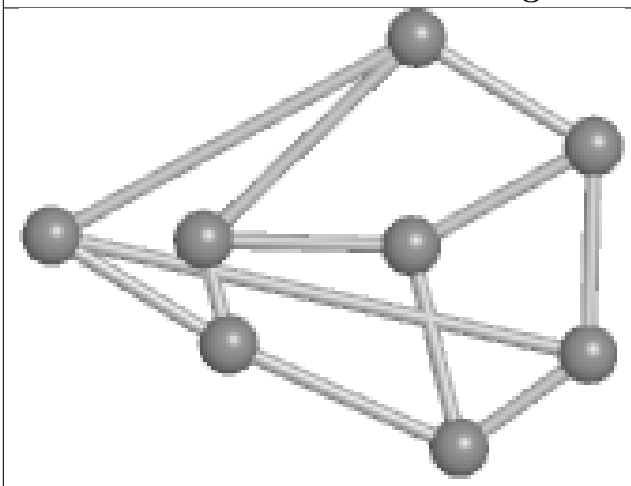


Torsions

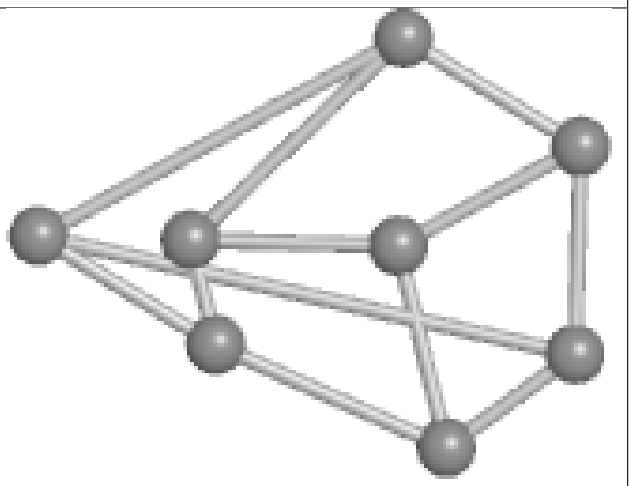


Rings

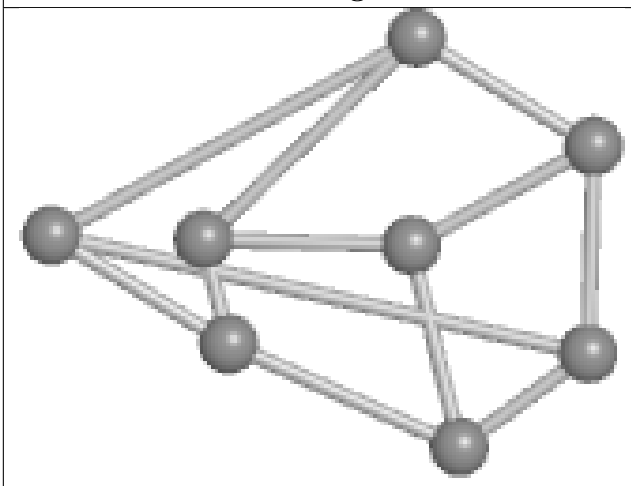
Ligand SF4 C 1104



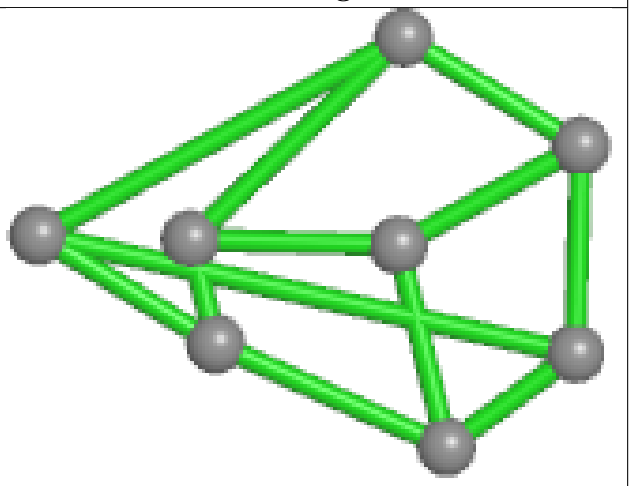
Bond lengths



Bond angles

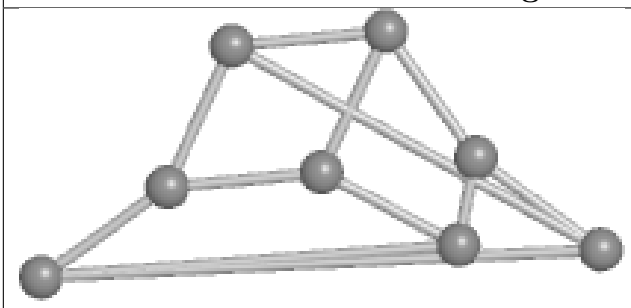


Torsions



Rings

Ligand SF4 D 1101



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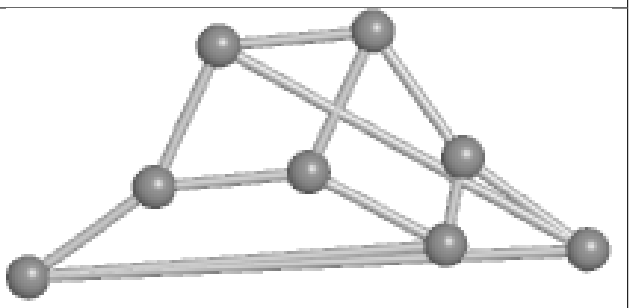
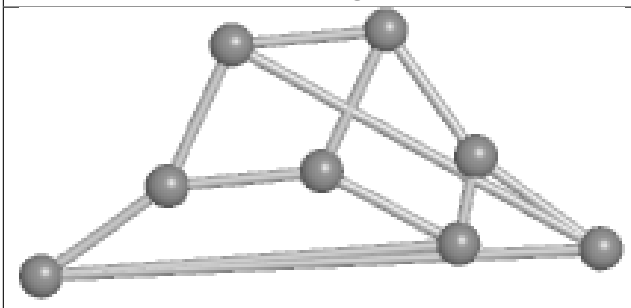


Bond angles



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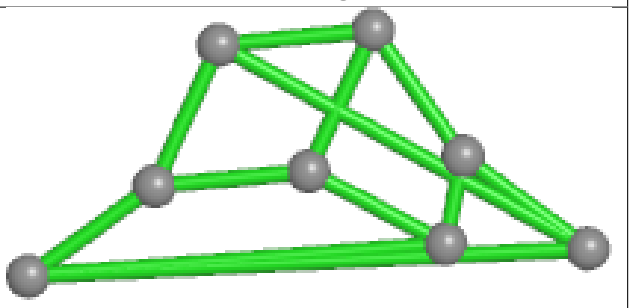
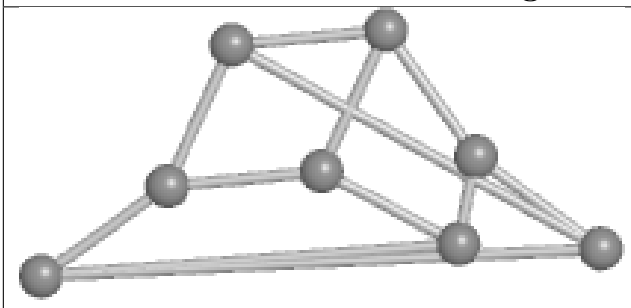


Rings

Ligand SF4 D 1104



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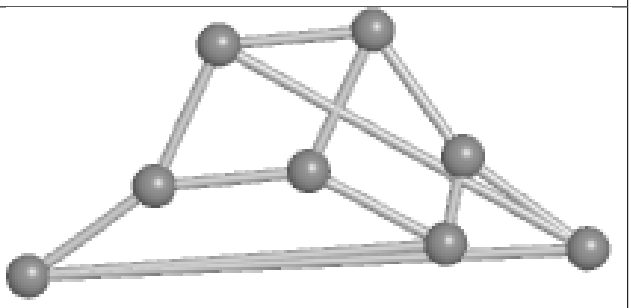
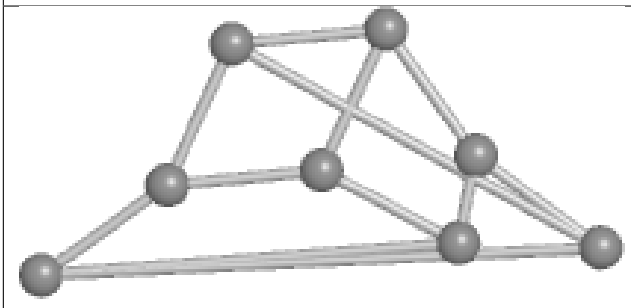


Bond angles



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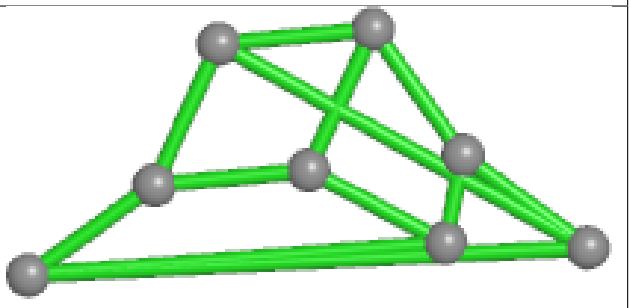
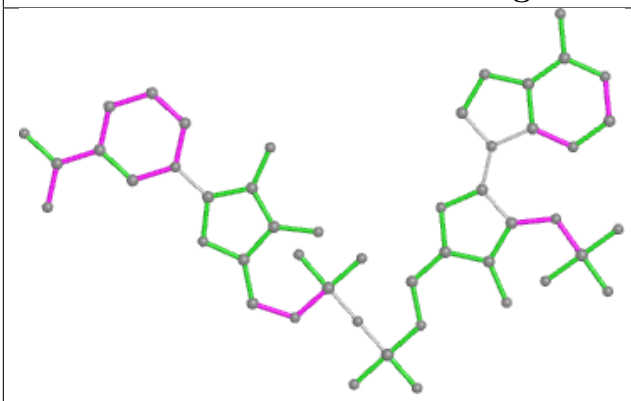


Rings

Ligand NAP B 1106



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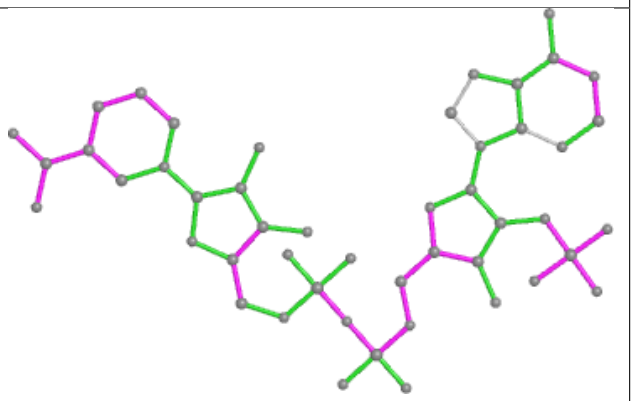
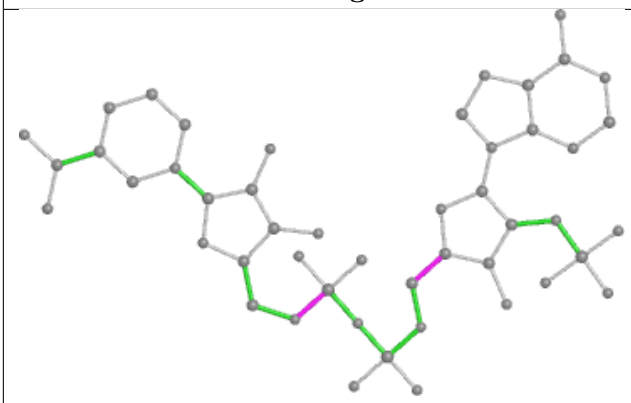
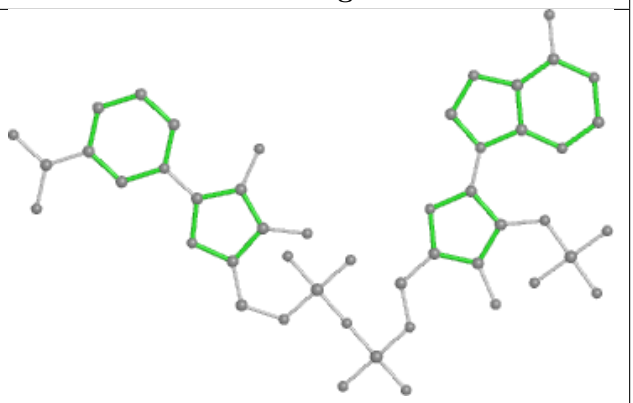


Bond angles

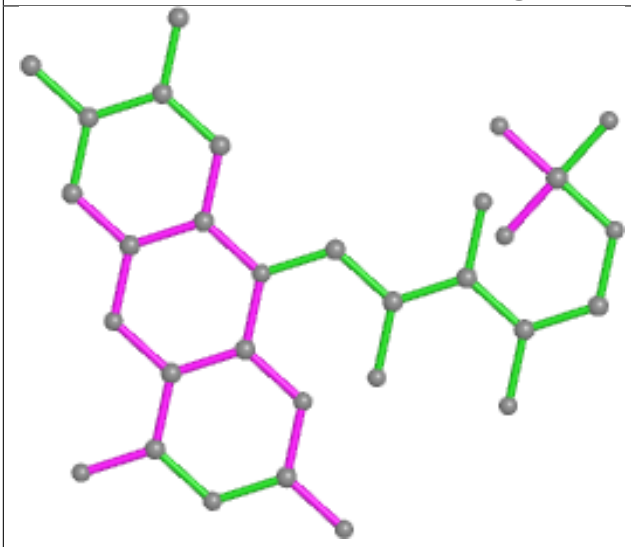


Torsions



Rings

Ligand FMN B 1108



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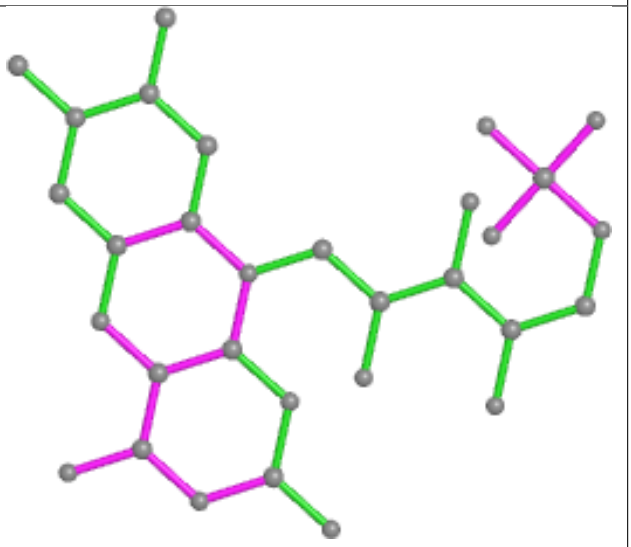
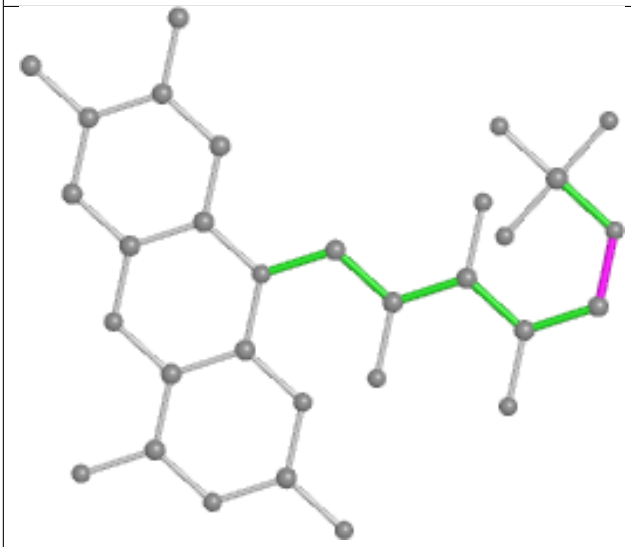


Bond angles



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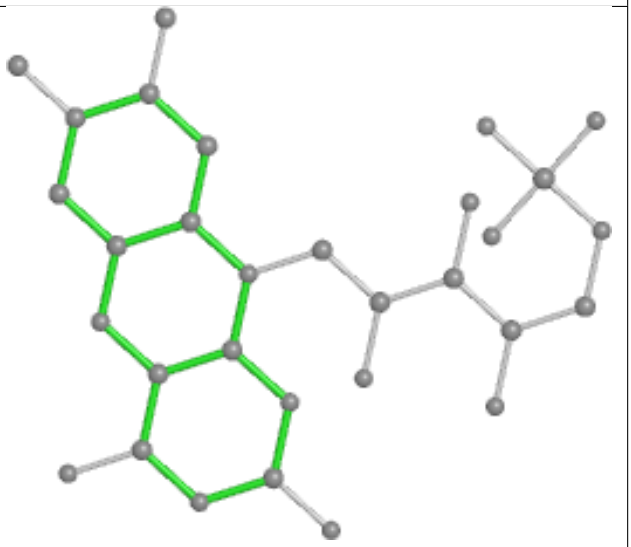
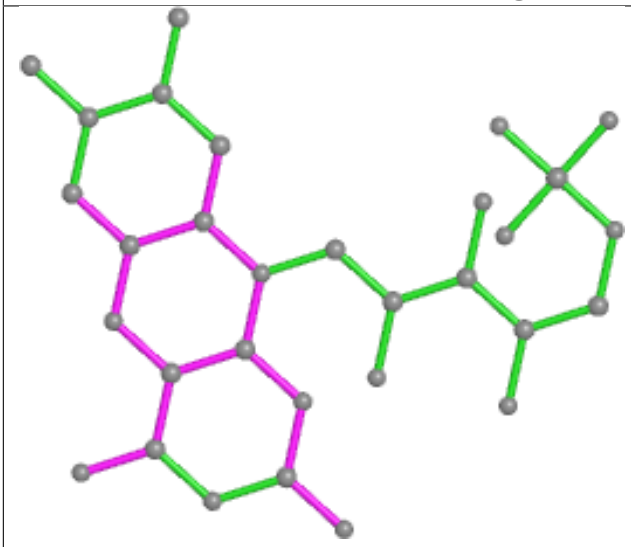


Rings

Ligand FMN C 1109



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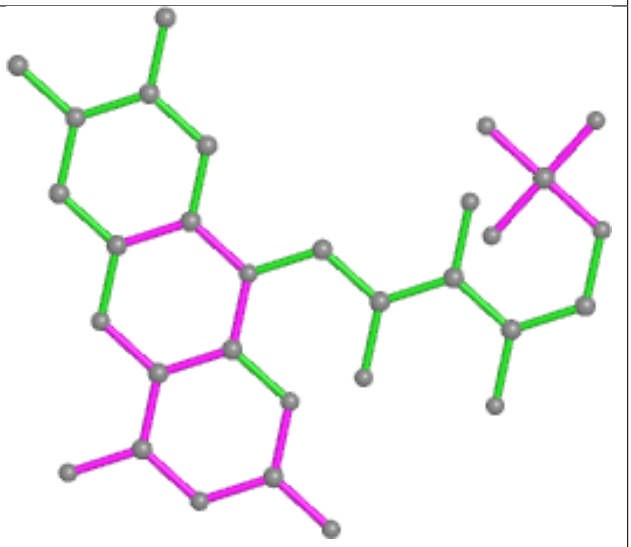
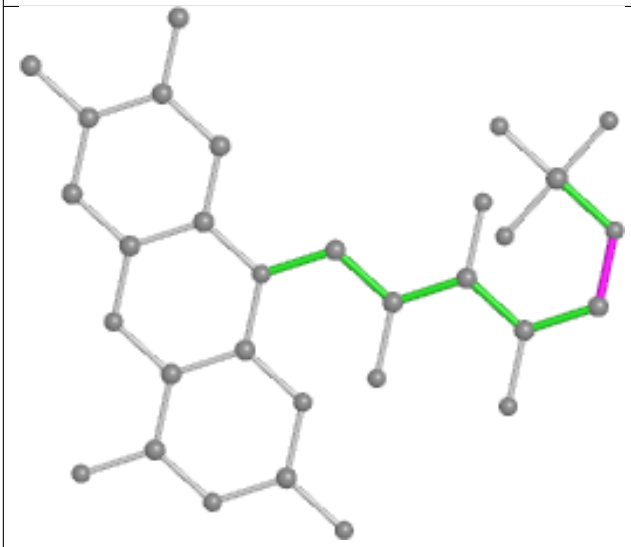


Bond angles



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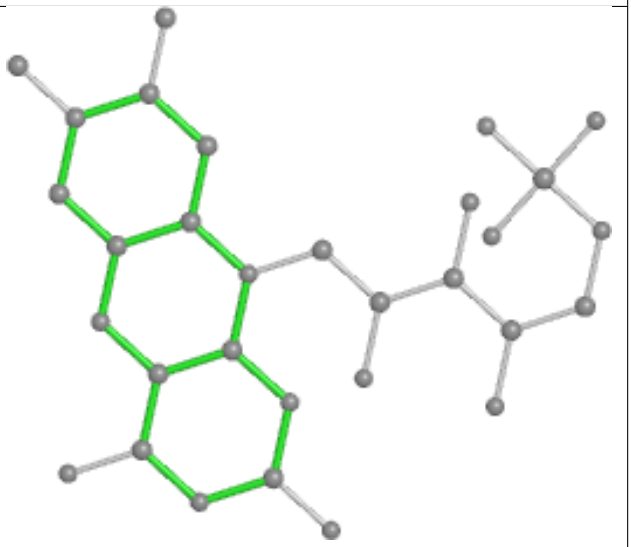
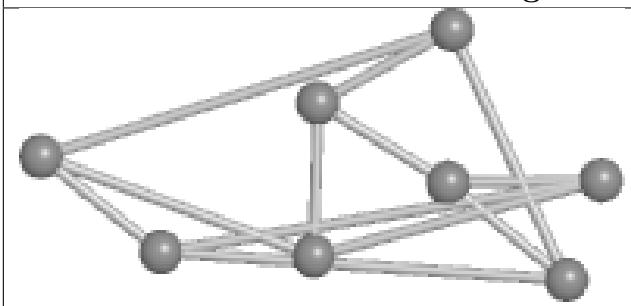


Rings

Ligand SF4 B 1101



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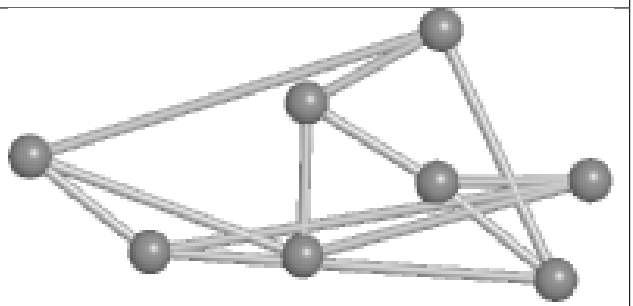
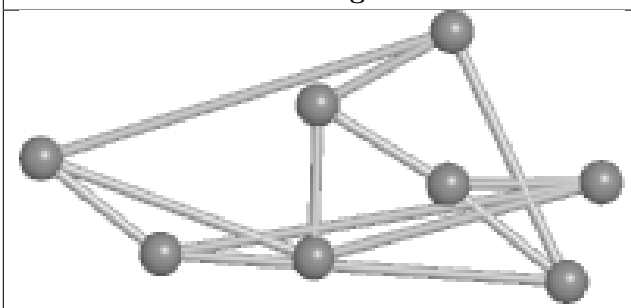
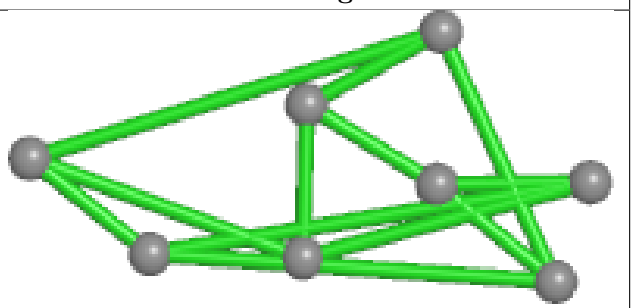


Bond angles

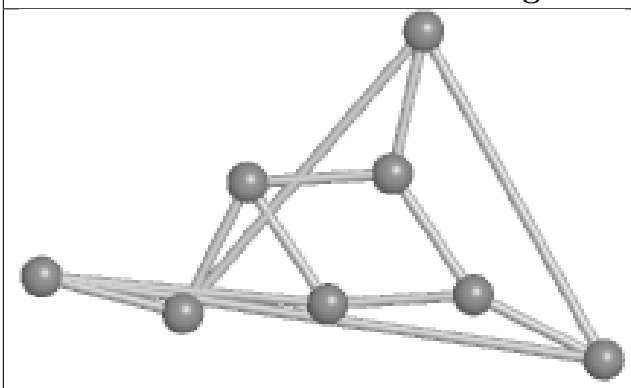


Torsions



Rings

Ligand SF4 B 1104



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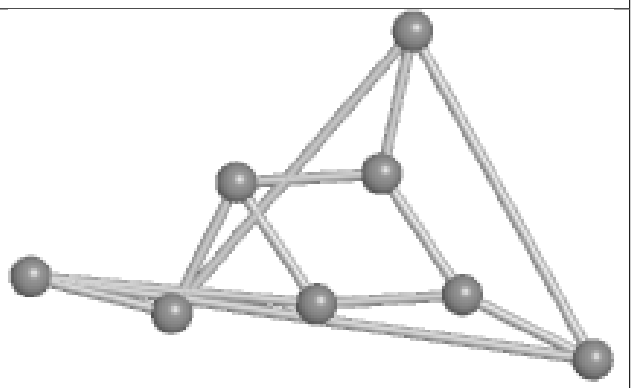
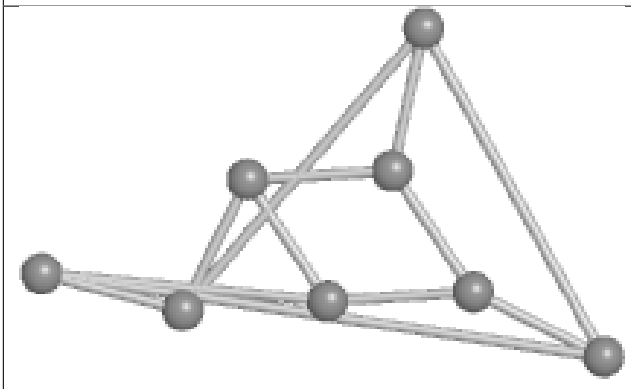


Bond angles



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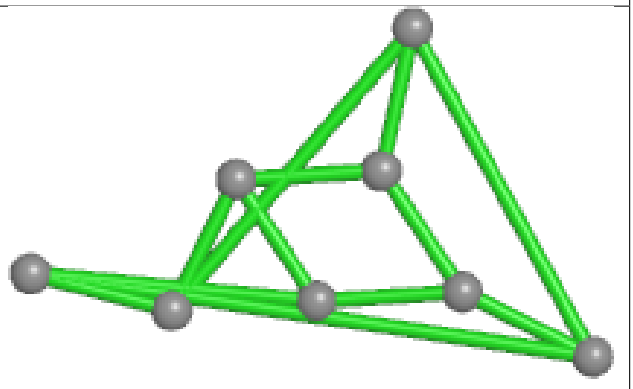
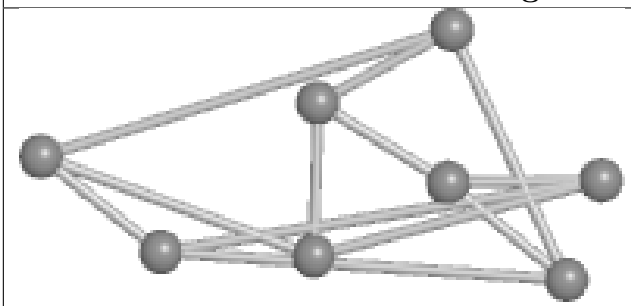


Rings

Ligand SF4 A 1103



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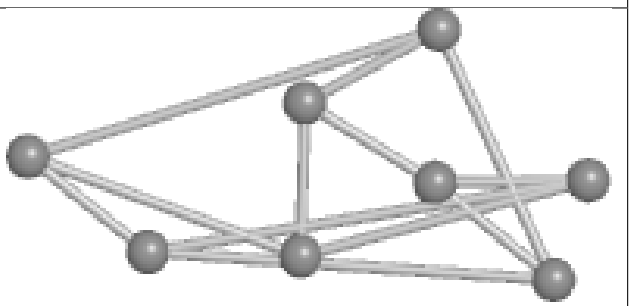
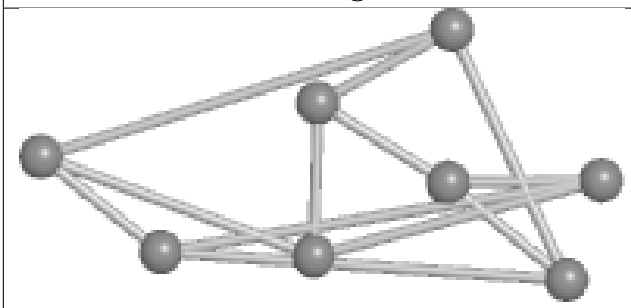
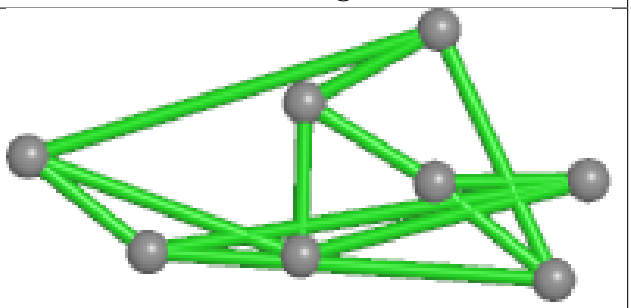


Bond angles

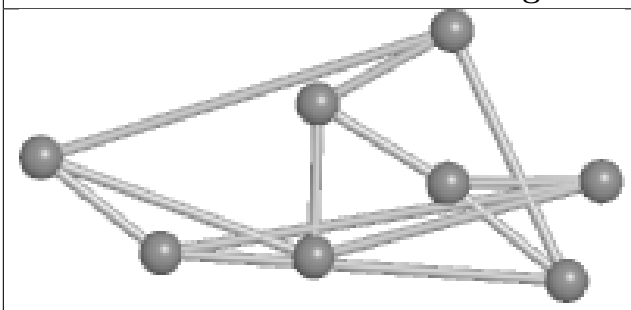


Torsions

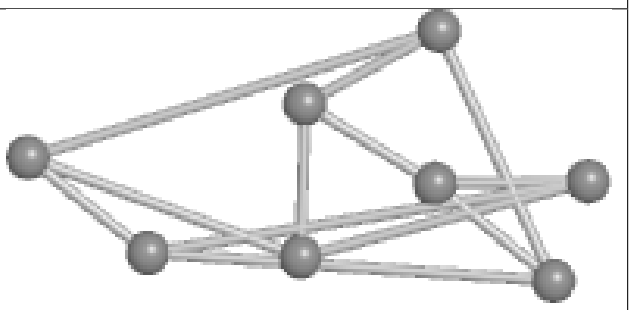


Rings

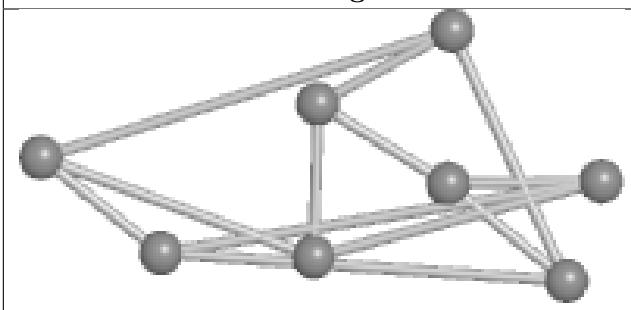
Ligand SF4 B 1102



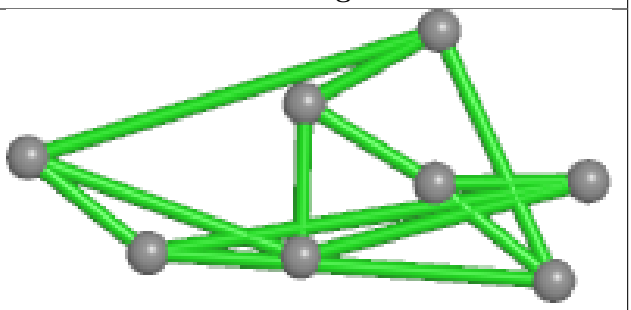
Bond lengths



Bond angles

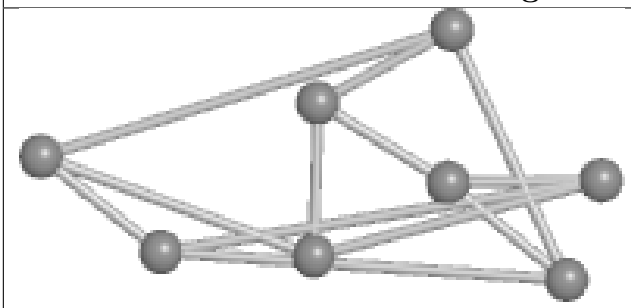


Torsions



Rings

Ligand SF4 A 1101



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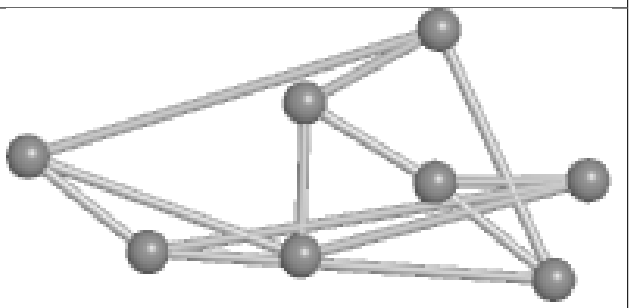
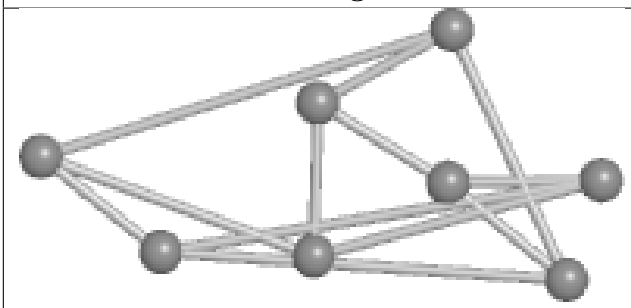
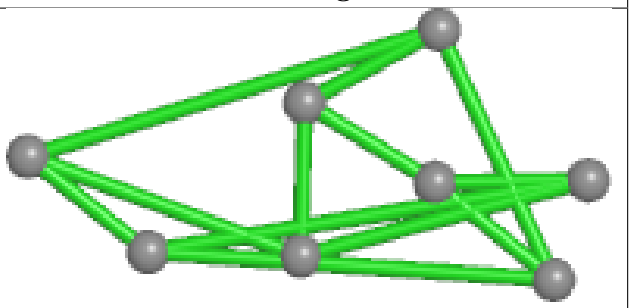


Bond angles

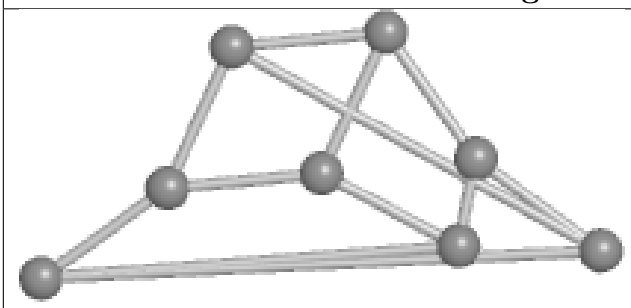


Torsions

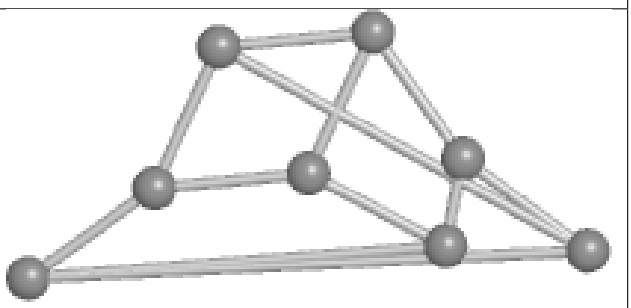


Rings

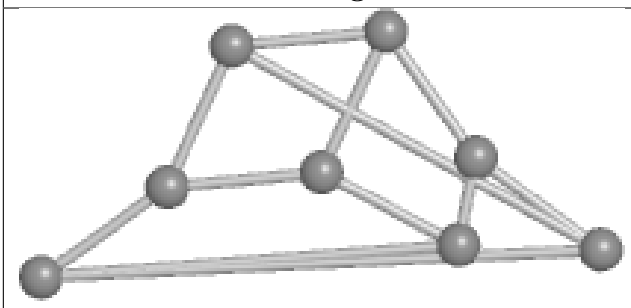
Ligand SF4 A 1102



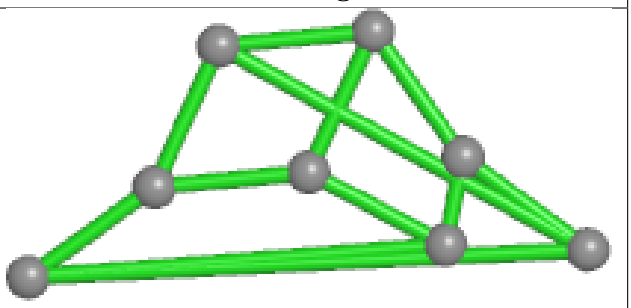
Bond lengths



Bond angles

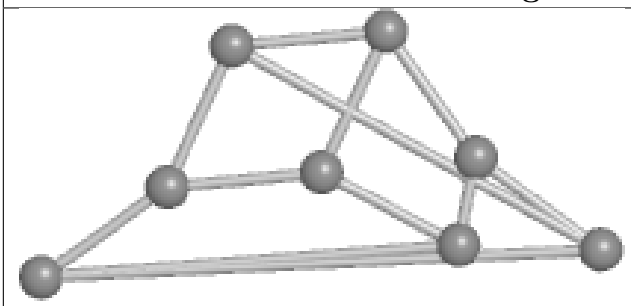


Torsions

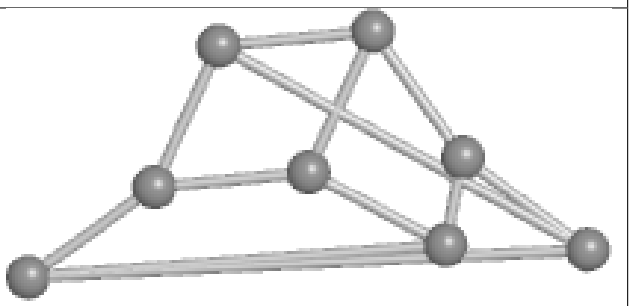


Rings

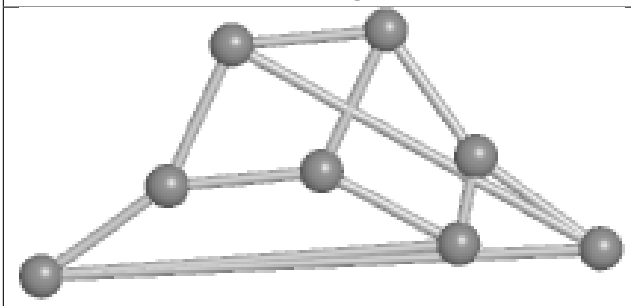
Ligand SF4 C 1105



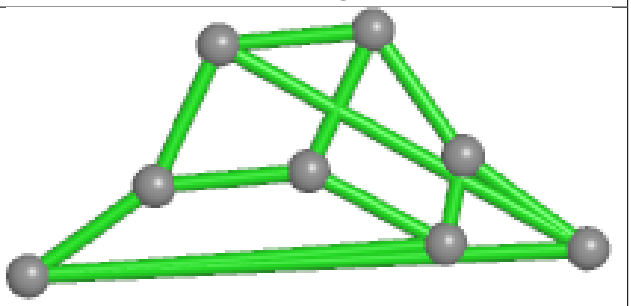
Bond lengths



Bond angles

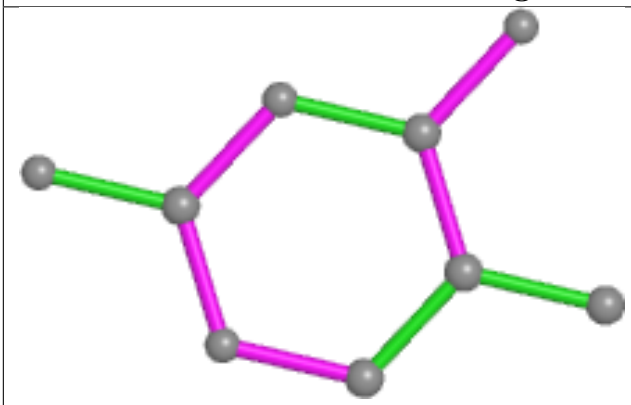


Torsions

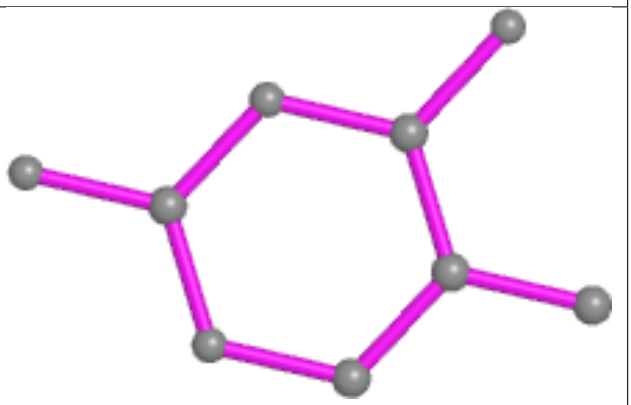


Rings

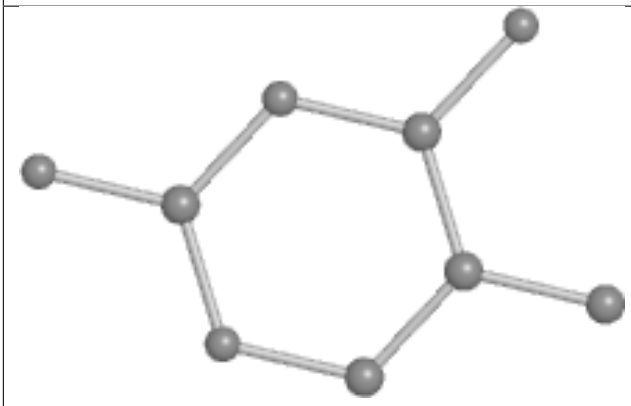
Ligand TDR C 1108



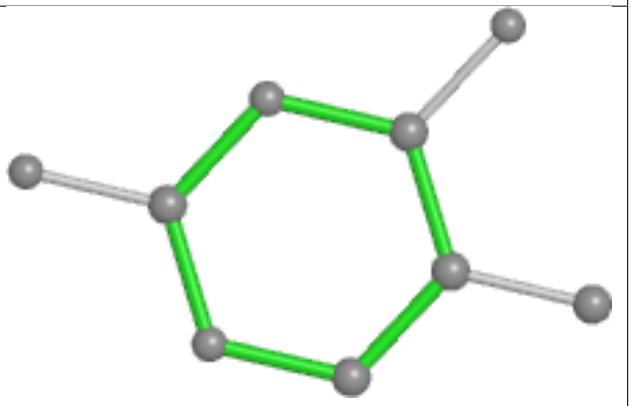
Bond lengths



Bond angles

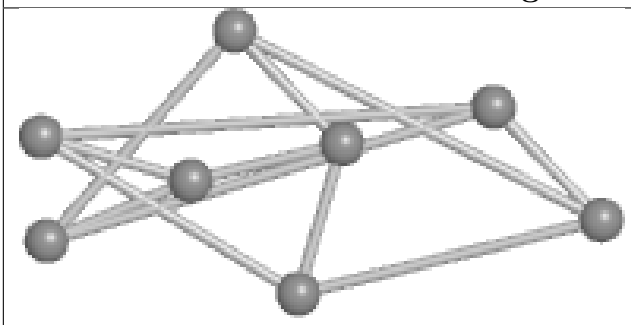


Torsions

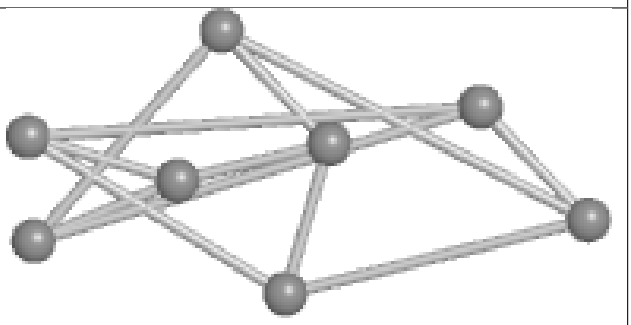


Rings

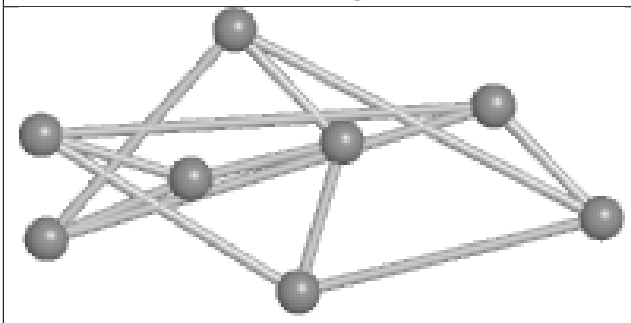
Ligand SF4 D 1103



Bond lengths



Bond angles



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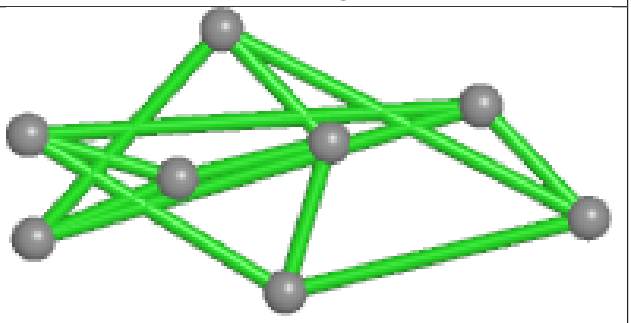
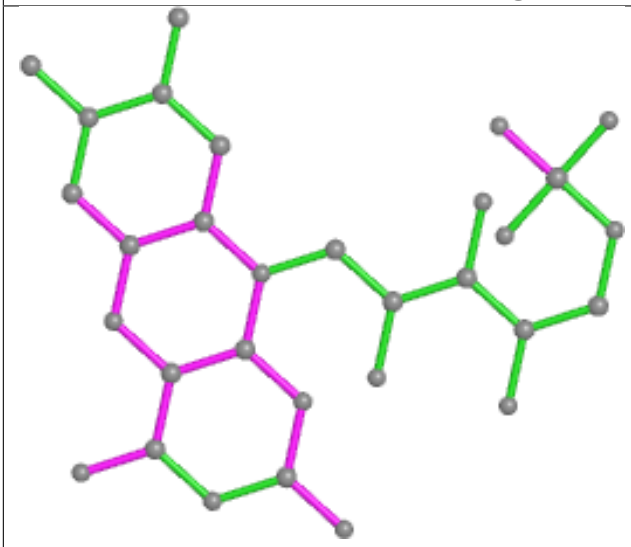
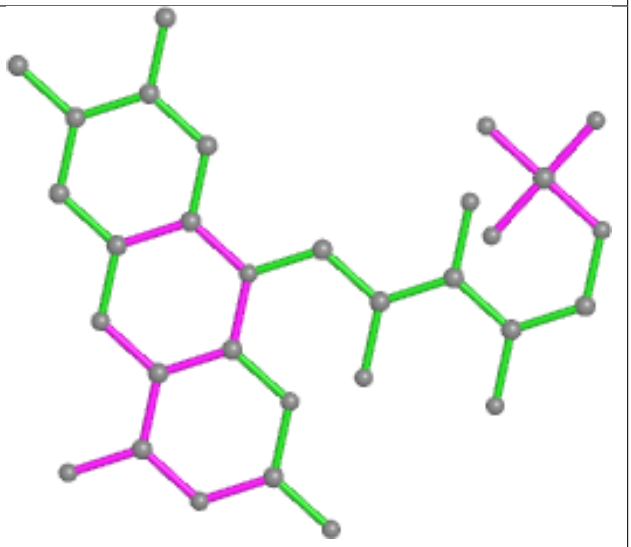


Rings

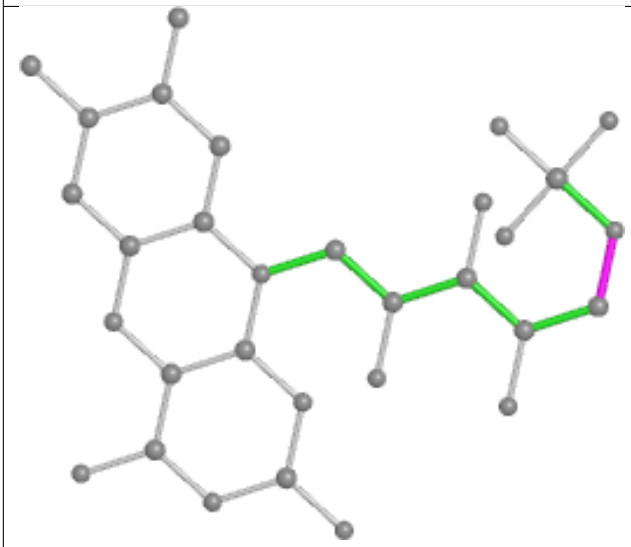
Ligand FMN A 1107



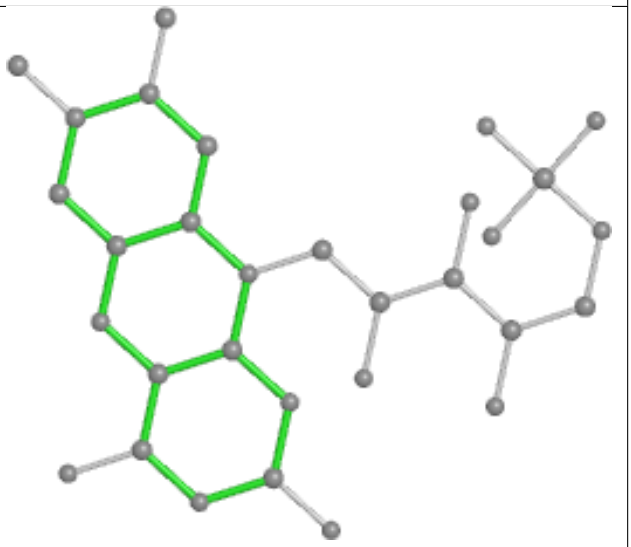
Bond lengths



Bond angles

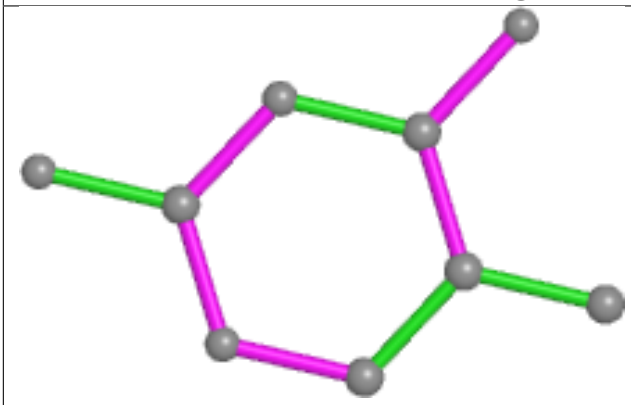


Torsions

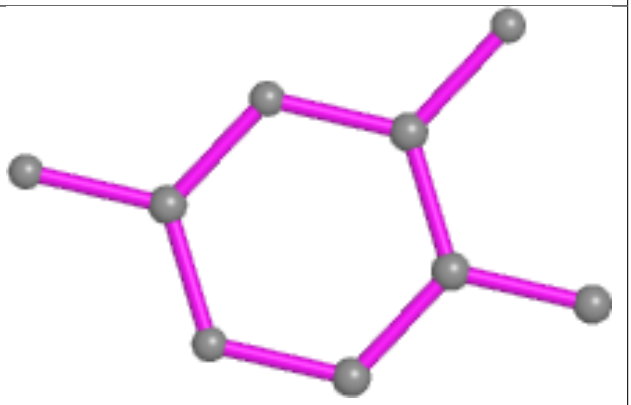


Rings

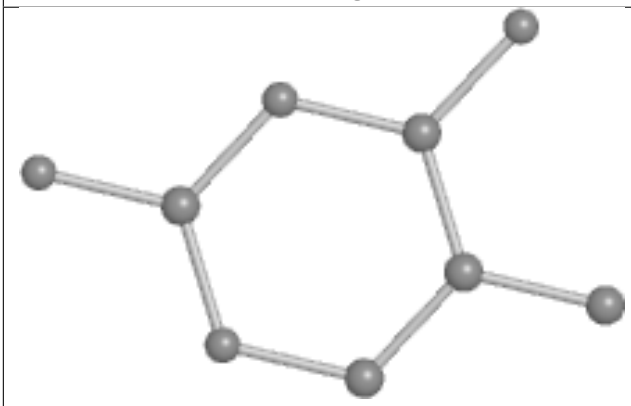
Ligand TDR A 1108



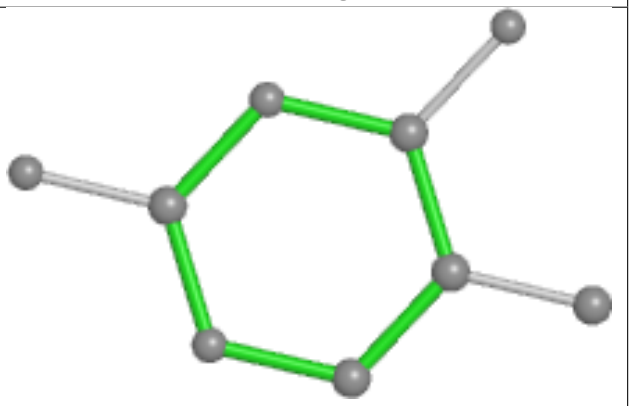
Bond lengths



Bond angles

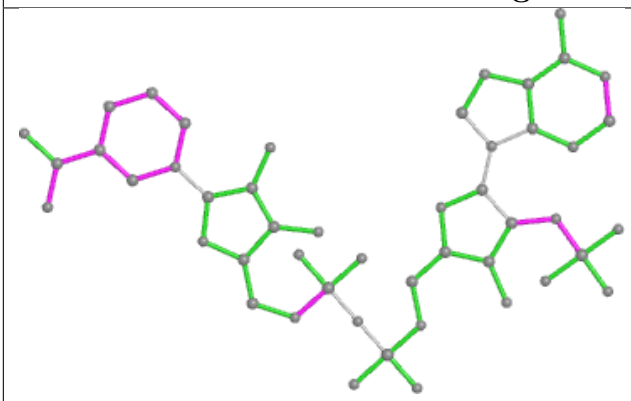


Torsions

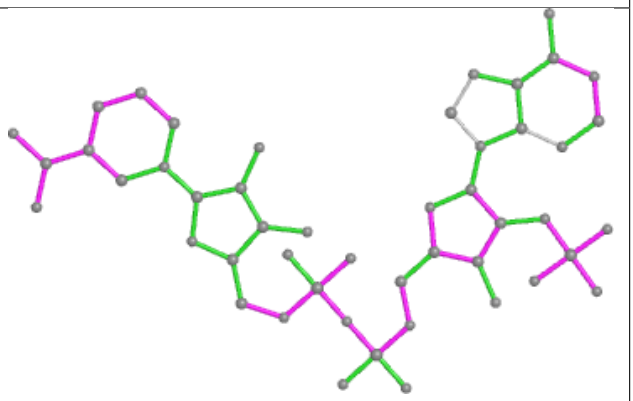


Rings

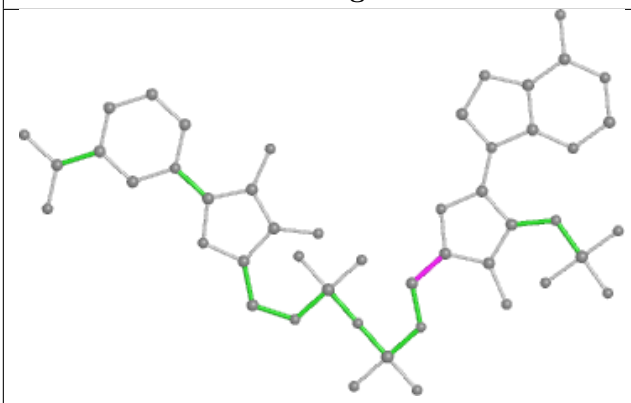
Ligand NAP C 1107



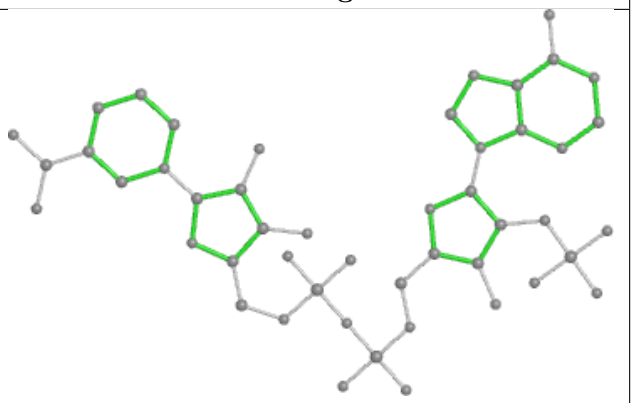
Bond lengths



Bond angles

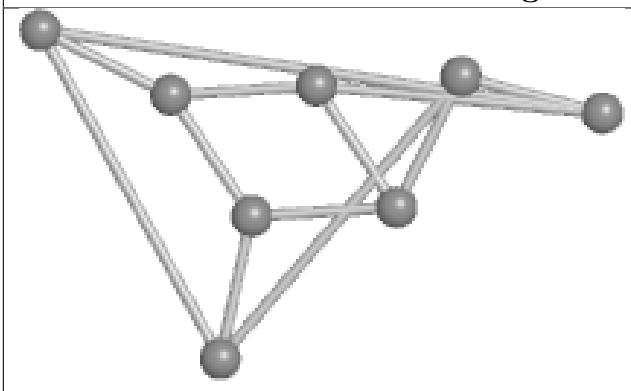


Torsions

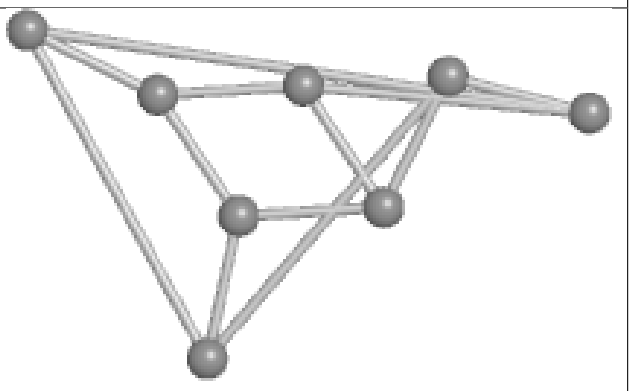


Rings

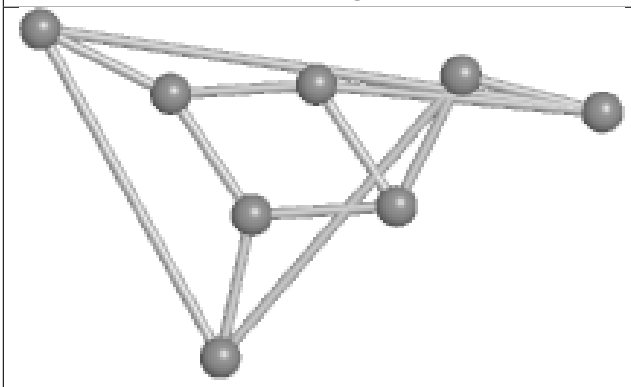
Ligand SF4 A 1104



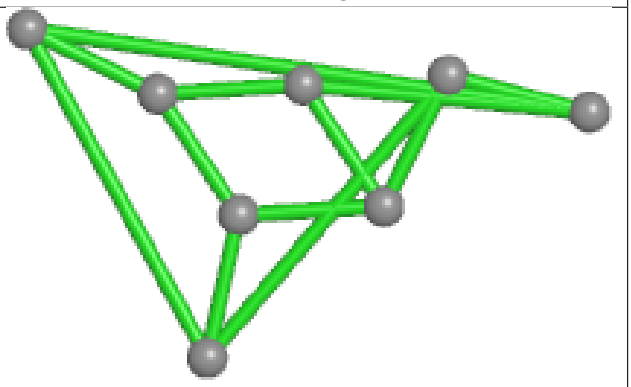
Bond lengths



Bond angles

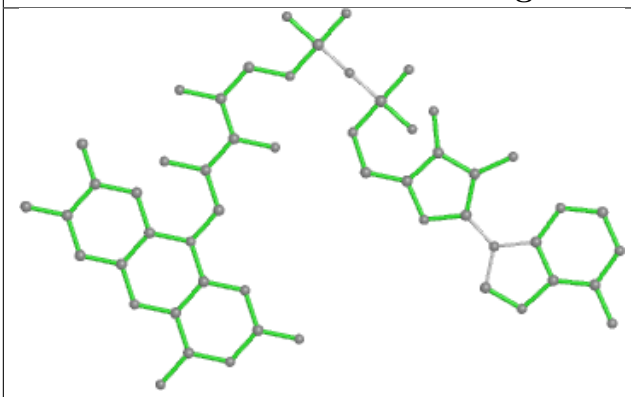


Torsions

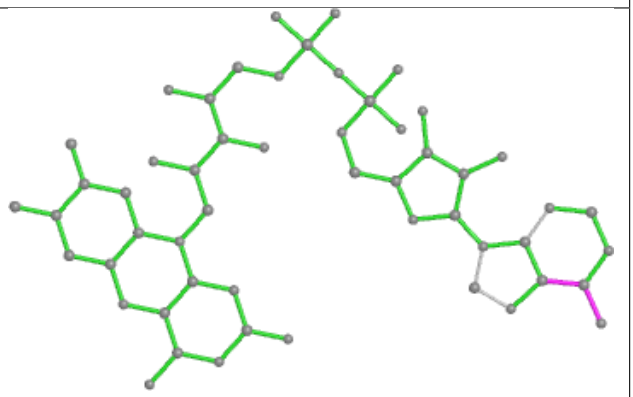


Rings

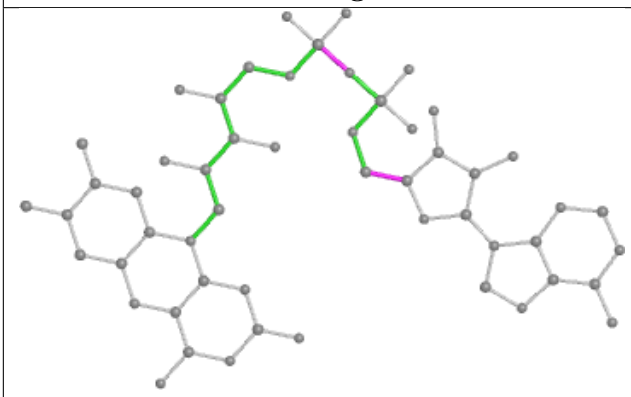
Ligand FAD D 1105



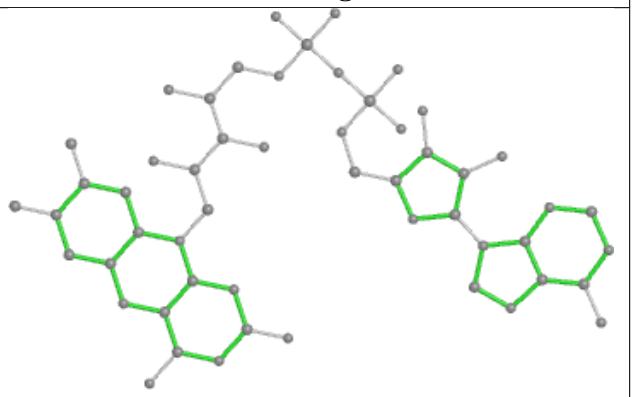
Bond lengths



Bond angles

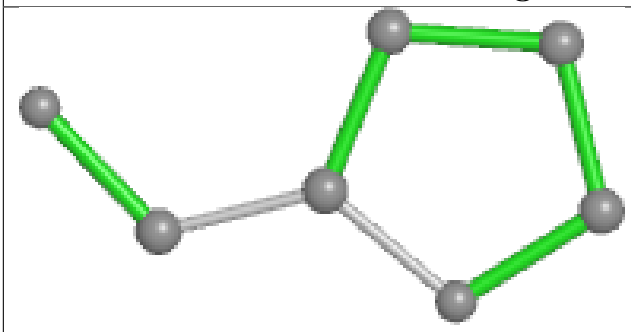


Torsions

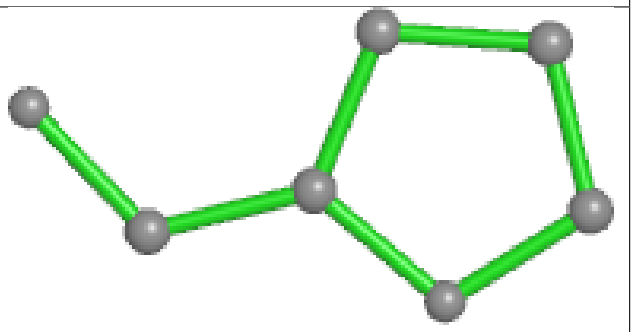


Rings

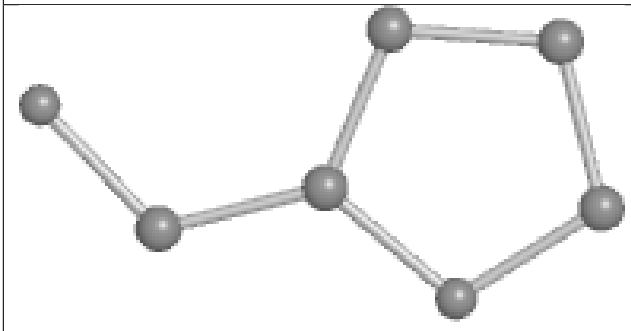
Ligand PRO C 1101



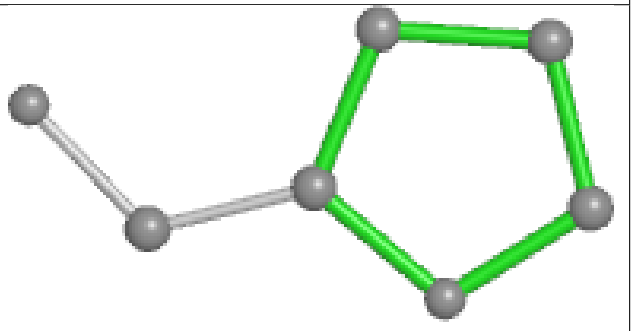
Bond lengths



Bond angles

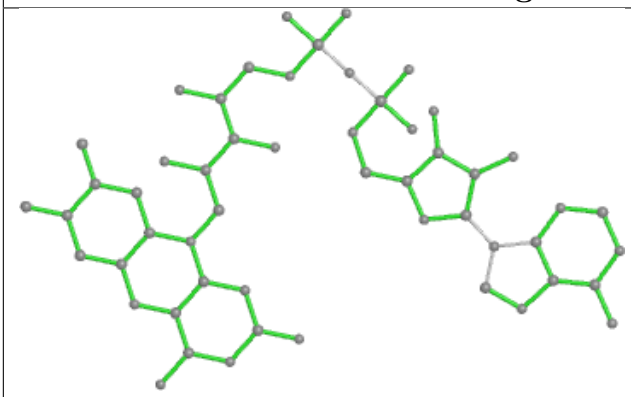


Torsions

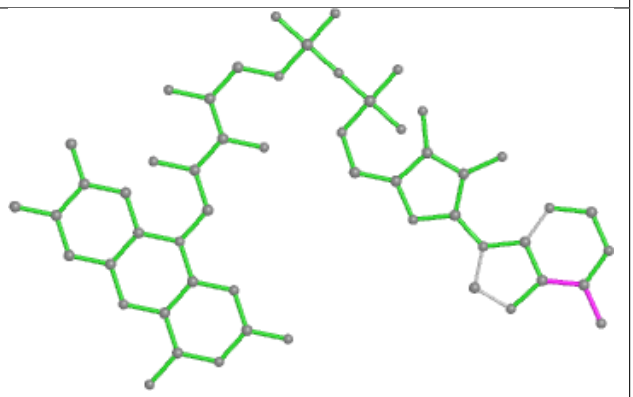


Rings

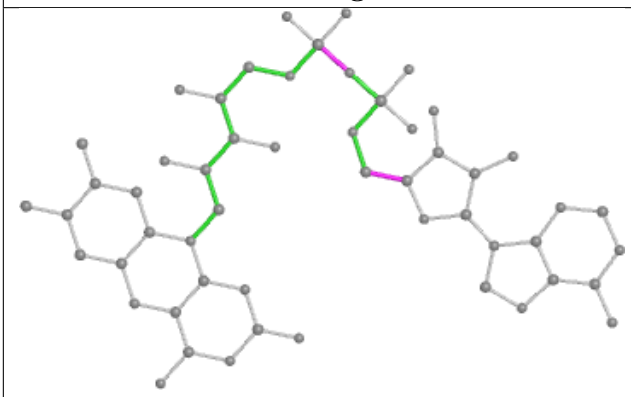
Ligand FAD A 1105



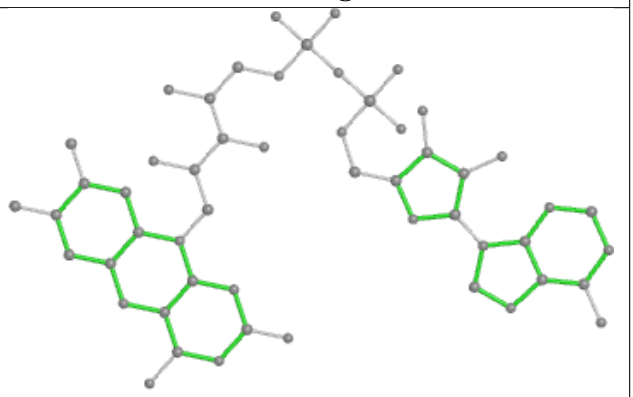
Bond lengths



Bond angles

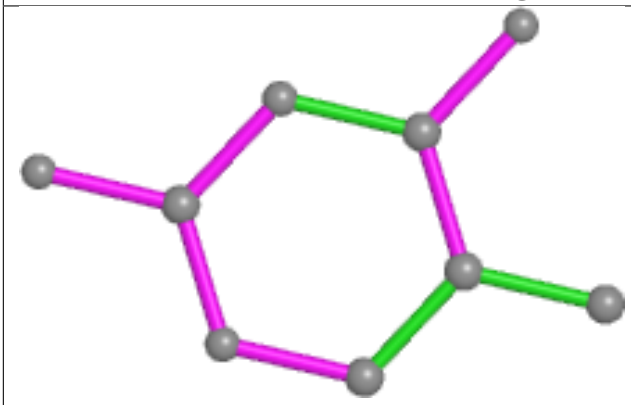


Torsions

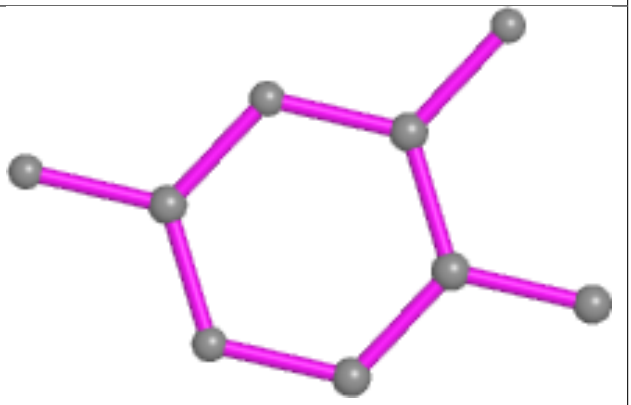


Rings

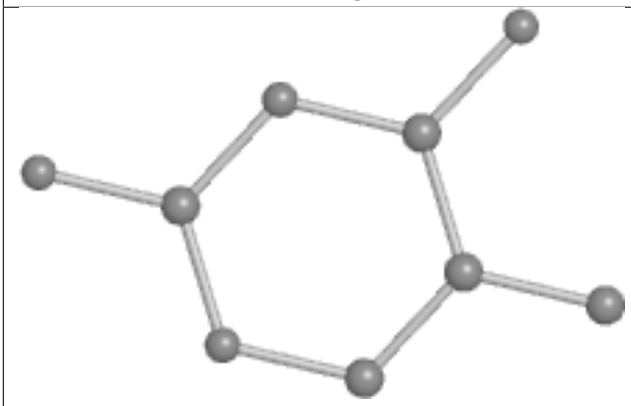
Ligand TDR B 1107



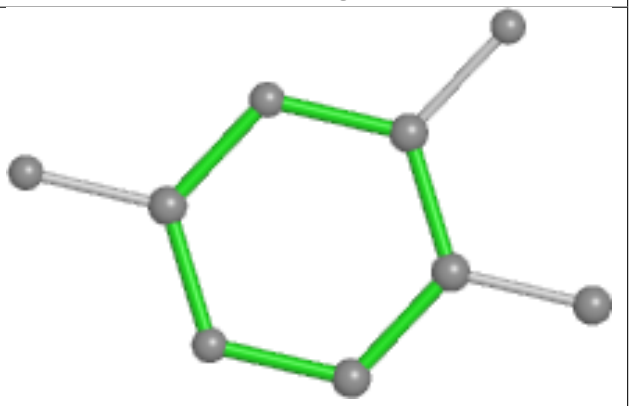
Bond lengths



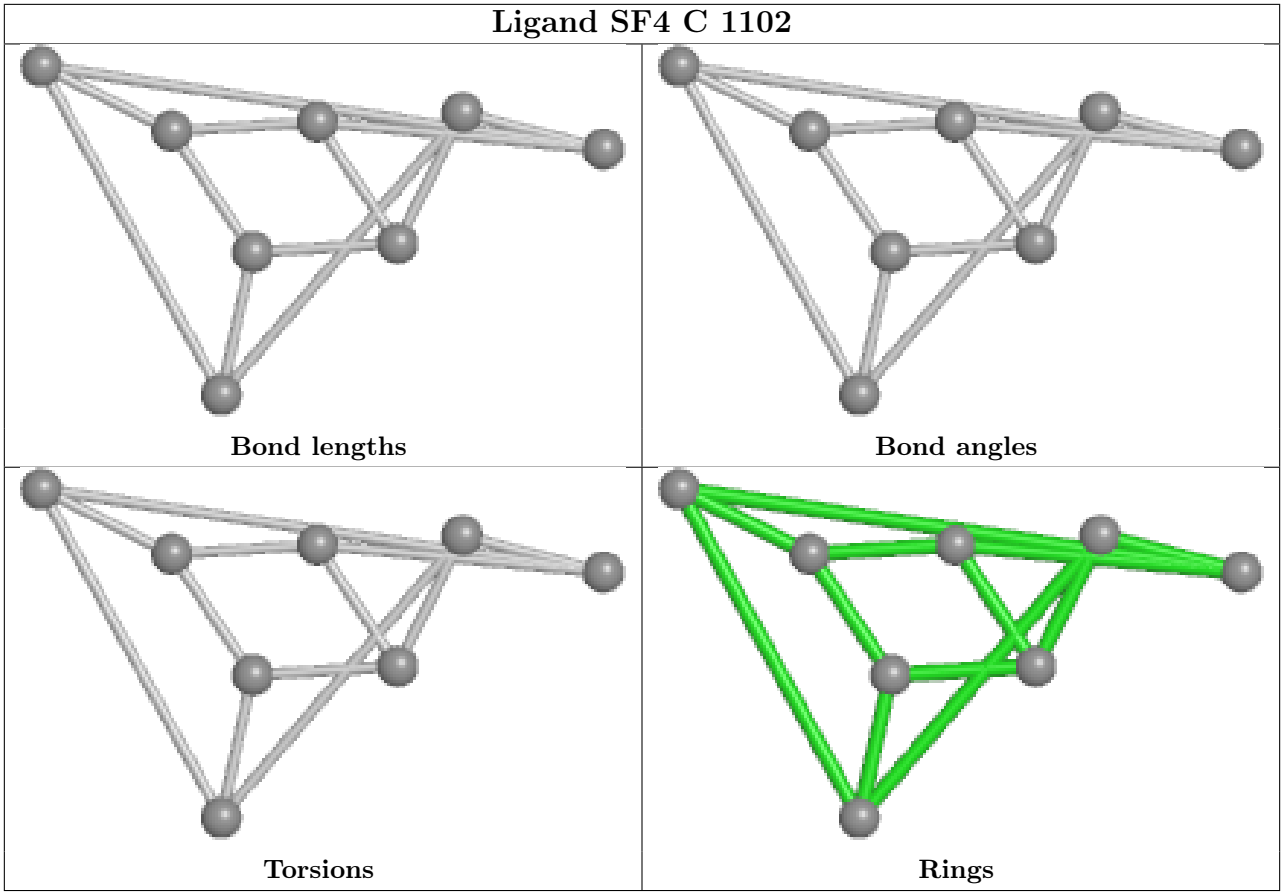
Bond angles



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	1005/1025 (98%)	-0.02	33 (3%)	46	51	15, 22, 45, 85	0
1	B	1006/1025 (98%)	-0.01	41 (4%)	37	41	16, 23, 48, 84	0
1	C	1007/1025 (98%)	-0.10	33 (3%)	46	51	12, 21, 45, 73	0
1	D	1011/1025 (98%)	-0.06	36 (3%)	42	47	13, 21, 46, 81	0
All	All	4029/4100 (98%)	-0.05	143 (3%)	44	49	12, 22, 47, 85	0

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	907	LEU	19.8
1	B	897	LEU	9.3
1	B	907	LEU	8.6
1	B	902	ALA	7.5
1	D	907	LEU	7.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

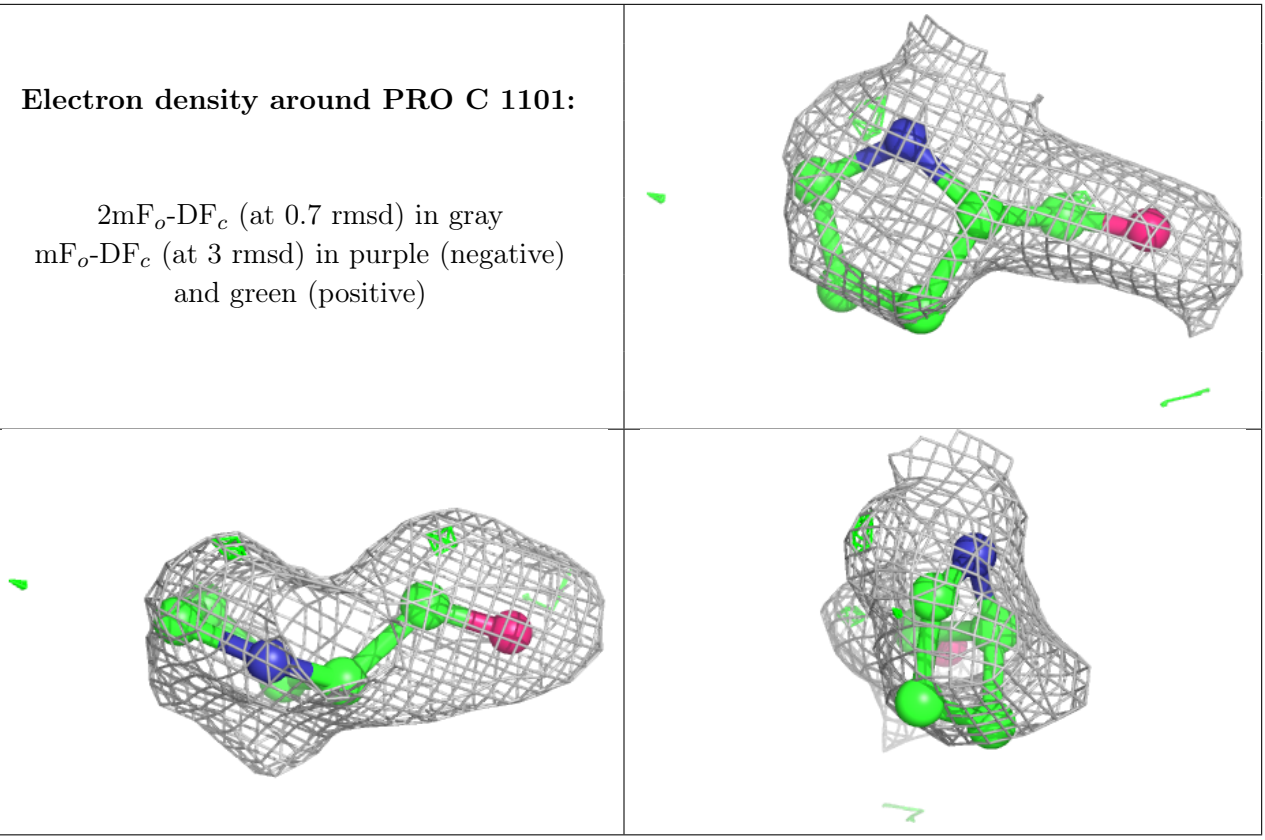
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
7	PRO	C	1101	7/8	0.68	0.17	53,55,57,59	0
4	NAP	B	1106	48/48	0.95	0.12	19,27,42,47	0
3	FAD	B	1105	53/53	0.96	0.08	16,20,26,28	0
4	NAP	D	1106	40/48	0.96	0.10	19,25,48,66	0
5	FMN	A	1107	31/31	0.96	0.11	14,18,23,28	0
4	NAP	A	1106	48/48	0.96	0.11	18,26,38,41	0
3	FAD	A	1105	53/53	0.97	0.08	15,19,23,27	0
3	FAD	C	1106	53/53	0.97	0.07	16,20,25,29	0
5	FMN	B	1108	31/31	0.97	0.08	14,19,22,30	0
5	FMN	C	1109	31/31	0.97	0.09	12,16,18,20	0
5	FMN	D	1108	31/31	0.97	0.10	13,16,20,27	0
6	TDR	C	1108	9/9	0.97	0.08	15,16,17,18	0
6	TDR	D	1107	9/9	0.97	0.08	14,15,17,20	0
4	NAP	C	1107	48/48	0.97	0.09	17,26,36,38	0
6	TDR	A	1108	9/9	0.98	0.09	16,18,20,22	0
3	FAD	D	1105	53/53	0.98	0.07	14,18,21,24	0
2	SF4	C	1103	8/8	0.99	0.05	15,16,16,16	0
2	SF4	C	1104	8/8	0.99	0.06	14,15,15,16	0
2	SF4	D	1103	8/8	0.99	0.07	15,15,15,15	0
2	SF4	D	1104	8/8	0.99	0.06	16,16,17,17	0
2	SF4	A	1103	8/8	0.99	0.05	17,18,18,19	0
2	SF4	B	1101	8/8	0.99	0.06	16,16,17,17	0
2	SF4	B	1102	8/8	0.99	0.07	17,18,18,18	0
6	TDR	B	1107	9/9	0.99	0.07	17,19,20,20	0
2	SF4	B	1103	8/8	0.99	0.05	18,18,19,19	0
2	SF4	B	1104	8/8	0.99	0.05	17,17,18,18	0
2	SF4	C	1102	8/8	0.99	0.05	15,16,16,16	0
2	SF4	A	1104	8/8	1.00	0.04	17,18,18,19	0
2	SF4	A	1102	8/8	1.00	0.06	16,16,17,17	0
2	SF4	C	1105	8/8	1.00	0.07	17,18,18,18	0
2	SF4	D	1101	8/8	1.00	0.04	16,16,17,17	0
2	SF4	D	1102	8/8	1.00	0.04	16,16,17,17	0
2	SF4	A	1101	8/8	1.00	0.06	17,17,18,18	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.

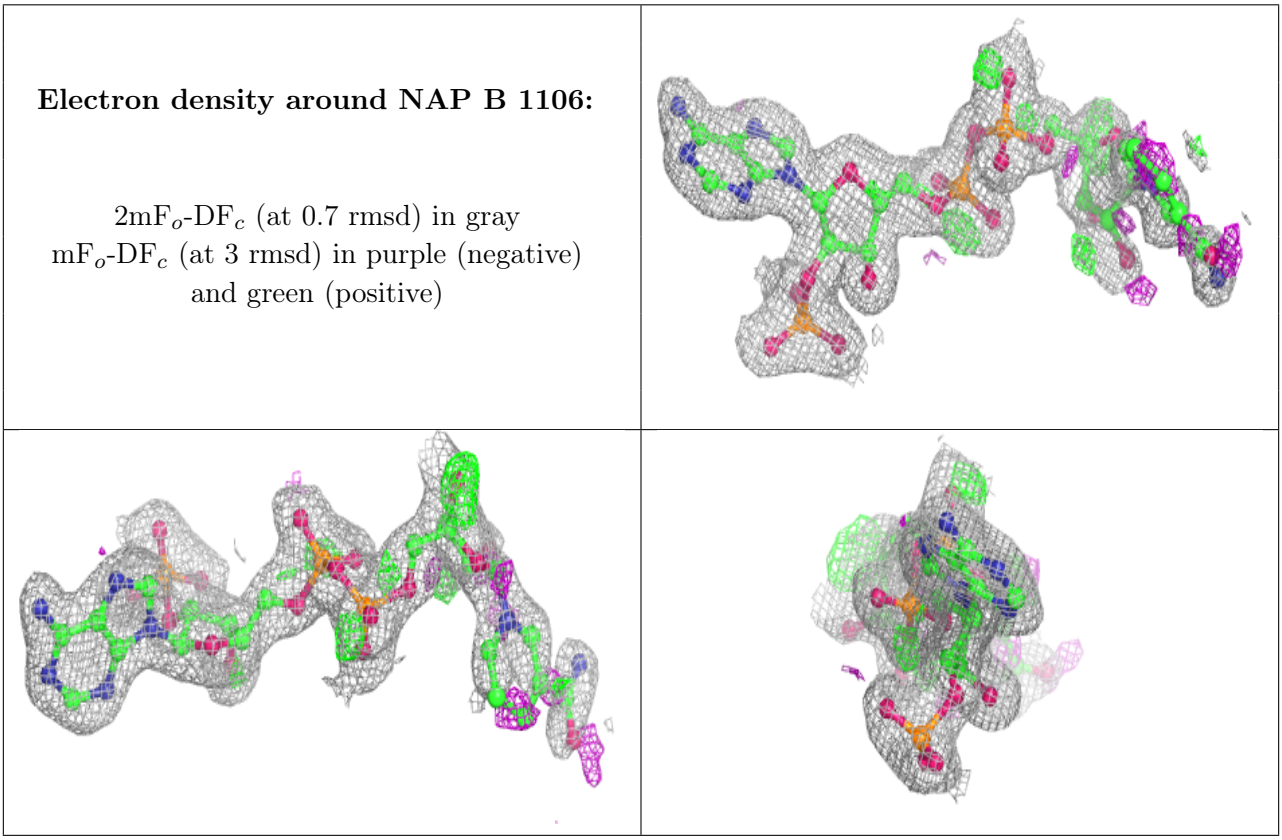
Electron density around PRO C 1101:

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



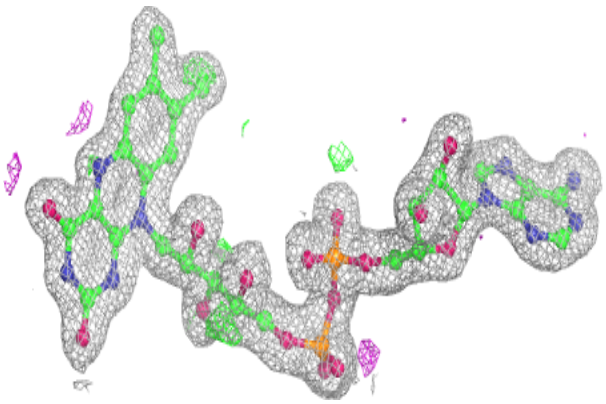
Electron density around NAP B 1106:

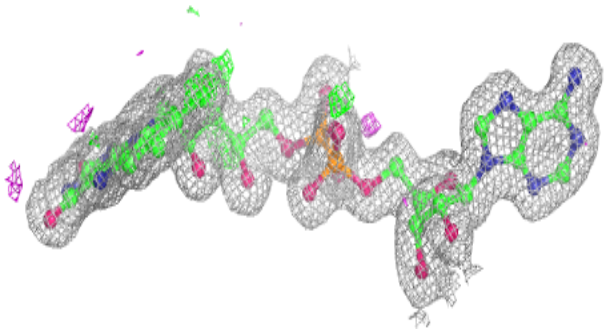
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

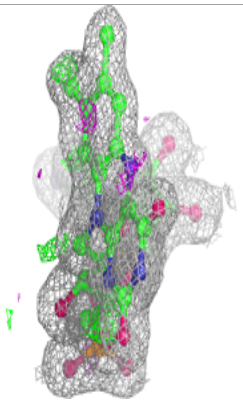


Electron density around FAD B 1105:

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

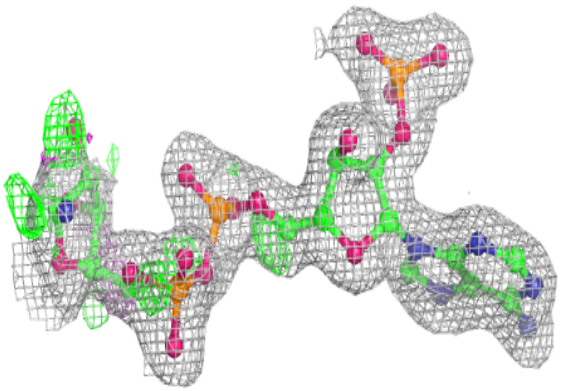


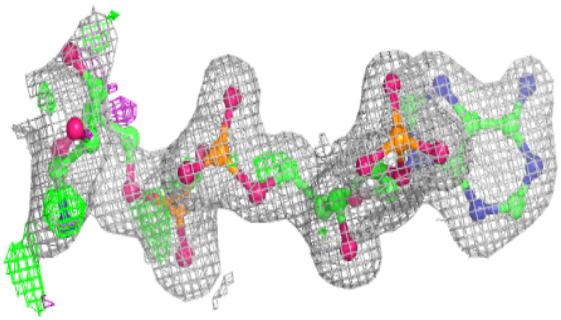


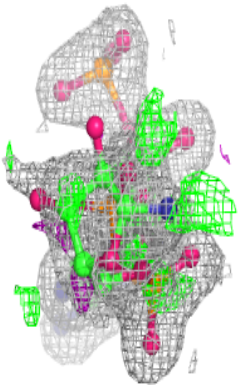


Electron density around NAP D 1106:

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

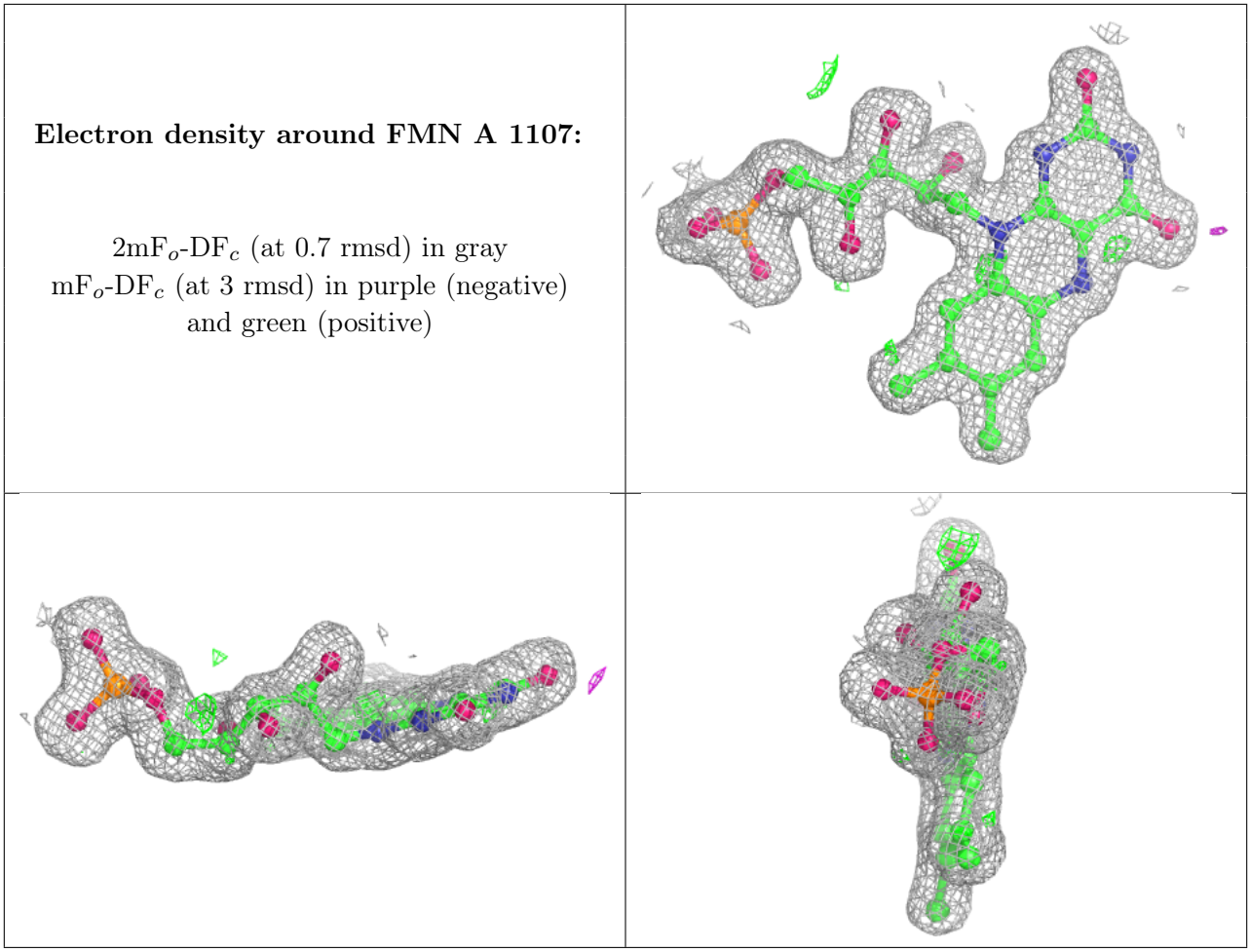






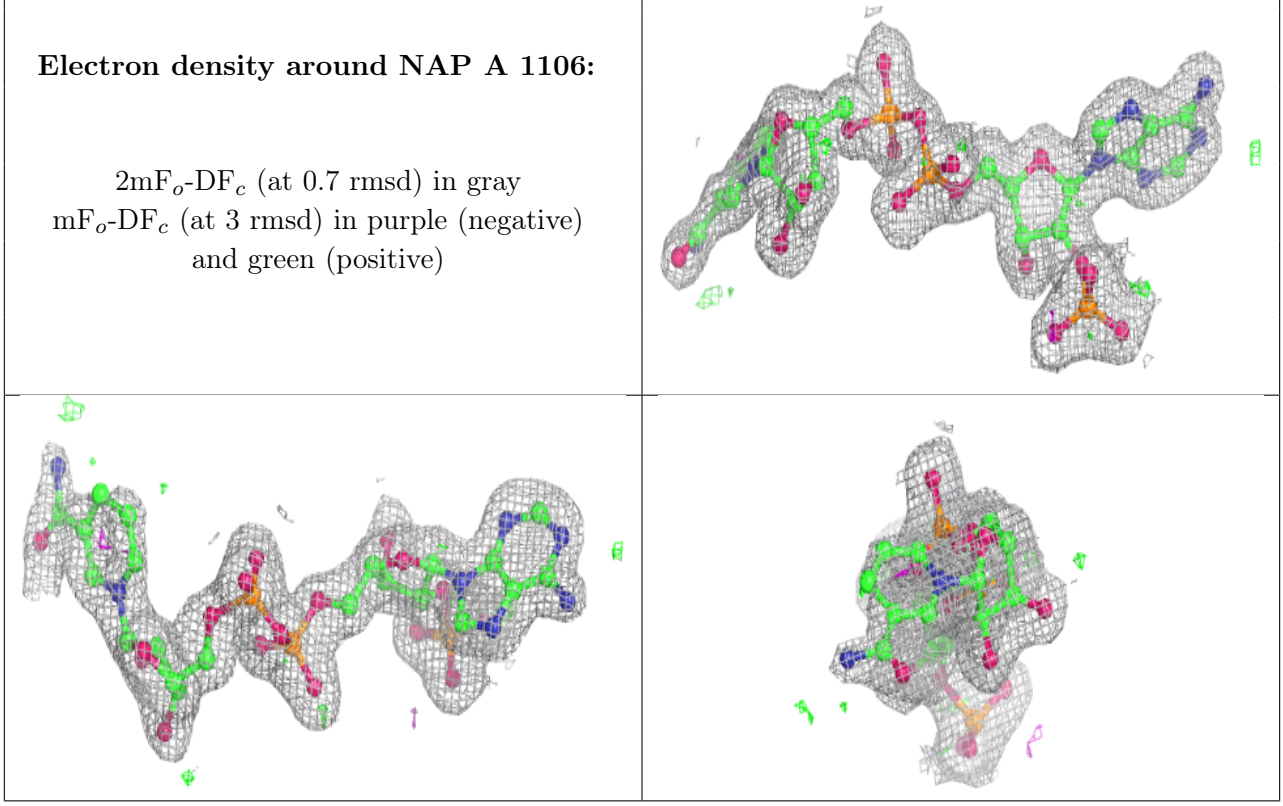
Electron density around FMN A 1107:

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



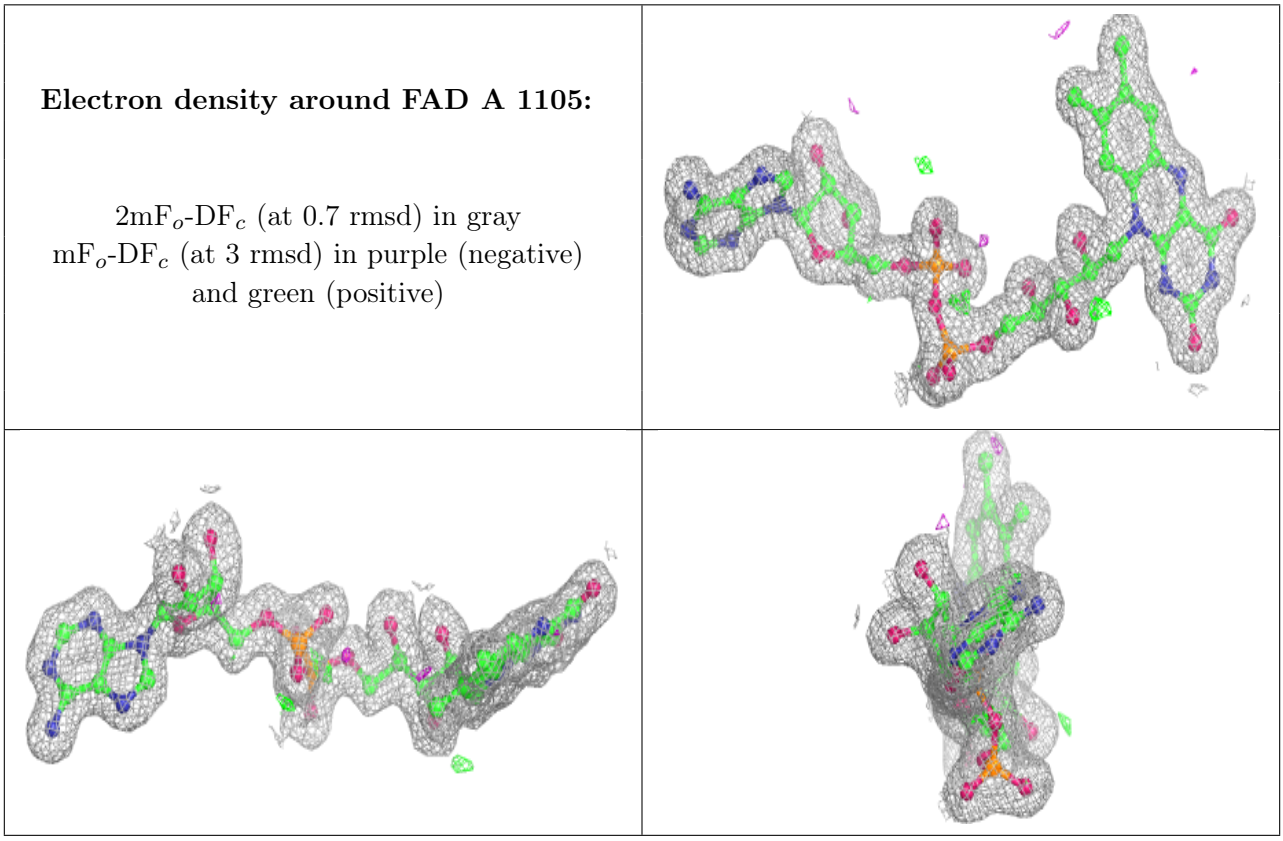
Electron density around NAP A 1106:

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



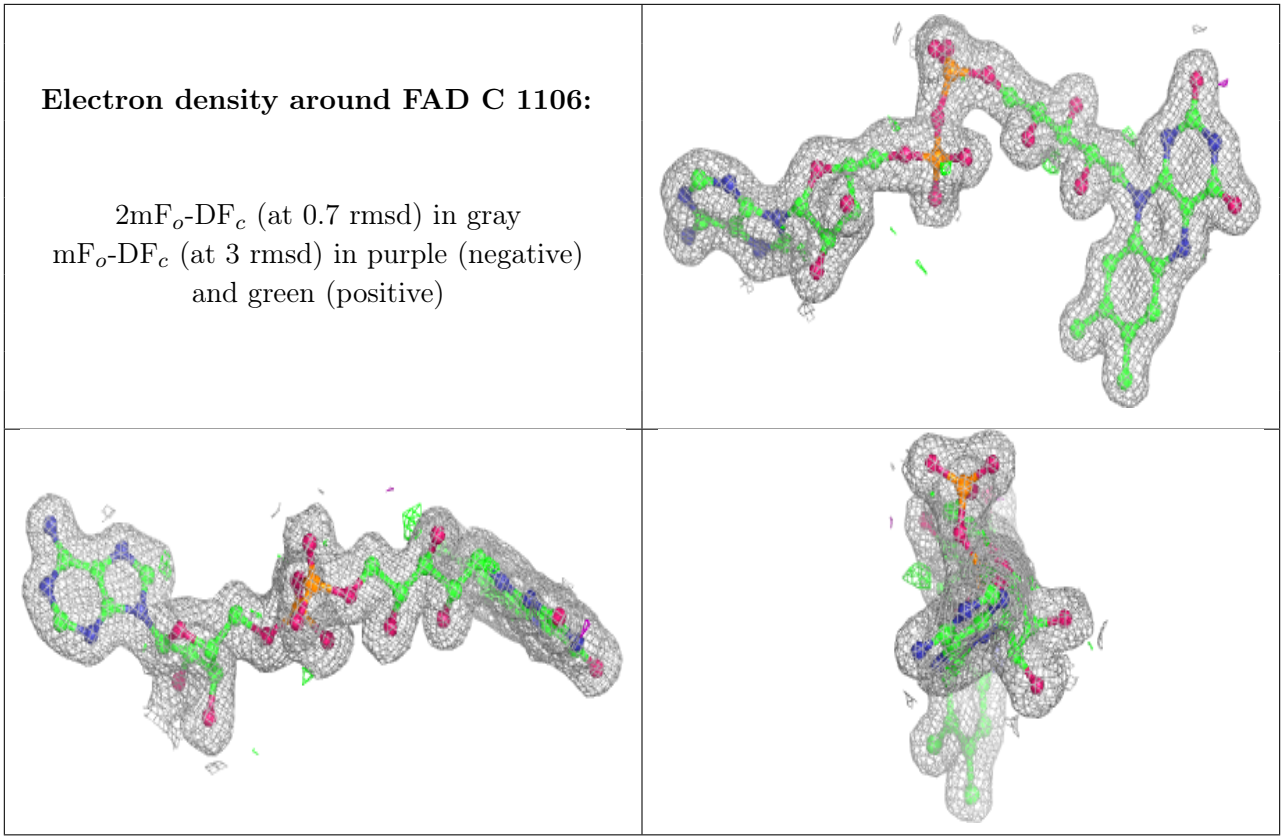
Electron density around FAD A 1105:

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



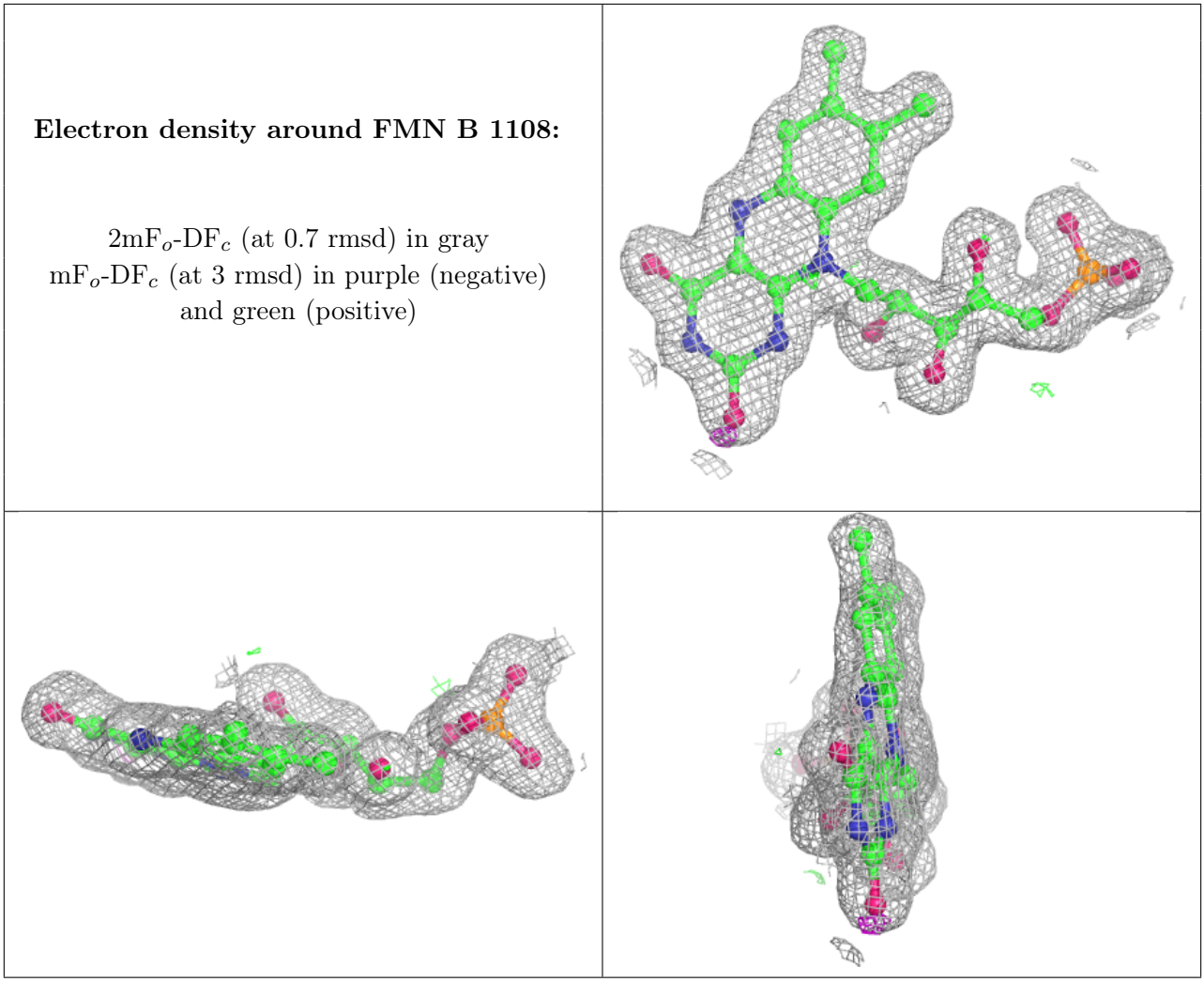
Electron density around FAD C 1106:

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



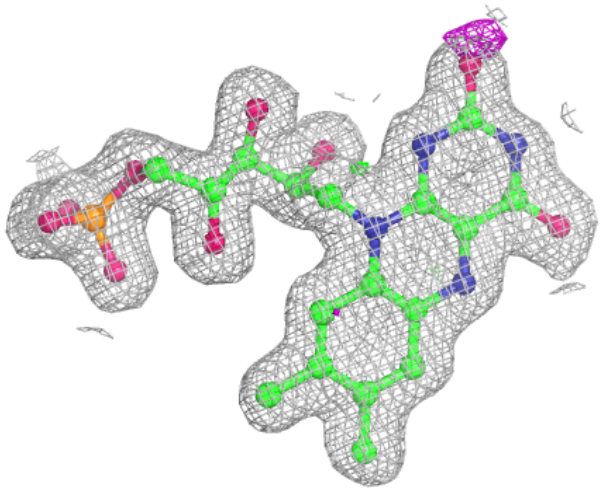
Electron density around FMN B 1108:

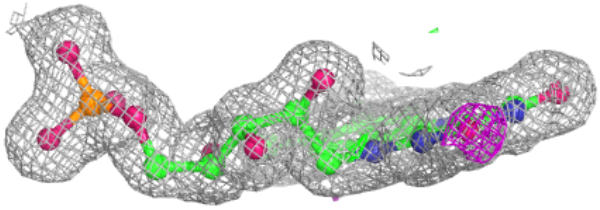
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

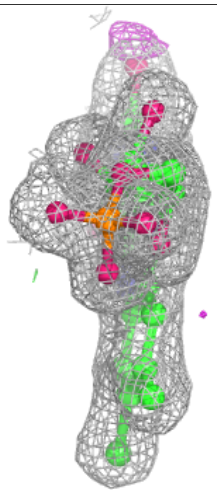


Electron density around FMN C 1109:

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

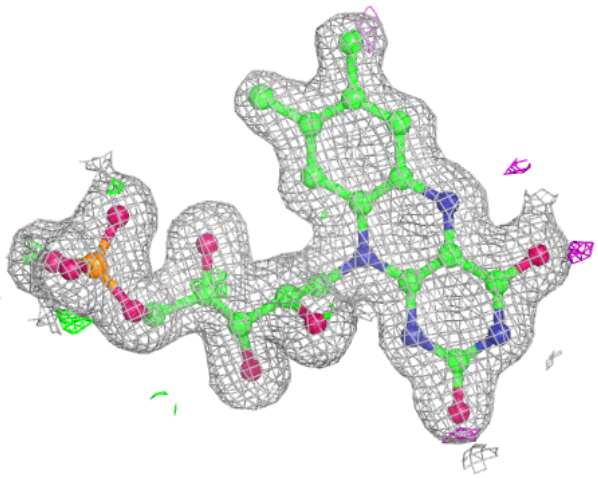


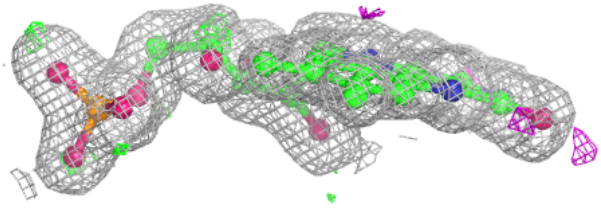


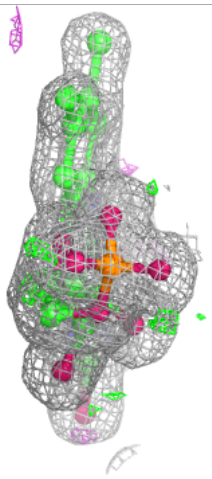


Electron density around FMN D 1108:

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

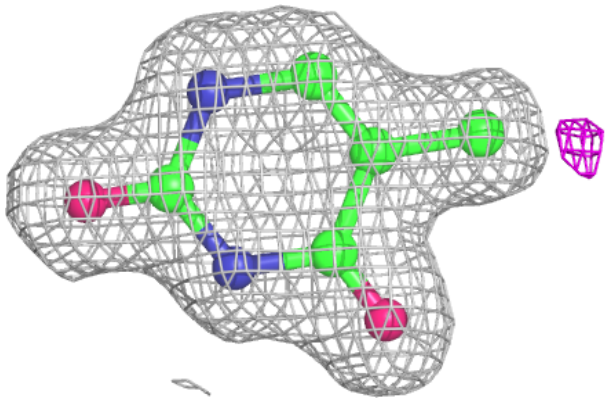


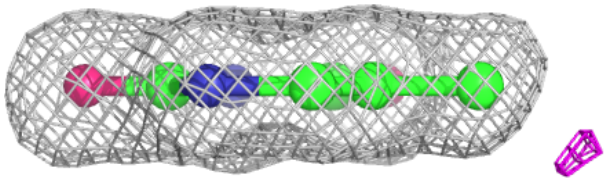


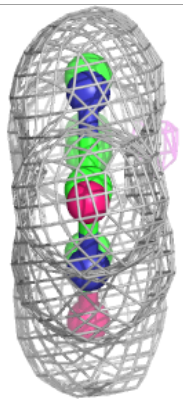


Electron density around TDR C 1108:

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

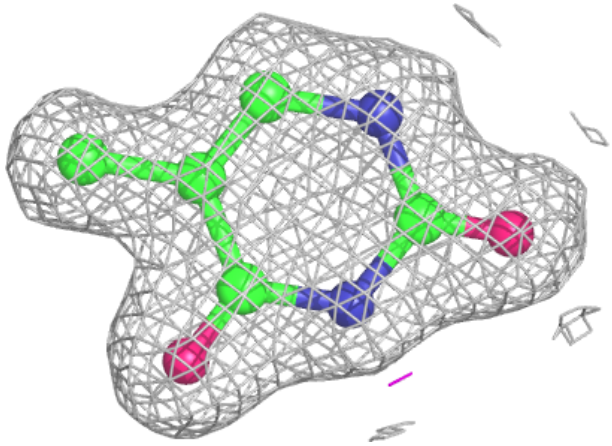


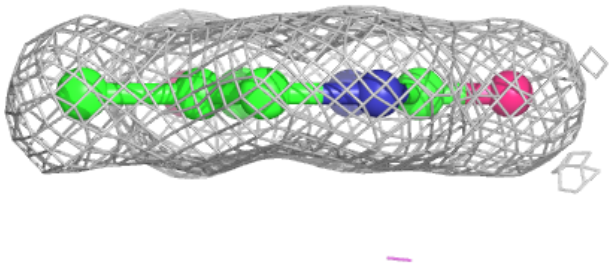


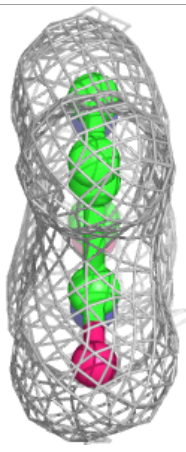


Electron density around TDR D 1107:

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

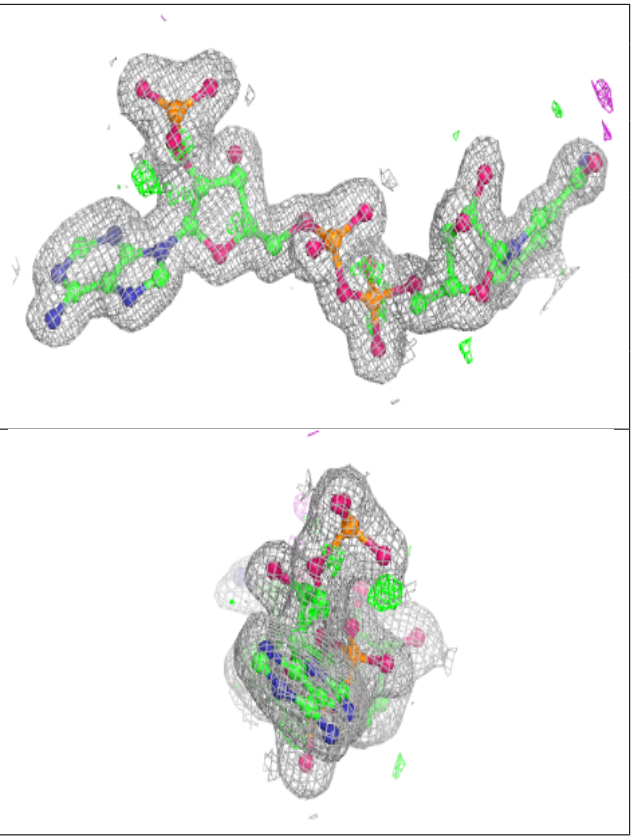






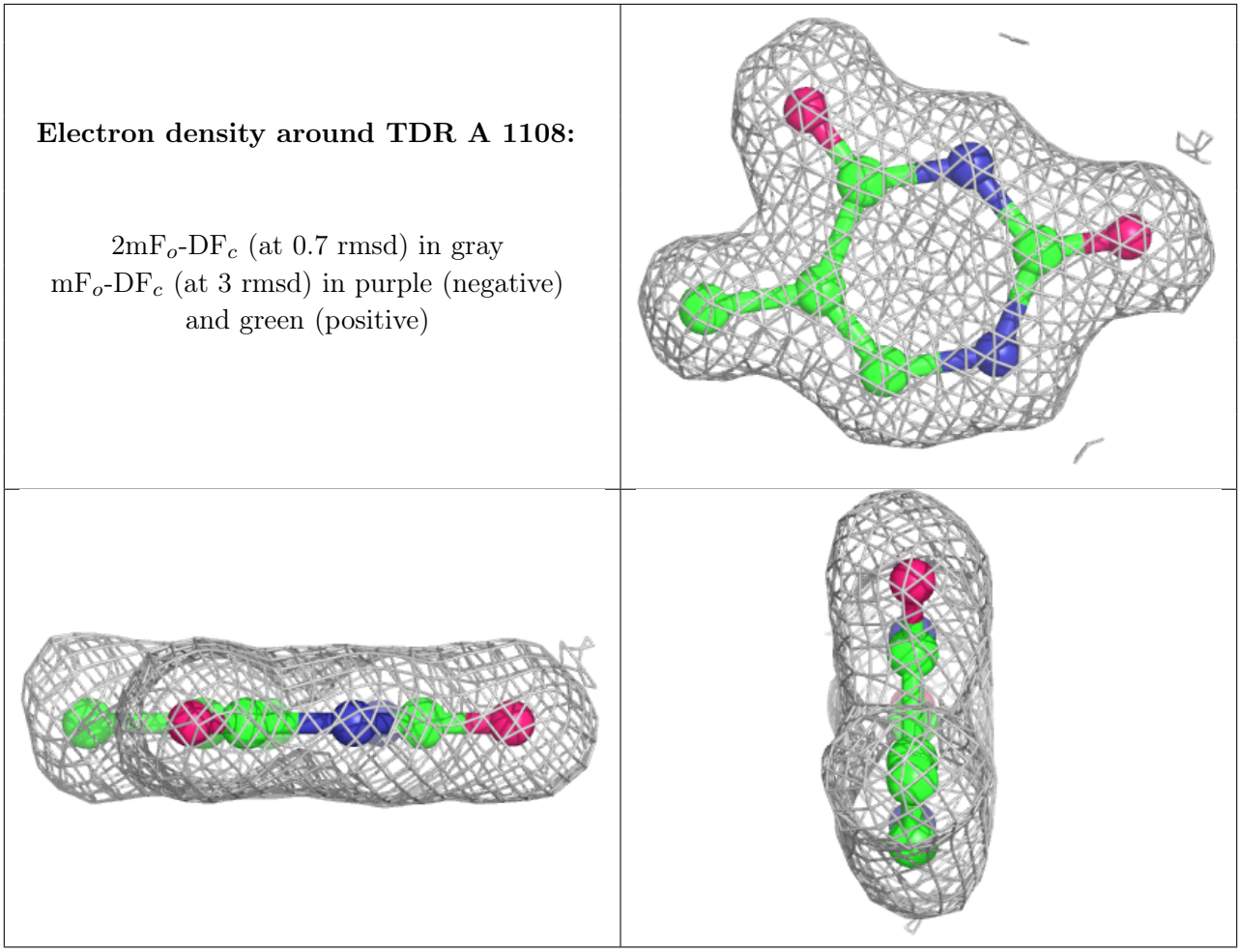
Electron density around NAP C 1107:

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



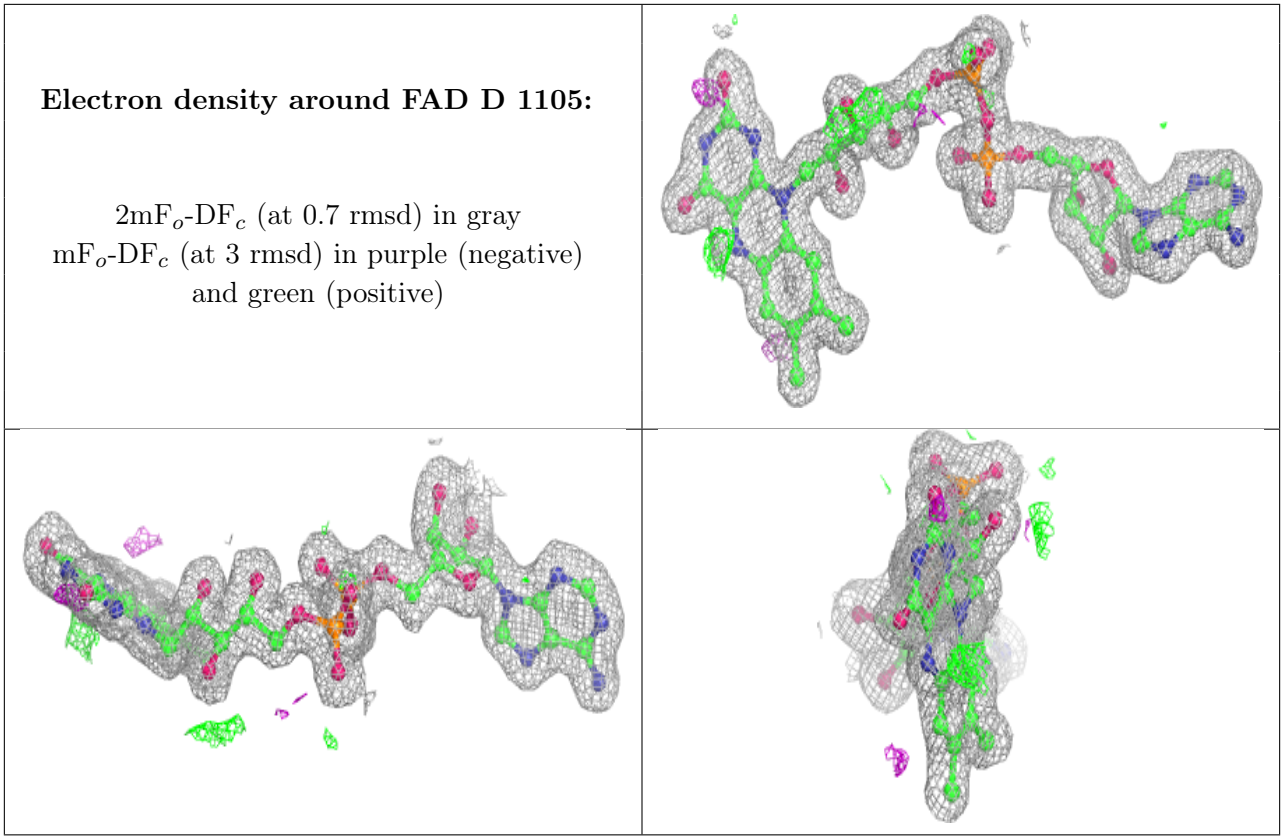
Electron density around TDR A 1108:

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



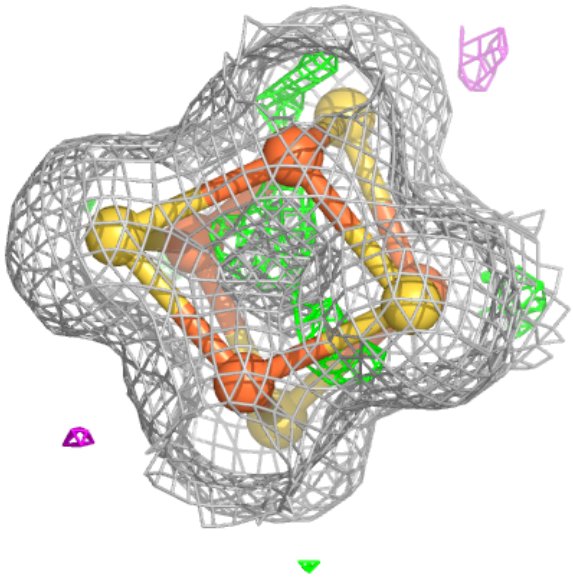
Electron density around FAD D 1105:

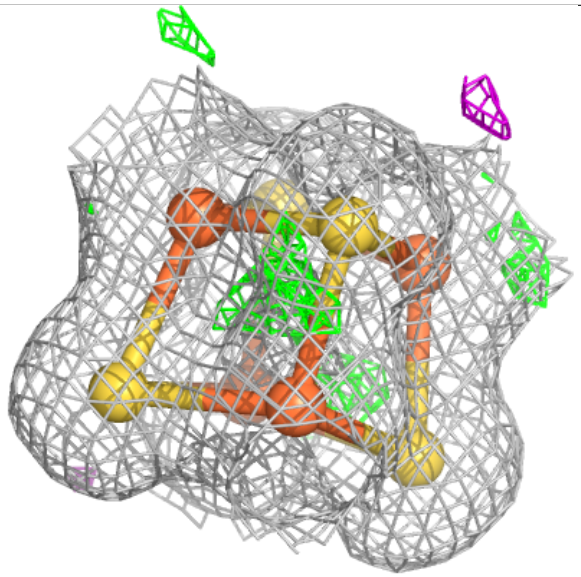
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

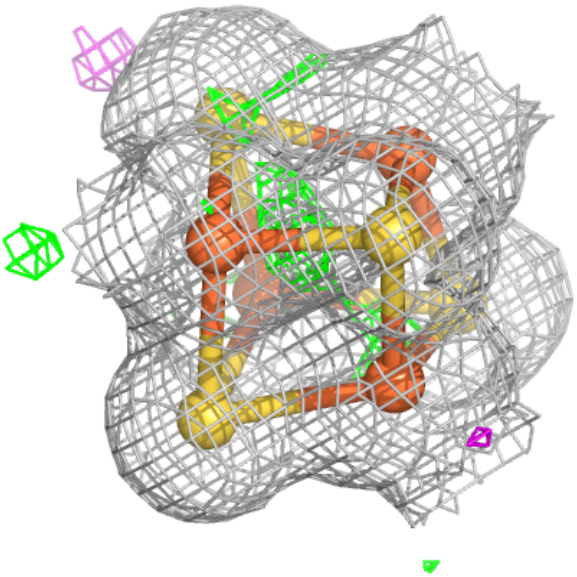


Electron density around SF4 C 1103:

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

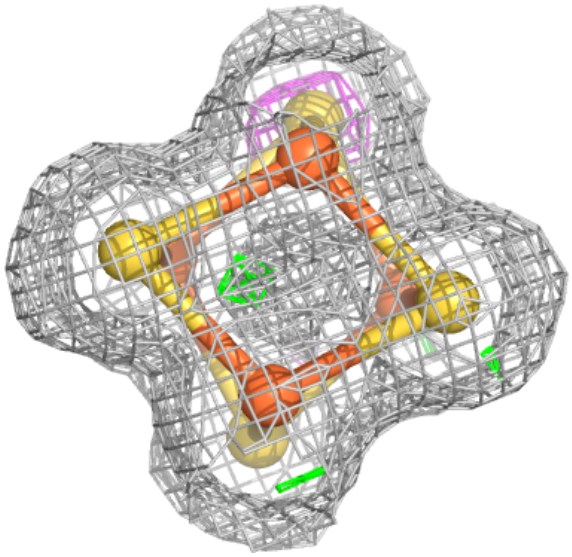


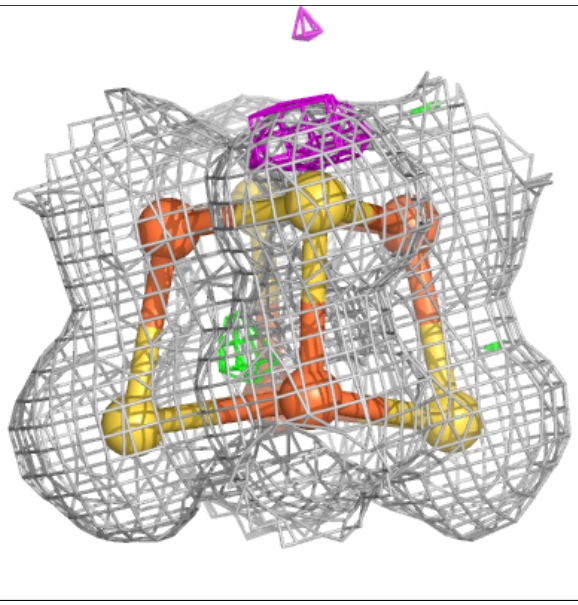


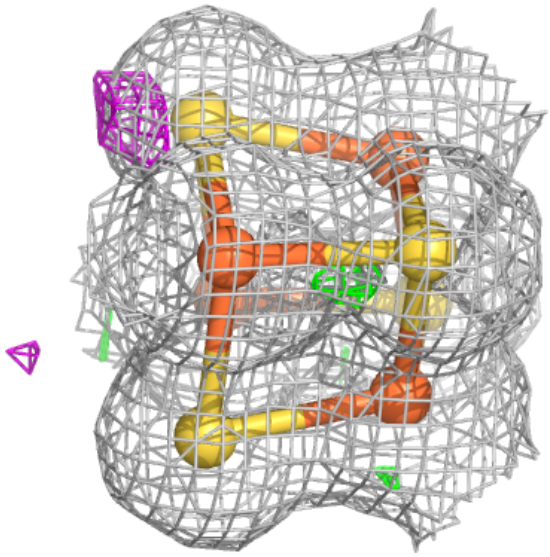


Electron density around SF4 C 1104:

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

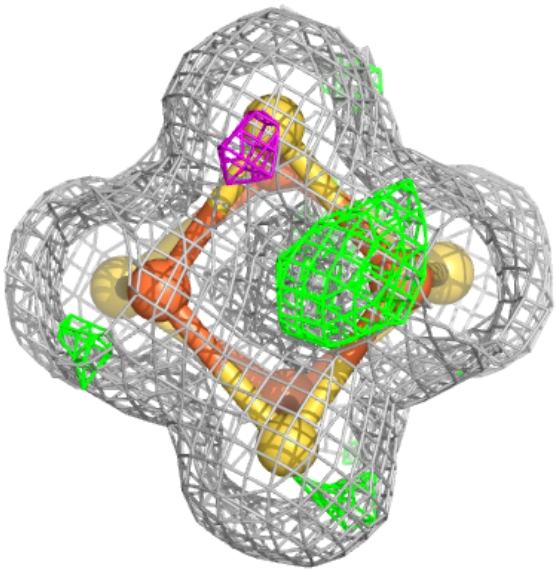


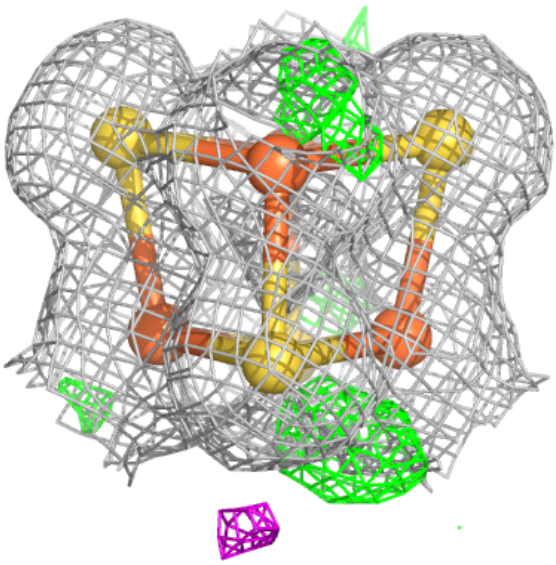


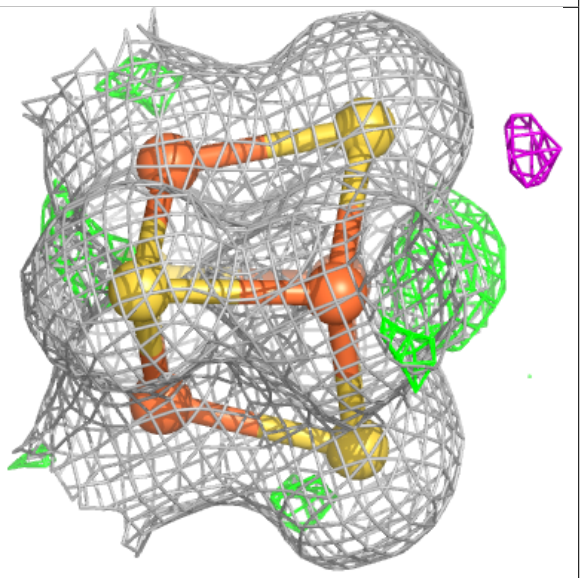


Electron density around SF4 D 1103:

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

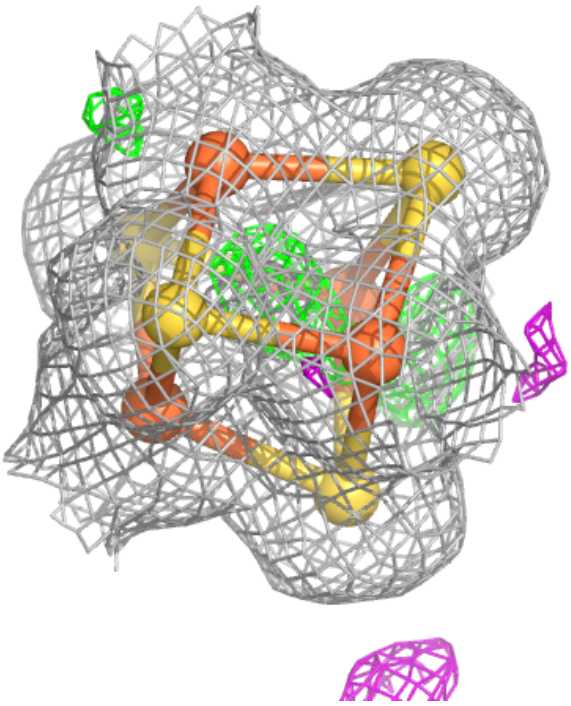


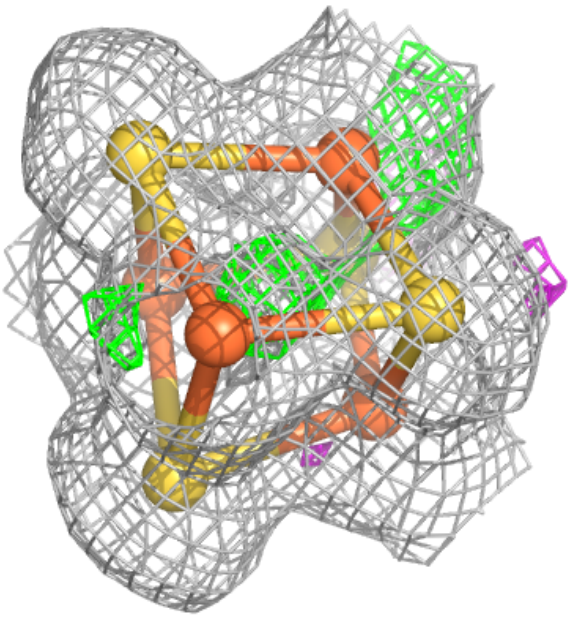


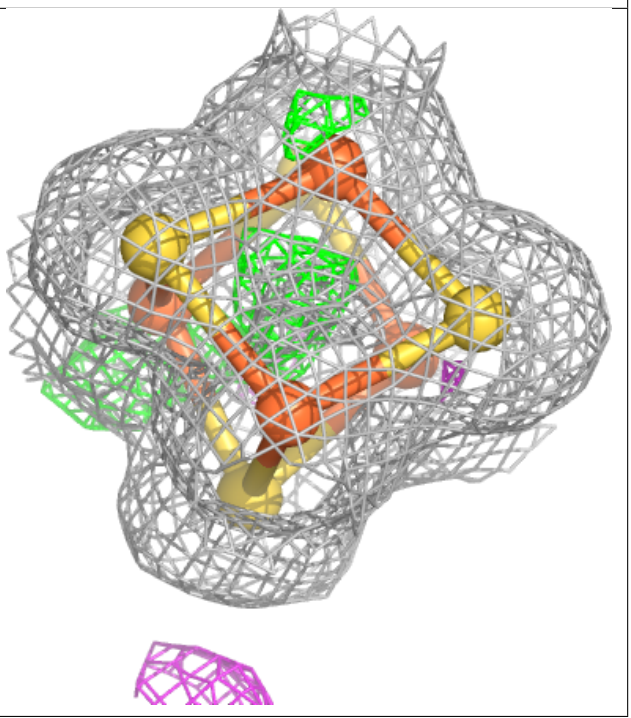


Electron density around SF4 D 1104:

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

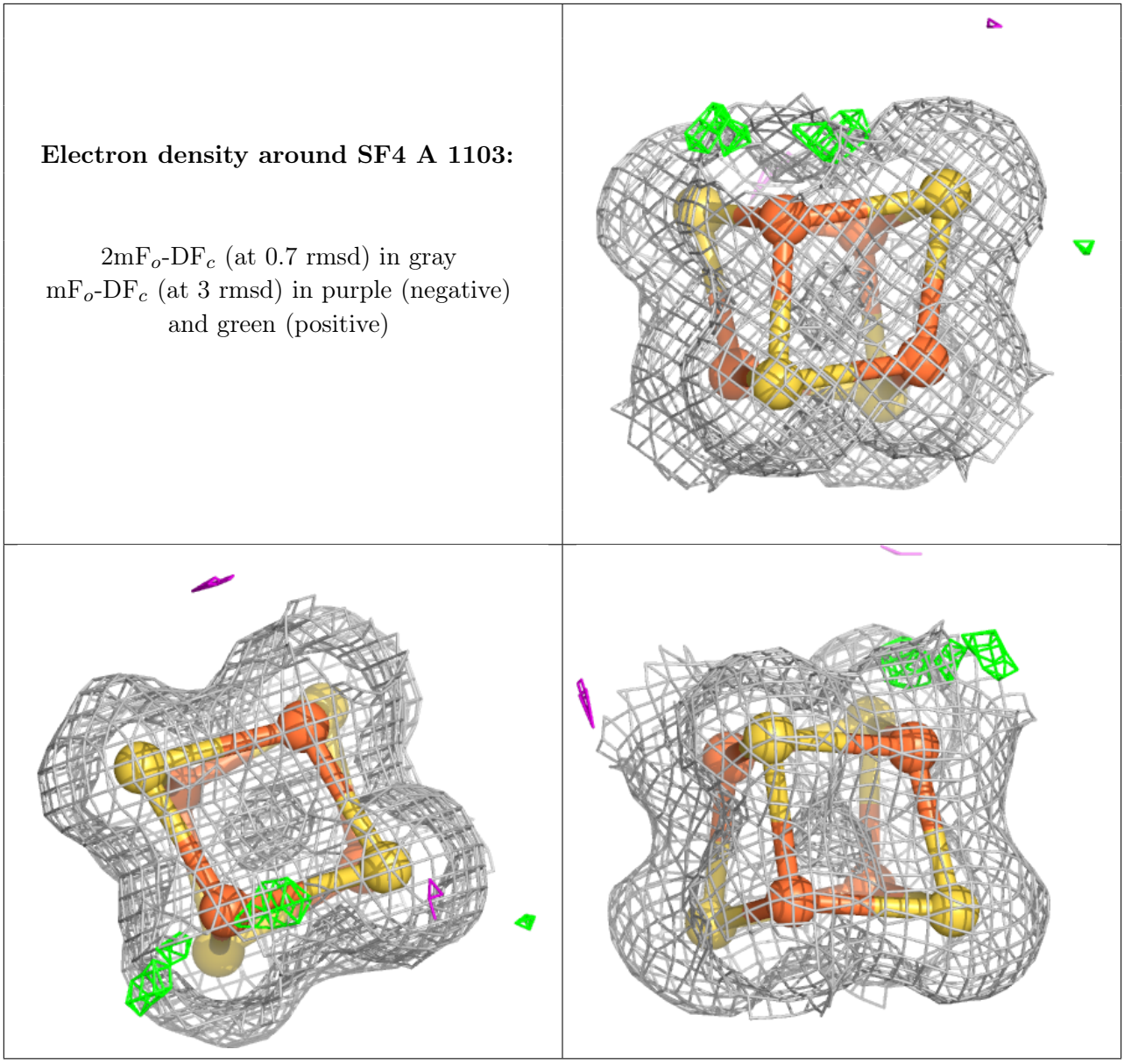






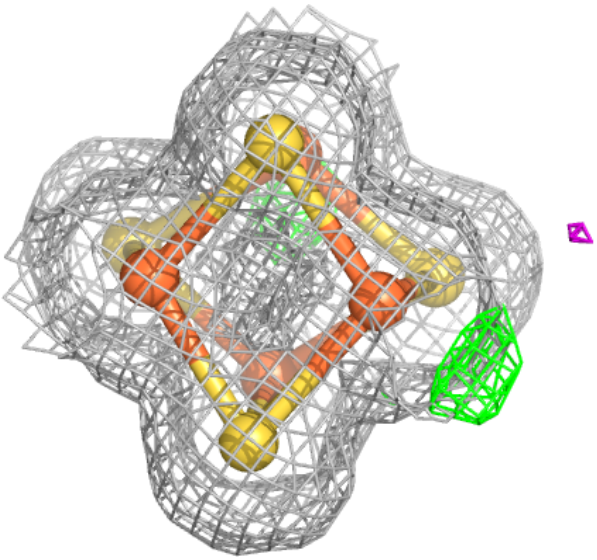
Electron density around SF4 A 1103:

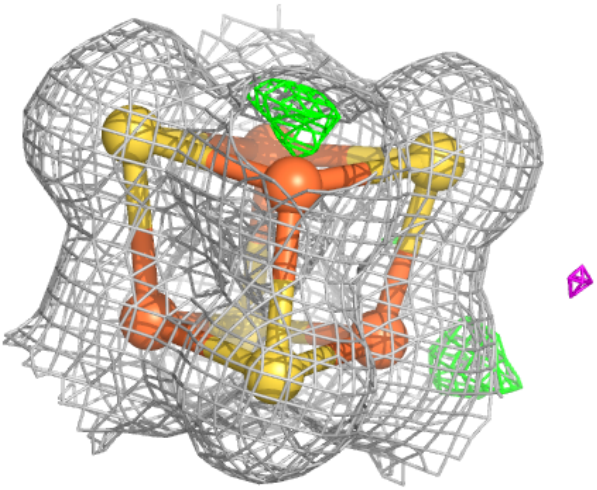
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

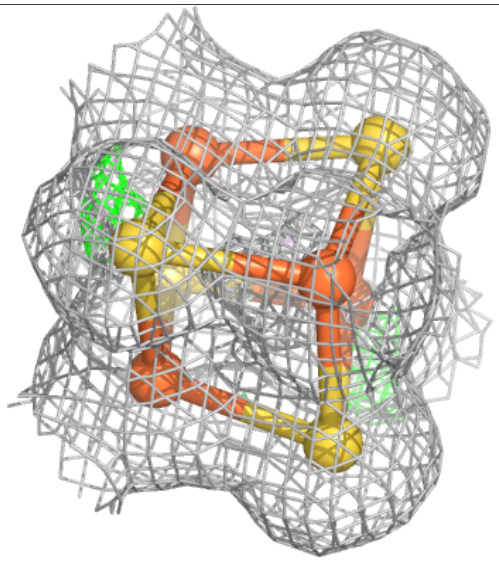


Electron density around SF4 B 1101:

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

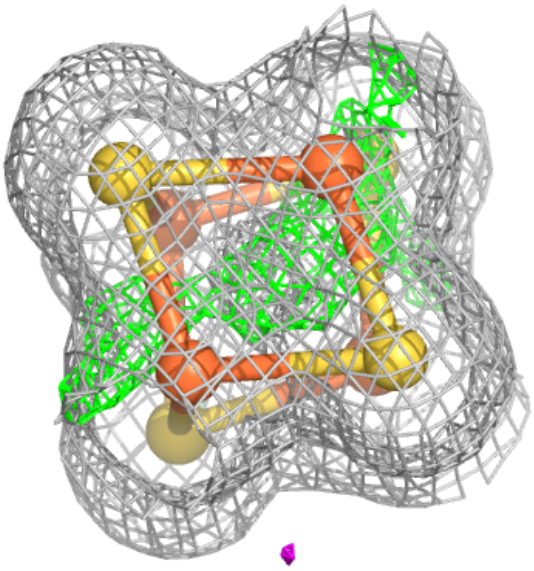


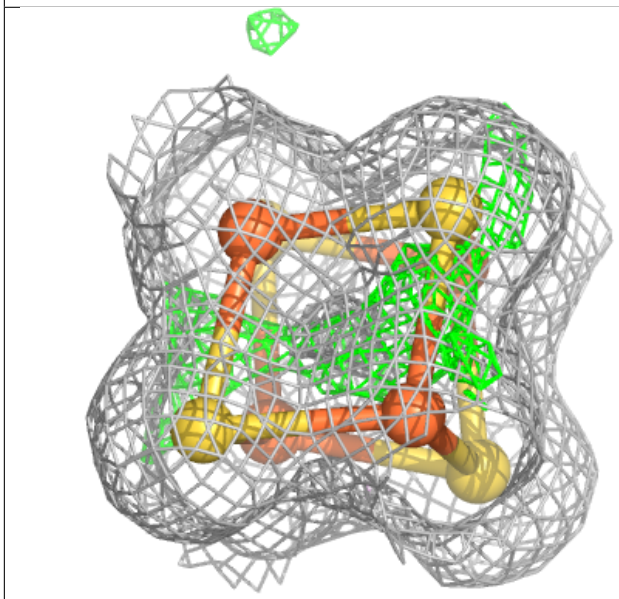


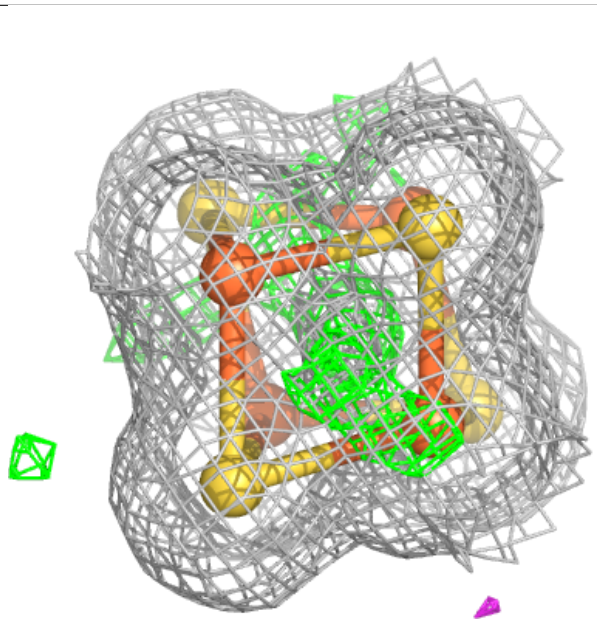


Electron density around SF4 B 1102:

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

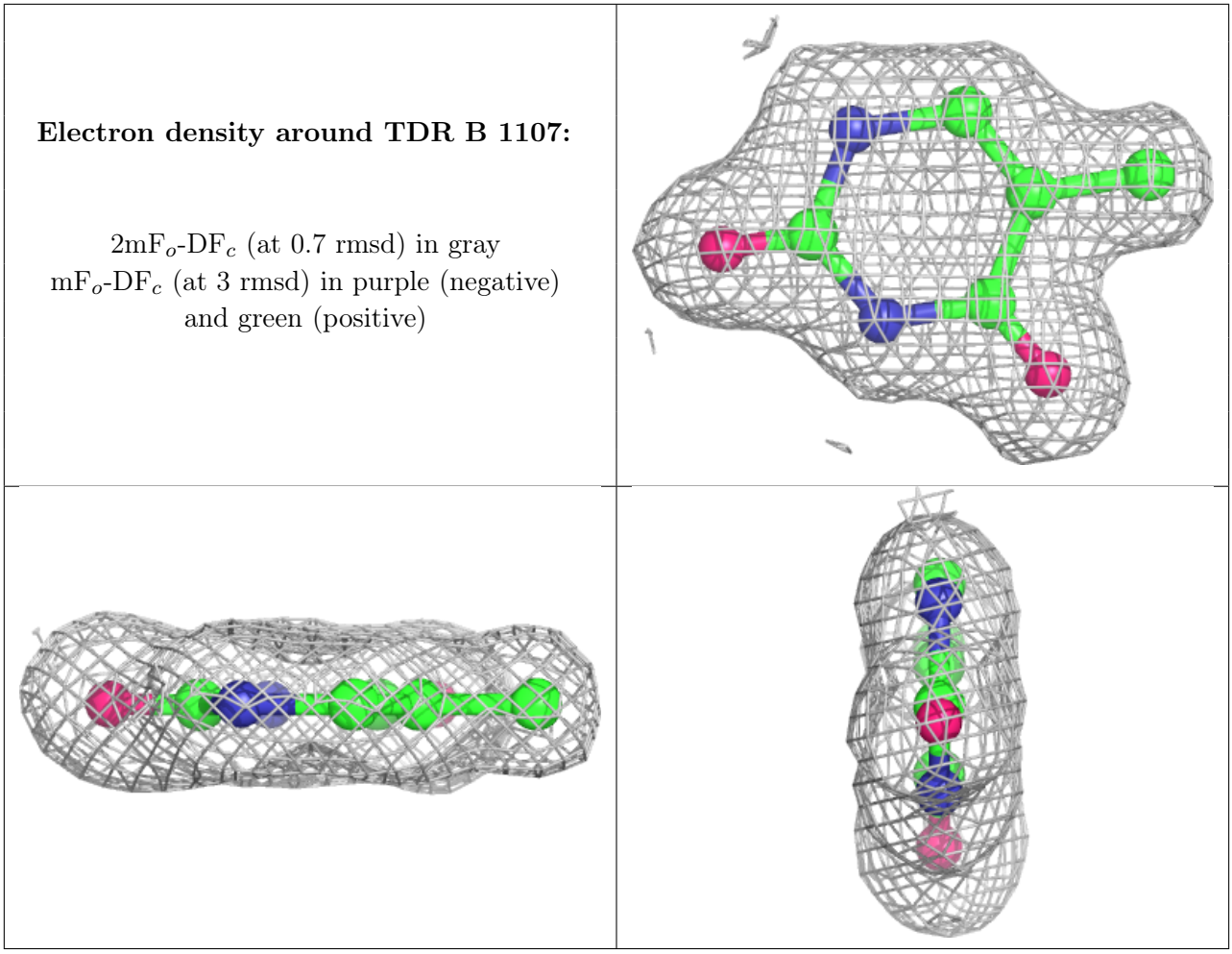






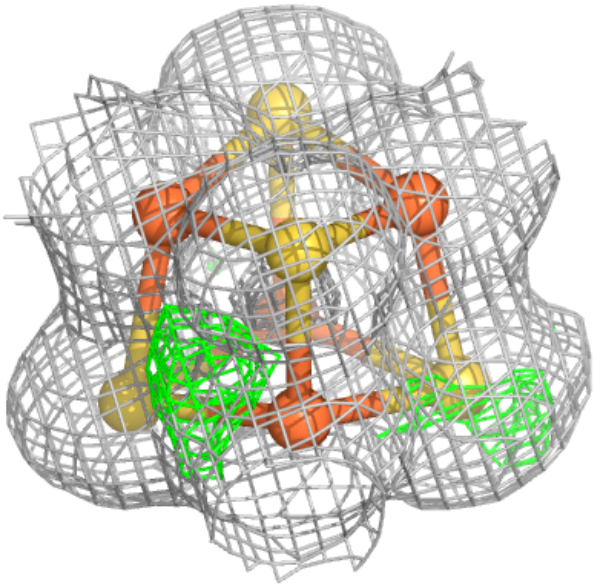
Electron density around TDR B 1107:

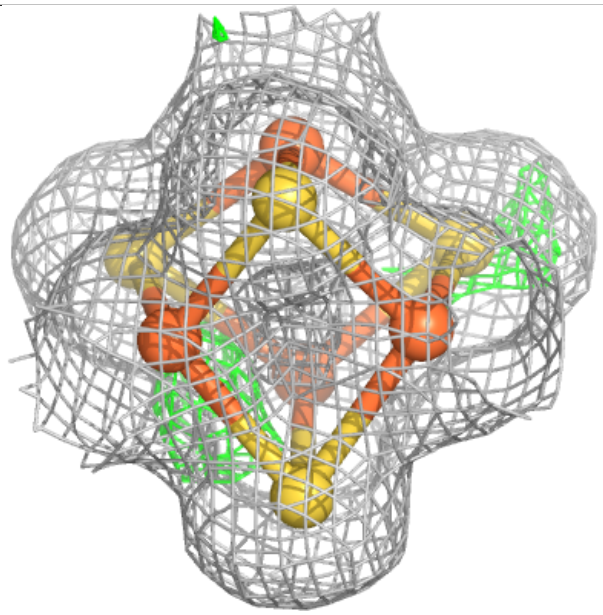
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

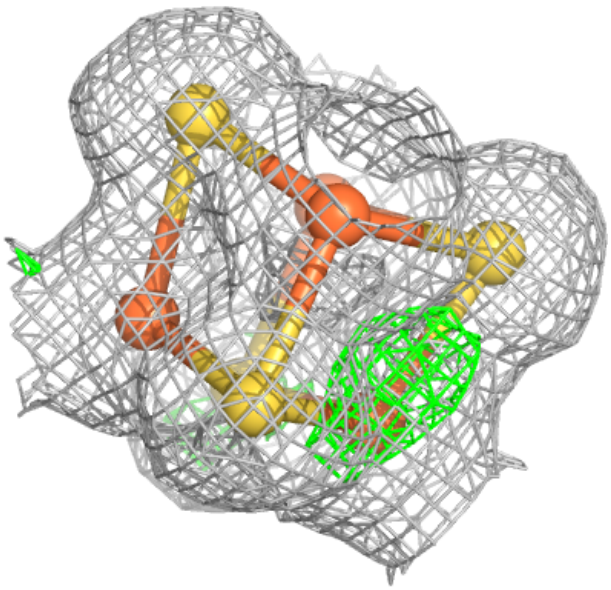


Electron density around SF4 B 1103:

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

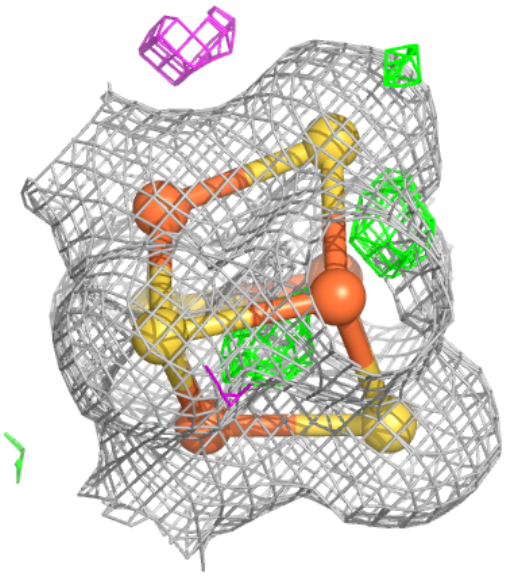


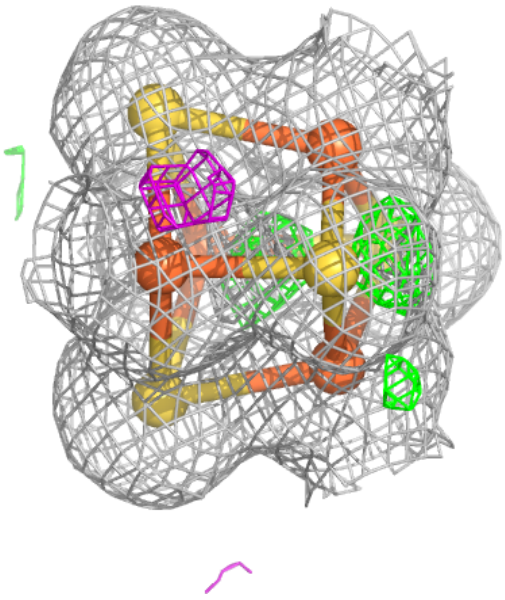


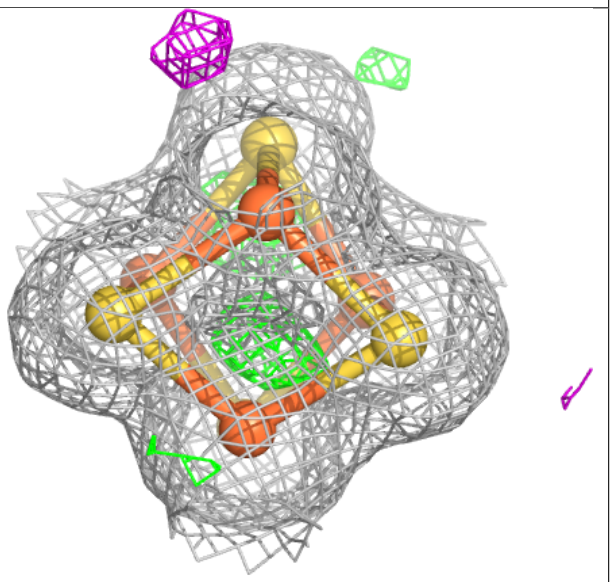


Electron density around SF4 B 1104:

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

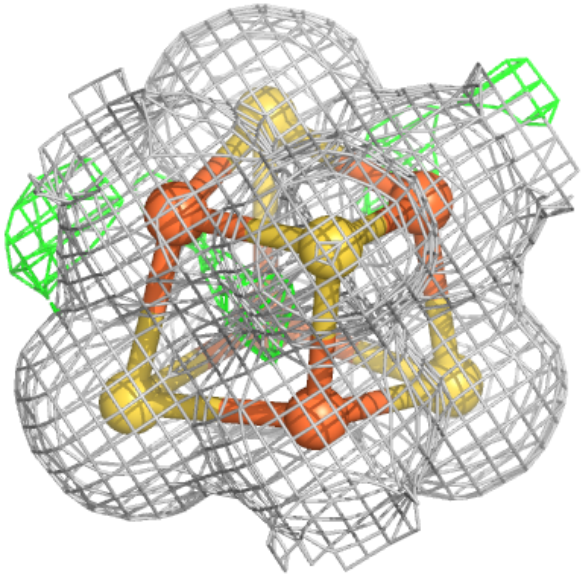


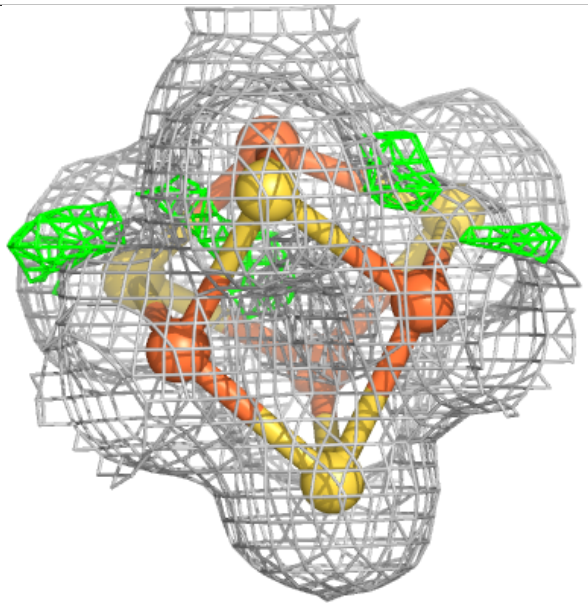


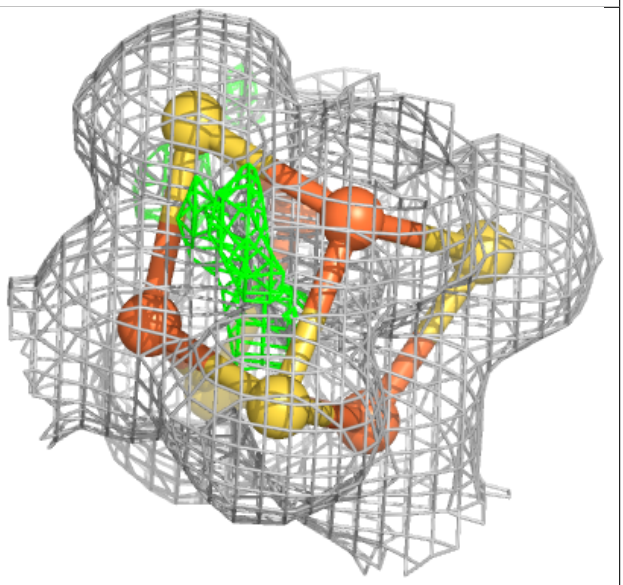


Electron density around SF4 C 1102:

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

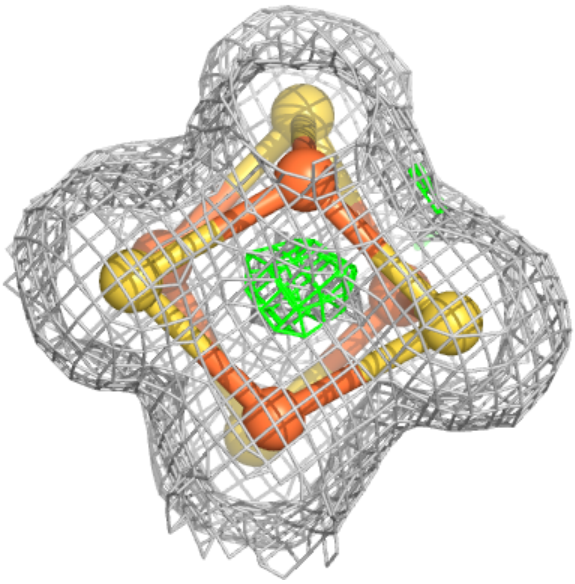


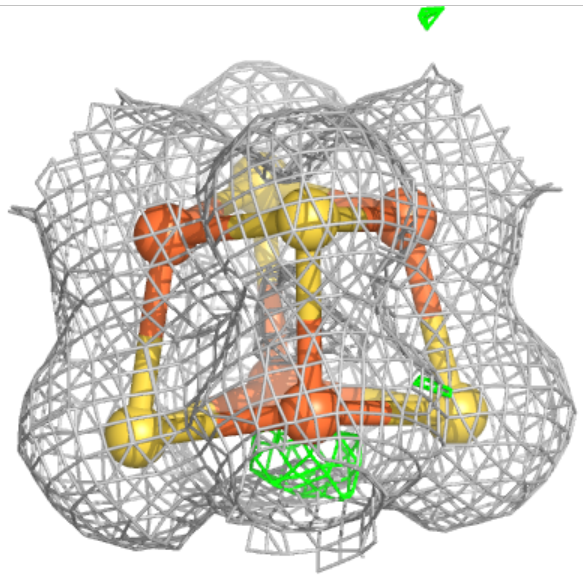


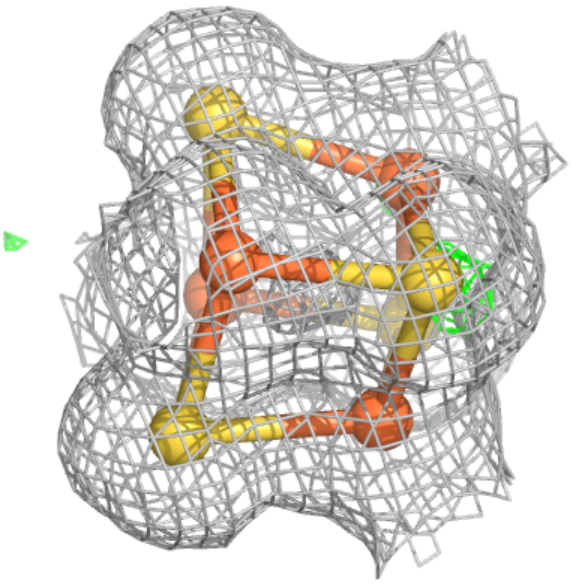


Electron density around SF4 A 1104:

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

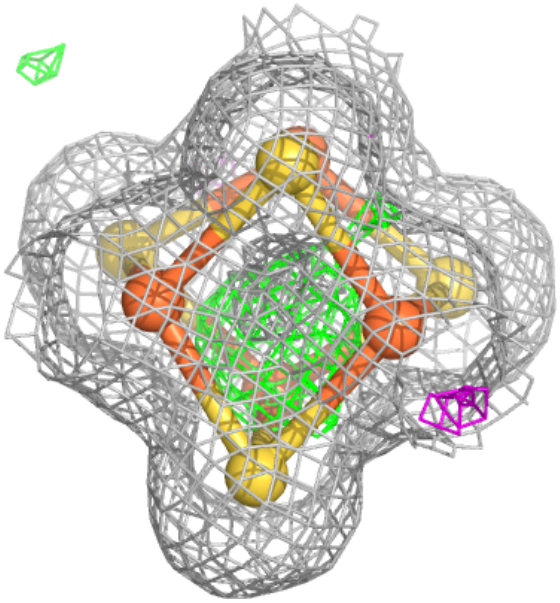


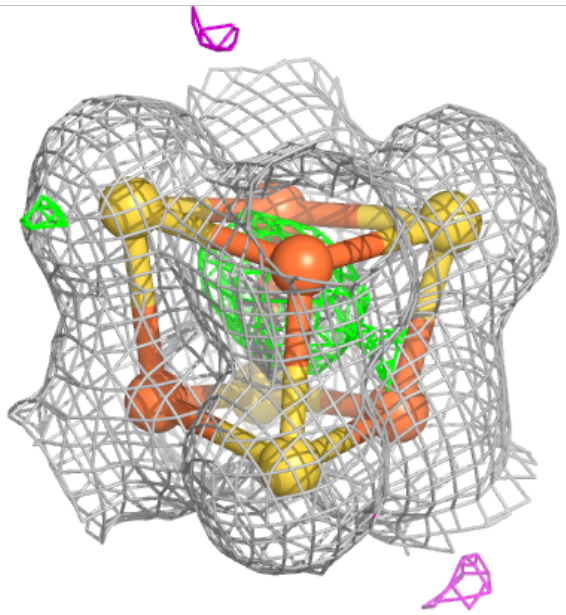


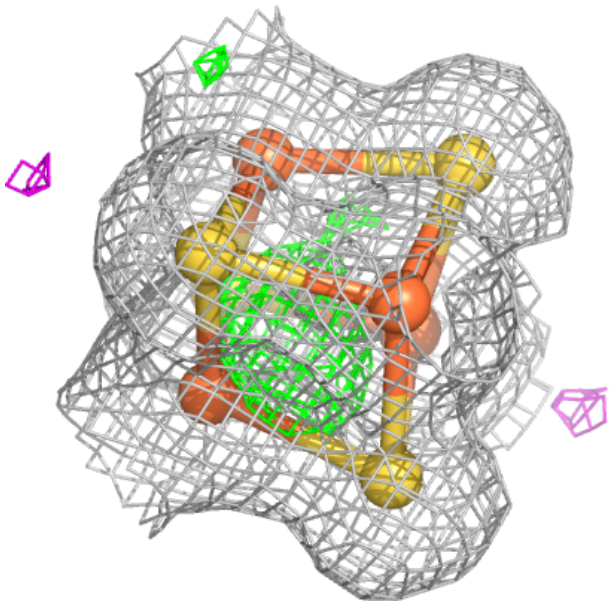


Electron density around SF4 A 1102:

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

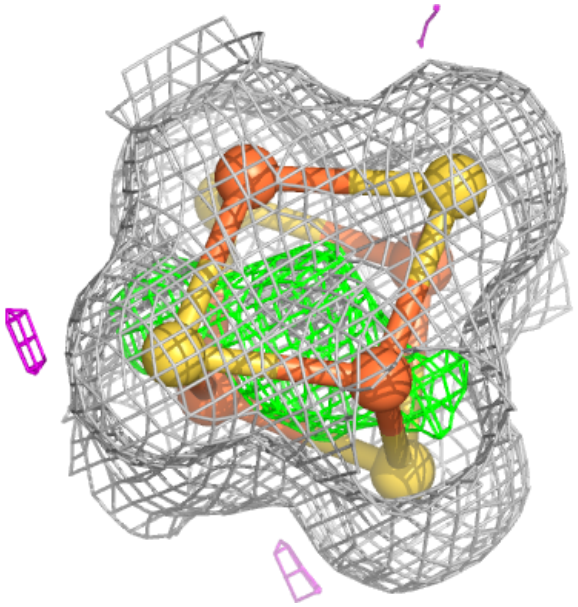


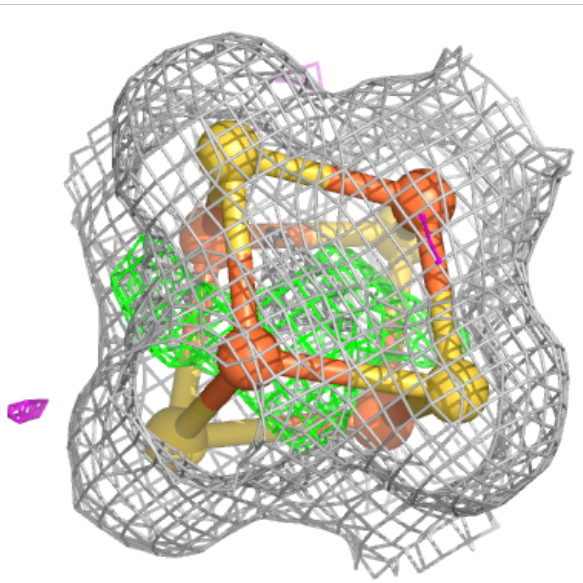


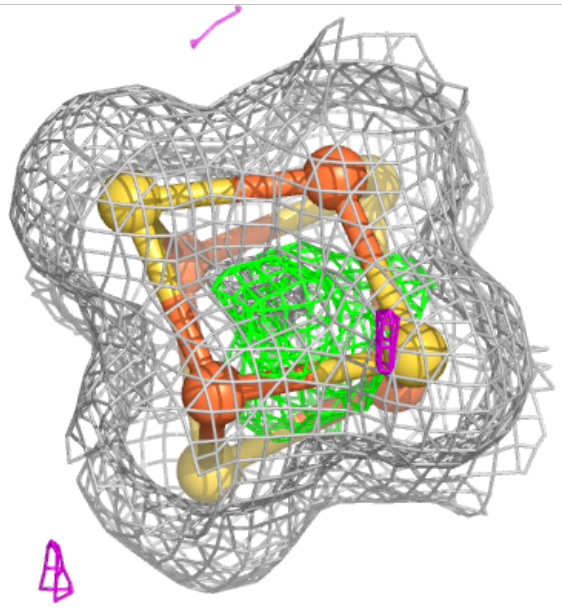


Electron density around SF4 C 1105:

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

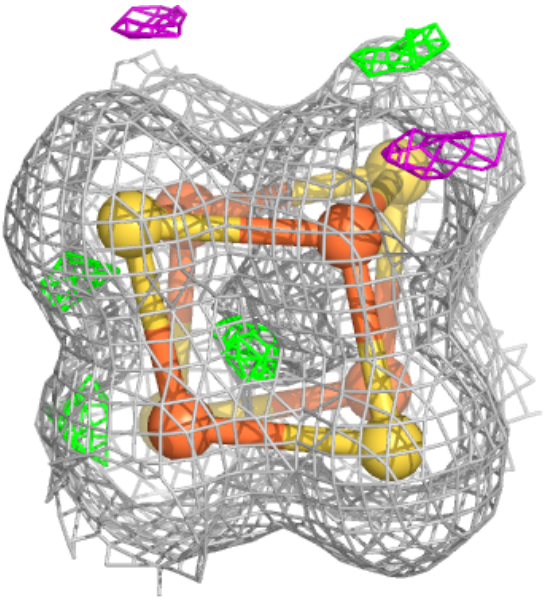


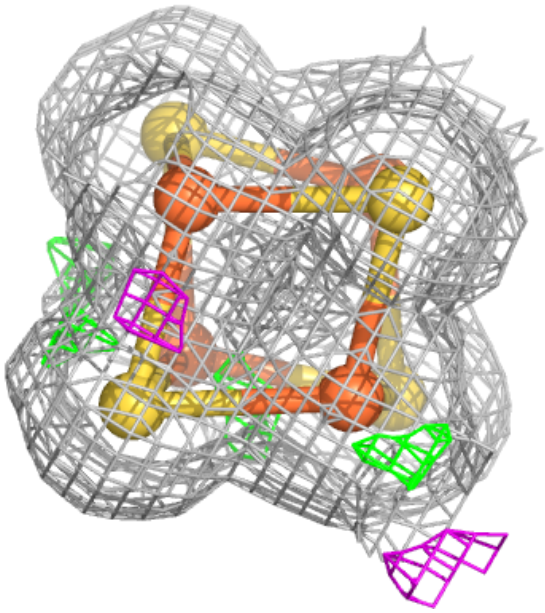


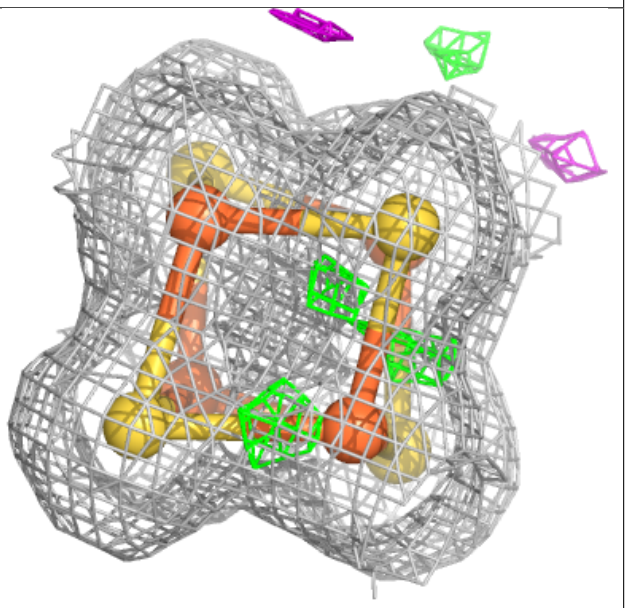


Electron density around SF4 D 1101:

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

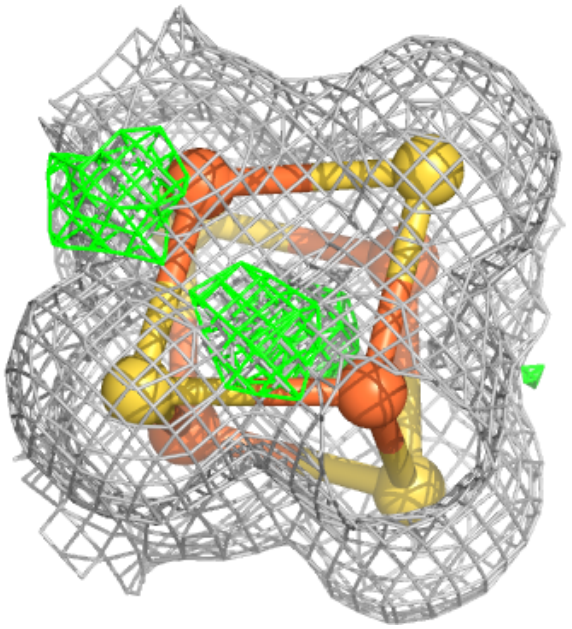


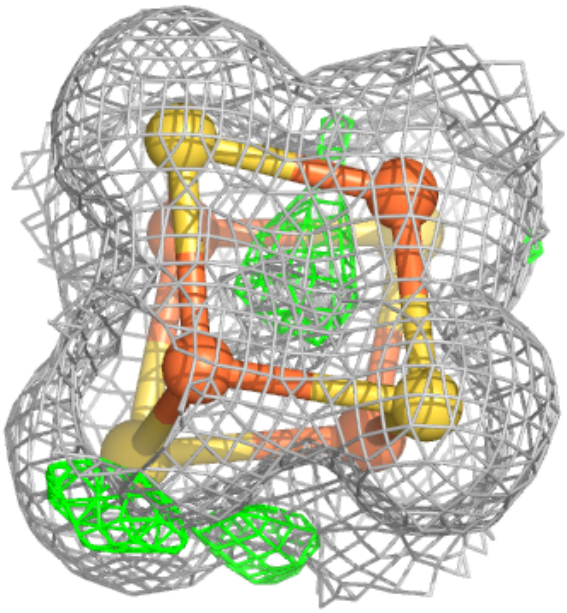


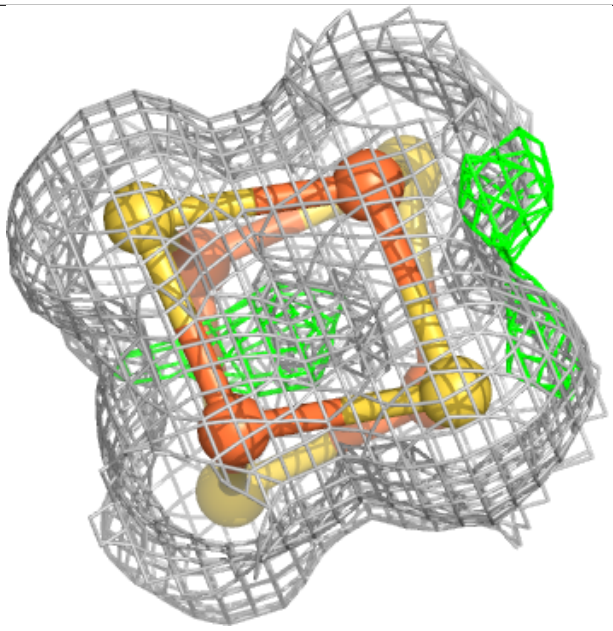


Electron density around SF4 D 1102:

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

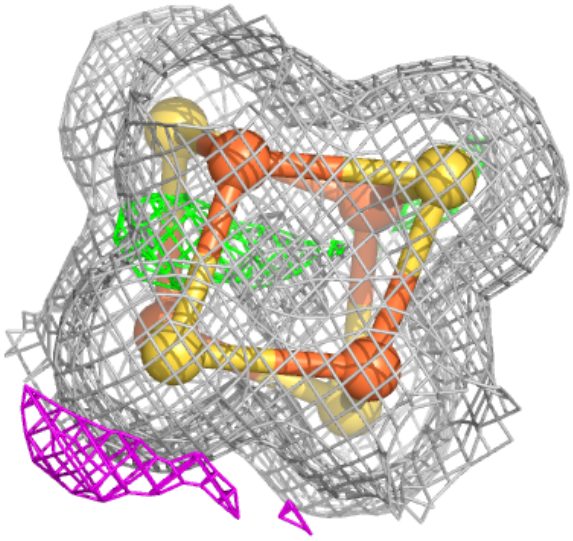


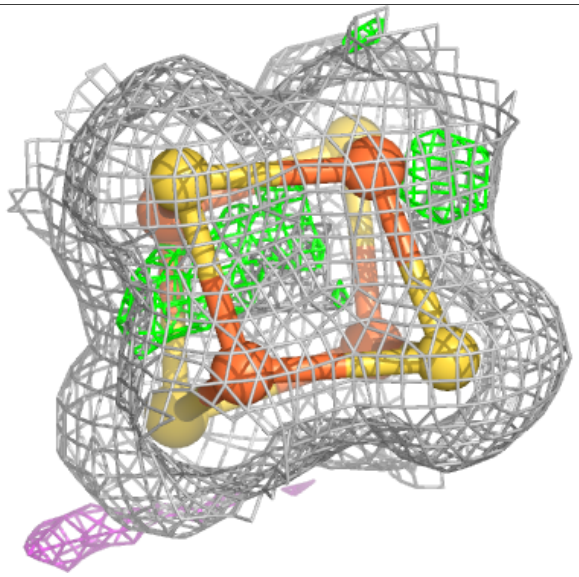


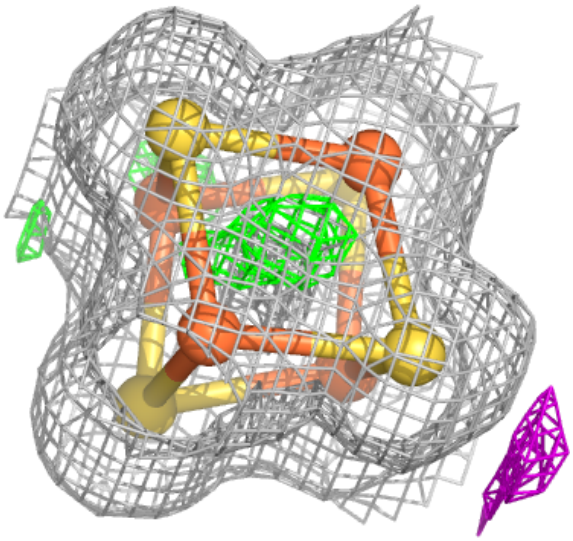


Electron density around SF4 A 1101:

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







6.5 Other polymers

There are no such residues in this entry.