wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 03:46 AM EDT

PDB ID	:	8F6N
Title	:	Dihydropyrimidine Dehydrogenase (DPD) C671S Mutant Soaked with Thymine Quasi-Anaerobically
Authors	:	Kaley, N.; Smith, M.; Forouzesh, D.; Liu, D.; Moran, G.
Deposited on	:	2022-11-16
Resolution	:	2.12 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:

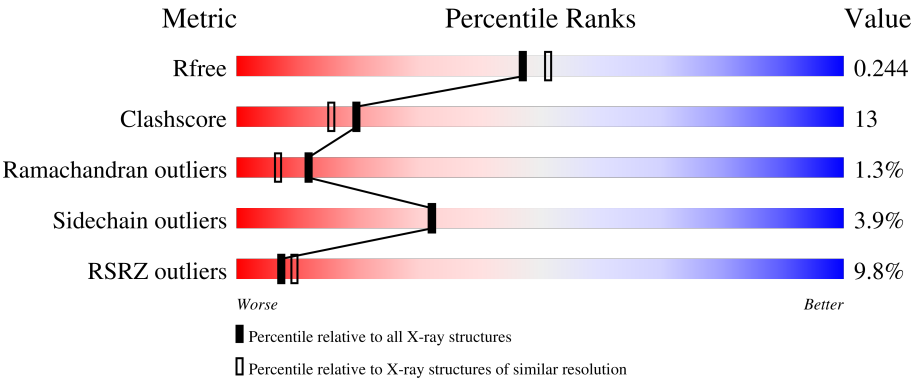
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	8% 61% 30% 6%
1	B	1025	10% 61% 30% 6%
1	C	1025	10% 63% 29% 6%
1	D	1025	10% 63% 29%

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
2	SF4	A	1103	-	-	X	-
2	SF4	C	1102	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 31607 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	996	Total	C	N	O	S	0	4	0
			7608	4829	1283	1443	53			
1	B	1001	Total	C	N	O	S	0	5	0
			7662	4860	1298	1450	54			
1	C	1002	Total	C	N	O	S	0	4	0
			7654	4856	1292	1453	53			
1	D	992	Total	C	N	O	S	0	5	0
			7590	4816	1282	1441	51			

There are 36 discrepancies between the modelled and reference sequences:

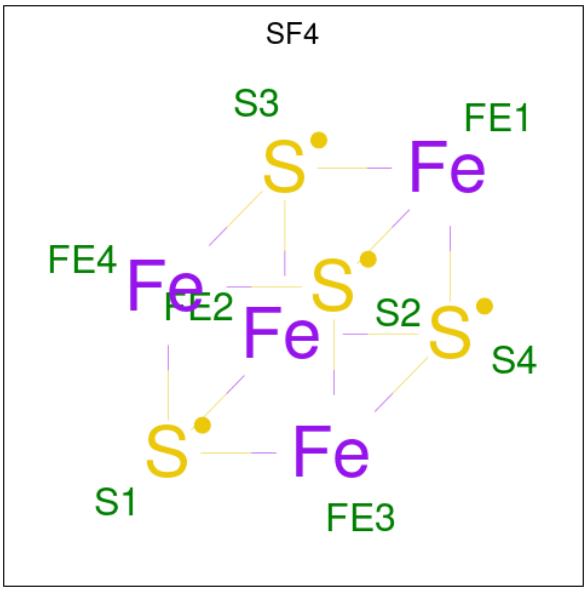
Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLY	conflict	UNP Q28943
A	671	SER	CYS	engineered mutation	UNP Q28943
A	1019	LEU	-	expression tag	UNP Q28943
A	1020	ALA	-	expression tag	UNP Q28943
A	1021	VAL	-	expression tag	UNP Q28943
A	1022	ASN	-	expression tag	UNP Q28943
A	1023	PRO	-	expression tag	UNP Q28943
A	1024	VAL	-	expression tag	UNP Q28943
A	1025	CYS	-	expression tag	UNP Q28943
B	60	ASP	GLY	conflict	UNP Q28943
B	671	SER	CYS	engineered mutation	UNP Q28943
B	1019	LEU	-	expression tag	UNP Q28943
B	1020	ALA	-	expression tag	UNP Q28943
B	1021	VAL	-	expression tag	UNP Q28943
B	1022	ASN	-	expression tag	UNP Q28943
B	1023	PRO	-	expression tag	UNP Q28943
B	1024	VAL	-	expression tag	UNP Q28943
B	1025	CYS	-	expression tag	UNP Q28943
C	60	ASP	GLY	conflict	UNP Q28943
C	671	SER	CYS	engineered mutation	UNP Q28943
C	1019	LEU	-	expression tag	UNP Q28943

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1020	ALA	-	expression tag	UNP Q28943
C	1021	VAL	-	expression tag	UNP Q28943
C	1022	ASN	-	expression tag	UNP Q28943
C	1023	PRO	-	expression tag	UNP Q28943
C	1024	VAL	-	expression tag	UNP Q28943
C	1025	CYS	-	expression tag	UNP Q28943
D	60	ASP	GLY	conflict	UNP Q28943
D	671	SER	CYS	engineered mutation	UNP Q28943
D	1019	LEU	-	expression tag	UNP Q28943
D	1020	ALA	-	expression tag	UNP Q28943
D	1021	VAL	-	expression tag	UNP Q28943
D	1022	ASN	-	expression tag	UNP Q28943
D	1023	PRO	-	expression tag	UNP Q28943
D	1024	VAL	-	expression tag	UNP Q28943
D	1025	CYS	-	expression tag	UNP Q28943

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



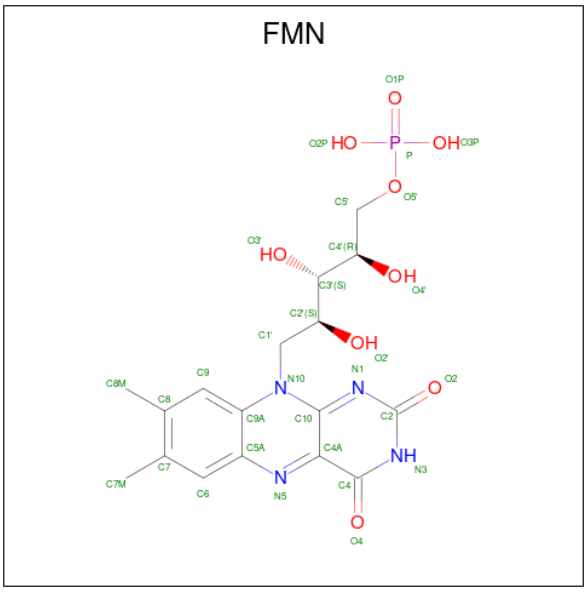
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0

Continued on next page...

Continued from previous page...

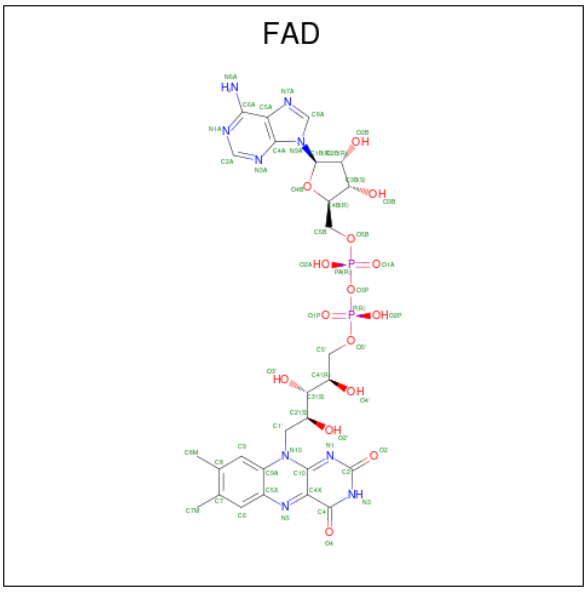
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe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

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



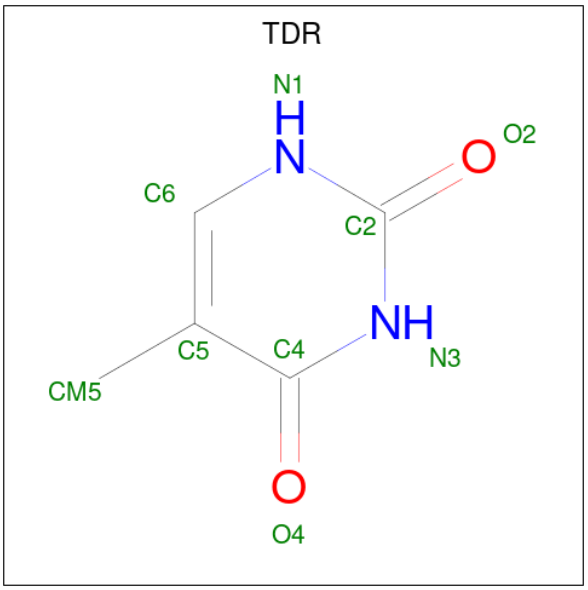
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 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
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 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
5	A	1	Total	C	N	O	0	0
			9	5	2	2		
5	B	1	Total	C	N	O	0	0
			9	5	2	2		
5	C	1	Total	C	N	O	0	0
			9	5	2	2		
5	D	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	149	Total	O	0	0
			149	149		

Continued on next page...

Continued from previous page...

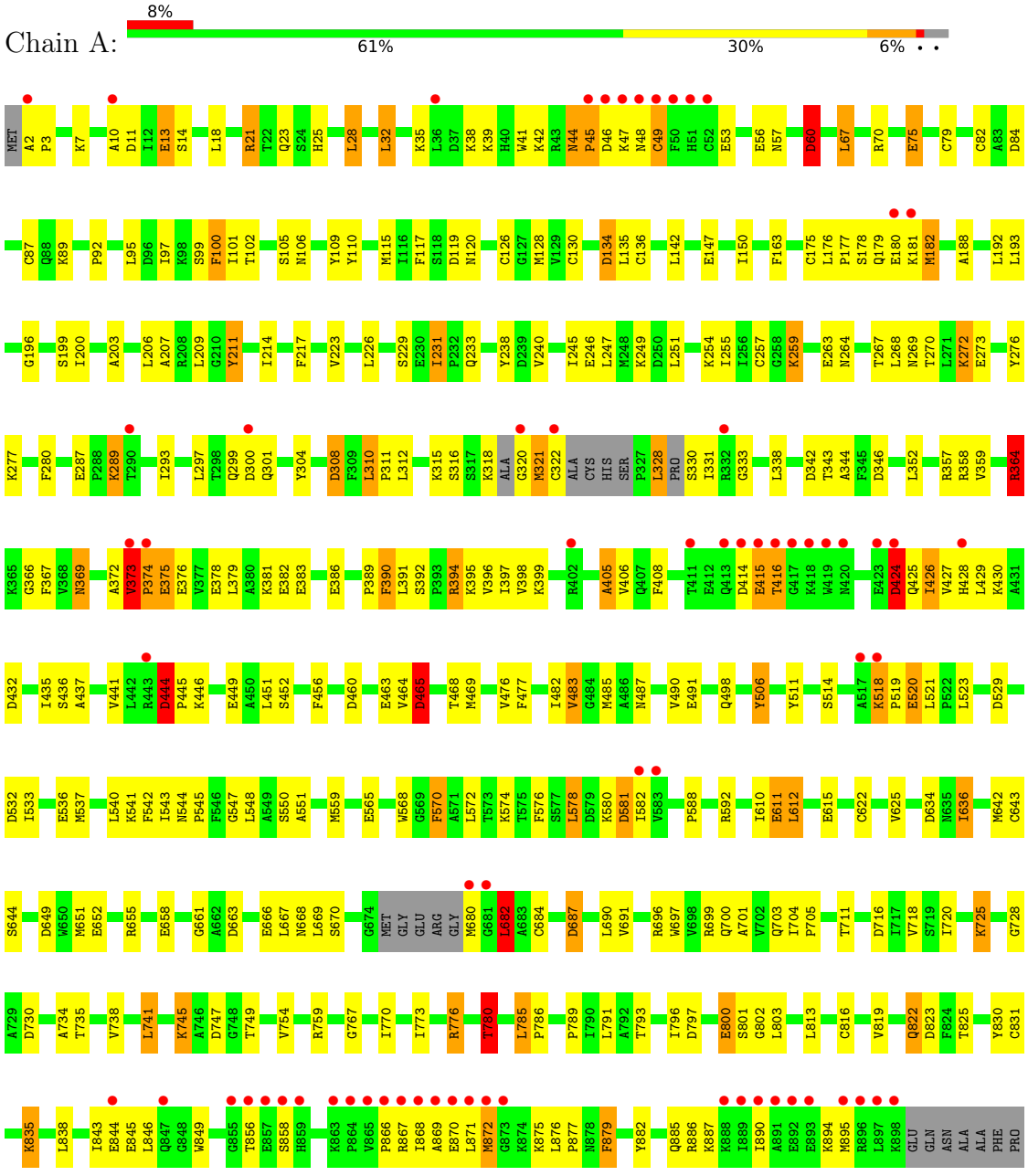
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	141	Total O 141 141	0	0
6	C	159	Total O 159 159	0	0
6	D	144	Total O 144 144	0	0

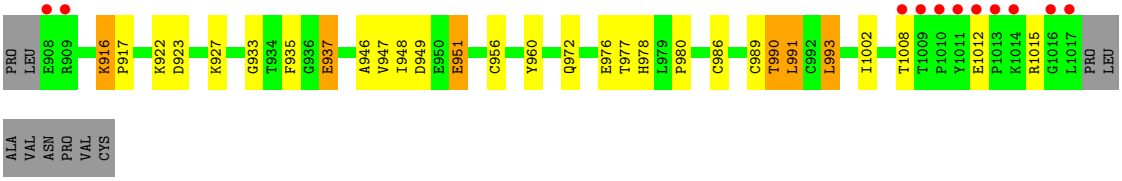
3 Residue-property plots (i)

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(+)]

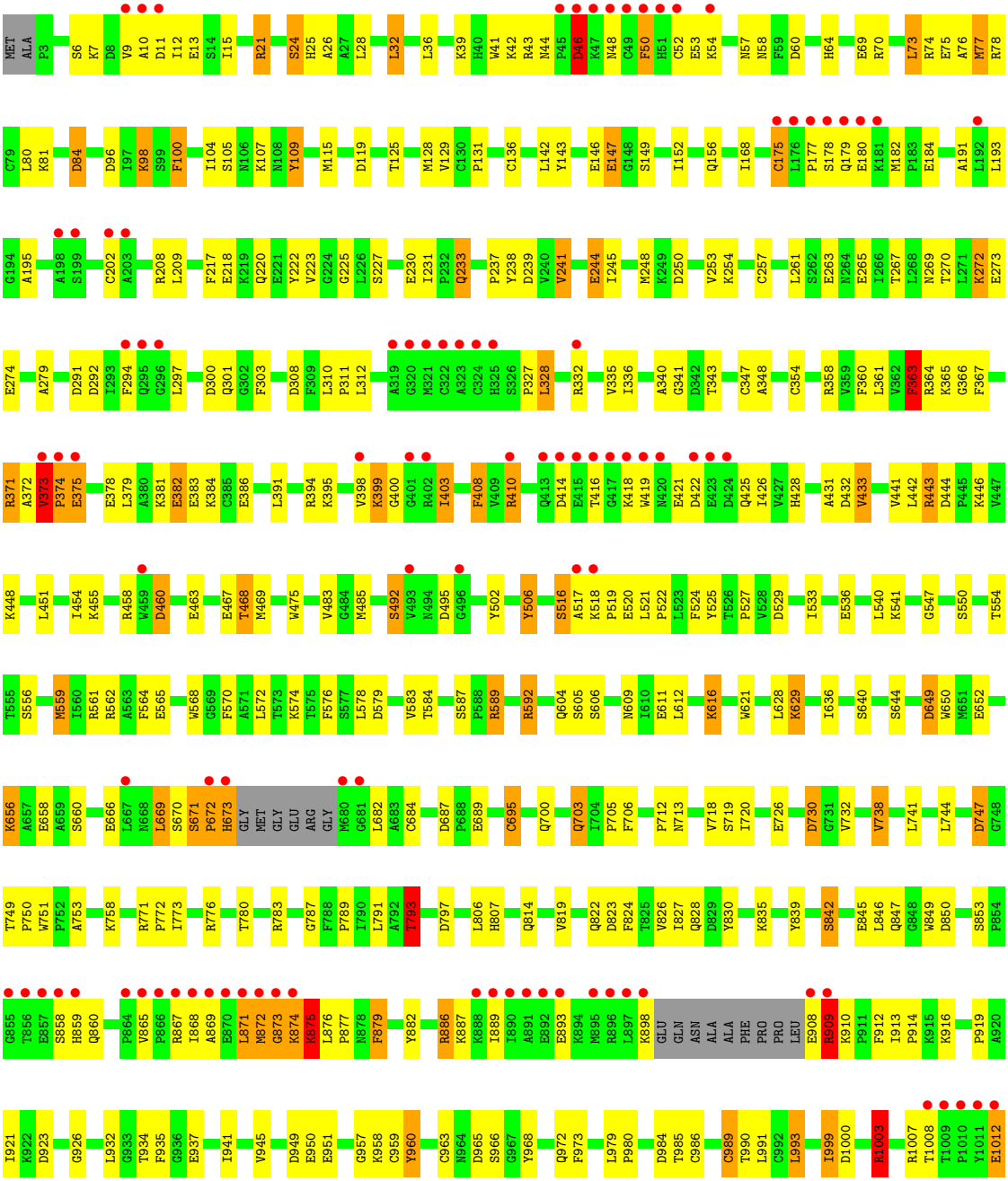
Chain A:

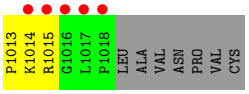




• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]

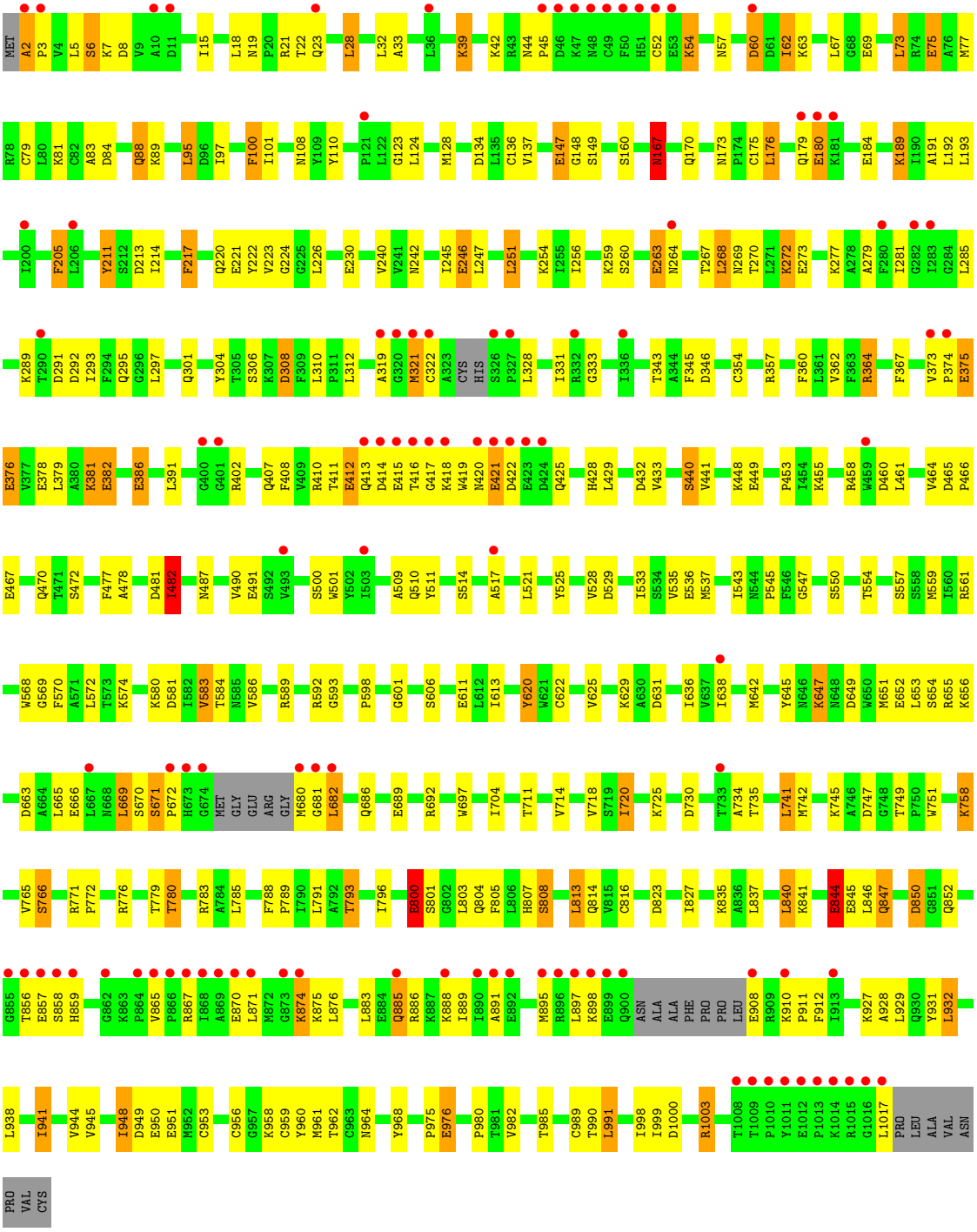
Chain B:





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

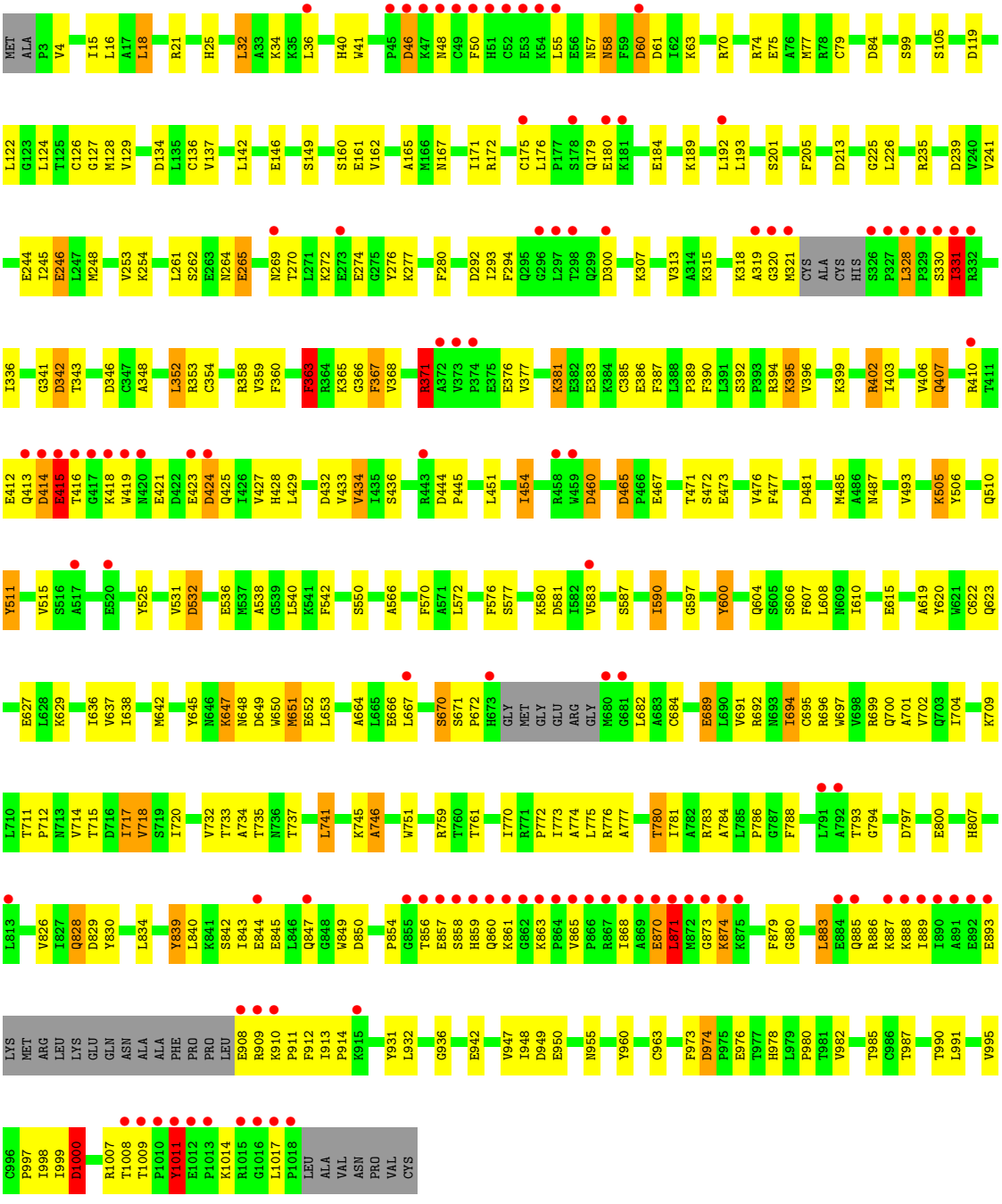
Chain C:



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

Chain D:


10%
63%
29%


MET ALA P3 V4 I15 L16 A17 L18 R21 H25 L32 A33 K34 K35 L36 H40 W41 P45 D46 K47 N48 C49 F50 H51 C52 E53 K54 L55 E56 N57 N58 F59 D60 D61 I62 K63 R70 R74 E75 A76 M77 R78 C79 D84 S99 S105 D119
L122 G123 L124 T125 C126 G127 M128 V129 D134 L135 C136 V137 L142 E146 S149 S160 E161 V162 A165 M166 N167 I171 R172 C175 L176 P177 S178 Q179 E180 K181 E184 K189 L192 L193 S201 F205 D213 G225 L226 R235 D239 V240 V241
E244 I245 E246 L247 M248 V253 K254 L261 S262 E263 N264 E265 N269 T270 L271 K272 E273 E274 G275 Y276 K277 F280 D292 I293 F294 Q295 G296 L297 T298 Q299 D300 K307 V313 A314 K315 K318 A319 G320 M321 CYS ALA CYS HIS S326 P327 L328 P329 S330 I331 R332
I336 G341 D342 T343 D346 C347 A348 L352 R353 C354 R358 V359 F360 F363 R364 K365 G366 F367 V368 R371 A372 V373 P374 E375 E376 V377 K381 E382 E383 K384 C385 E386 F387 L388 P389 F390 L391 S392 P393 R394 K395 V396 K399 R402 I403 V406 Q407 R410 T411
E412 Q413 D414 E415 T416 G417 K418 W419 N420 E421 D422 E423 D424 Q425 I426 V427 H428 L429 D432 V433 V434 I435 S436 R443 D444 P445 L451 I454 R458 W459 D460 D465 P466 E467 T471 S472 E473 V476 F477 D481 M485 A486 N487 V493 K505 Y506 Q510
Y511 V515 S516 A517 E520 Y525 V531 D532 E536 M537 A538 G539 L540 K541 F542 S550 A566 F570 A571 L572 F576 S577 K580 D581 I582 V583 S587 I590 G597 Y600 Q604 S605 S606 F607 L608 N609 I610 E615 A619 Y620 W621 C622 Q623
E627 L628 K629 I636 V637 I638 M642 Y645 N646 K647 N648 D649 W650 M651 E652 L653 A664 L665 E666 L667 S670 S671 P672 H673 GLY MET GLY GLU ARG GLY M680 G681 L682 A683 C684 E689 L690 V691 R692 N693 I694 C695 R696 W697 V698 R699 Q700 A701 V702 Q703 I704 K709
L710 T711 P712 N713 V714 T715 D716 I717 V718 S719 I720 V732 T733 A734 T735 N736 T737 L741 K745 A746 W751 R759 T760 T761 I770 R771 P772 I773 A774 L775 R776 A777 T780 I781 A782 R783 A784 L785 P786 G787 F788 L791 A792 T793 G794 D797 E800 H807
L813 V826 I827 Q828 D829 Y830 L834 Y839 L840 K841 S842 I843 E844 E845 L846 Q847 G848 W849 D850 P854 G855 T856 E857 S858 H859 Q860 K861 G862 K863 P864 V865 P866 R867 I868 A869 E870 L871 M872 G873 K874 K875 F879 G880 L883 E884 Q885 R886 K887 K888 I889 E890 A891 E892 E893
LYS MET ARG LEU LYS GLU GLN ASN ALA ALA PHE PRO PRO LEU E908 R909 K910 P911 F912 I913 P914 K915 Y931 L932 G936 E942 V947 I948 D949 E950 N955 Y960 C963 E973 D974 P975 E976 T977 H978 L979 P980 T981 V982 T985 C986 T987 T990 L991 V995
C996 P997 I998 I999 D1000 R1007 T1008 T1009 P1010 Y1011 E1012 P1013 K1014 R1015 G1016 L1017 P1018 LEU ALA VAL ASN PRO VAL CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.44Å 158.14Å 165.71Å 90.00° 96.78° 90.00°	Depositor
Resolution (Å)	26.98 – 2.12 26.98 – 2.12	Depositor EDS
% Data completeness (in resolution range)	61.4 (26.98-2.12) 61.4 (26.98-2.12)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.182 , 0.244 0.182 , 0.244	Depositor DCC
R_{free} test set	7333 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 61.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	31607	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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, TDR, 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	1.53	105/7773 (1.4%)	1.40	91/10525 (0.9%)
1	B	1.54	109/7839 (1.4%)	1.36	72/10620 (0.7%)
1	C	1.50	93/7823 (1.2%)	1.39	80/10598 (0.8%)
1	D	1.44	82/7765 (1.1%)	1.36	63/10522 (0.6%)
All	All	1.50	389/31200 (1.2%)	1.38	306/42265 (0.7%)

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	8
1	B	0	12
1	C	0	4
1	D	0	7
All	All	0	31

The worst 5 of 389 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	671	SER	C-N	-19.68	0.96	1.34
1	B	175	CYS	CB-SG	14.29	2.06	1.82
1	A	652	GLU	CG-CD	14.04	1.73	1.51
1	B	670	SER	C-N	-13.25	1.03	1.34
1	B	695	CYS	CB-SG	12.80	2.04	1.82

The worst 5 of 306 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	670	SER	O-C-N	-18.09	93.76	122.70
1	D	32	LEU	CB-CG-CD1	-14.83	85.79	111.00
1	C	670	SER	CA-C-N	12.78	145.31	117.20
1	A	444	ASP	CB-CG-OD2	-11.51	107.94	118.30
1	D	15	ILE	CG1-CB-CG2	-11.37	86.39	111.40

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ARG	Sidechain
1	A	364	ARG	Sidechain
1	A	415	GLU	Peptide
1	A	44	ASN	Peptide
1	A	70	ARG	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	7608	0	7645	212	0
1	B	7662	0	7694	218	0
1	C	7654	0	7686	219	0
1	D	7590	0	7612	190	0
2	A	32	0	0	3	0
2	B	32	0	0	2	0
2	C	32	0	0	3	0
2	D	32	0	0	1	0
3	A	31	0	19	1	0
3	B	31	0	19	1	0
3	C	31	0	19	1	0
3	D	31	0	19	1	0
4	A	53	0	31	2	0
4	B	53	0	31	3	0
4	C	53	0	31	1	0
4	D	53	0	31	2	0
5	A	9	0	6	1	0
5	B	9	0	6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	9	0	6	0	0
5	D	9	0	6	0	0
6	A	149	0	0	23	0
6	B	141	0	0	22	0
6	C	159	0	0	18	0
6	D	144	0	0	8	0
All	All	31607	0	30861	788	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 13.

The worst 5 of 788 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:A:259:LYS:NZ	1:A:259:LYS:CE	1.70	1.53
1:B:695:CYS:CB	1:B:695:CYS:SG	2.04	1.46
1:B:175:CYS:SG	1:B:175:CYS:CB	2.06	1.42
1:B:414:ASP:HB3	1:B:416:THR:HG22	1.32	1.09
1:B:115:MET:SD	6:B:1334:HOH:O	2.08	1.08

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	988/1025 (96%)	895 (91%)	80 (8%)	13 (1%)	12 7
1	B	1000/1025 (98%)	904 (90%)	83 (8%)	13 (1%)	12 7
1	C	998/1025 (97%)	913 (92%)	70 (7%)	15 (2%)	10 5
1	D	989/1025 (96%)	892 (90%)	85 (9%)	12 (1%)	13 8
All	All	3975/4100 (97%)	3604 (91%)	318 (8%)	53 (1%)	12 7

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	PRO
1	A	415	GLU
1	B	875	LYS
1	C	52	CYS
1	C	176	LEU

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	834/854 (98%)	801 (96%)	33 (4%)	31	31
1	B	842/854 (99%)	815 (97%)	27 (3%)	39	40
1	C	839/854 (98%)	807 (96%)	32 (4%)	33	33
1	D	834/854 (98%)	792 (95%)	42 (5%)	24	22
All	All	3349/3416 (98%)	3215 (96%)	134 (4%)	32	31

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	415	GLU
1	D	460	ASP
1	D	932[B]	LEU
1	B	703	GLN
1	B	673	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	413	GLN
1	D	407	GLN
1	C	508	GLN
1	D	220	GLN
1	C	413	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

28 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	$\#\|Z\| > 2$
5	TDR	B	1107	-	9,9,9	1.49	2 (22%)	12,12,12	1.43	1 (8%)
2	SF4	A	1103	1	0,12,12	-	-	-		
2	SF4	C	1103	1	0,12,12	-	-	-		
2	SF4	A	1104	1	0,12,12	-	-	-		
4	FAD	A	1106	-	53,58,58	0.96	3 (5%)	68,89,89	1.22	9 (13%)
2	SF4	A	1102	1	0,12,12	-	-	-		
3	FMN	D	1105	-	33,33,33	1.97	11 (33%)	48,50,50	2.26	17 (35%)
5	TDR	D	1107	-	9,9,9	2.57	5 (55%)	12,12,12	1.70	2 (16%)
2	SF4	C	1102	1	0,12,12	-	-	-		
5	TDR	A	1107	-	9,9,9	1.01	1 (11%)	12,12,12	1.58	2 (16%)
2	SF4	B	1103	1	0,12,12	-	-	-		
5	TDR	C	1107	-	9,9,9	1.37	1 (11%)	12,12,12	2.61	4 (33%)
3	FMN	C	1105	-	33,33,33	1.75	6 (18%)	48,50,50	2.27	18 (37%)
2	SF4	B	1104	1	0,12,12	-	-	-		
2	SF4	D	1102	1	0,12,12	-	-	-		
2	SF4	D	1104	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FAD	D	1106	-	53,58,58	0.98	4 (7%)	68,89,89	0.95	5 (7%)
3	FMN	B	1105	-	33,33,33	1.46	6 (18%)	48,50,50	2.38	20 (41%)
2	SF4	C	1101	1	0,12,12	-	-	-		
2	SF4	B	1101	1	0,12,12	-	-	-		
2	SF4	C	1104	1	0,12,12	-	-	-		
4	FAD	C	1106	-	53,58,58	1.15	2 (3%)	68,89,89	0.80	1 (1%)
3	FMN	A	1105	-	33,33,33	1.87	7 (21%)	48,50,50	2.39	17 (35%)
2	SF4	A	1101	1	0,12,12	-	-	-		
2	SF4	B	1102	1	0,12,12	-	-	-		
4	FAD	B	1106	-	53,58,58	1.14	3 (5%)	68,89,89	1.35	7 (10%)
2	SF4	D	1101	1	0,12,12	-	-	-		
2	SF4	D	1103	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
5	TDR	B	1107	-	-	-	0/1/1/1
2	SF4	A	1103	1	-	-	0/6/5/5
2	SF4	C	1103	1	-	-	0/6/5/5
2	SF4	A	1104	1	-	-	0/6/5/5
4	FAD	A	1106	-	-	3/30/50/50	0/6/6/6
2	SF4	A	1102	1	-	-	0/6/5/5
3	FMN	D	1105	-	-	4/18/18/18	0/3/3/3
5	TDR	D	1107	-	-	-	0/1/1/1
2	SF4	C	1102	1	-	-	0/6/5/5
5	TDR	A	1107	-	-	-	0/1/1/1
2	SF4	B	1103	1	-	-	0/6/5/5
5	TDR	C	1107	-	-	-	0/1/1/1
3	FMN	C	1105	-	-	2/18/18/18	0/3/3/3
2	SF4	B	1104	1	-	-	0/6/5/5
2	SF4	D	1102	1	-	-	0/6/5/5
2	SF4	D	1104	1	-	-	0/6/5/5
4	FAD	D	1106	-	-	1/30/50/50	0/6/6/6
3	FMN	B	1105	-	-	2/18/18/18	0/3/3/3
2	SF4	C	1101	1	-	-	0/6/5/5
2	SF4	B	1101	1	-	-	0/6/5/5
2	SF4	C	1104	1	-	-	0/6/5/5
4	FAD	C	1106	-	-	1/30/50/50	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	A	1105	-	-	1/18/18/18	0/3/3/3
2	SF4	A	1101	1	-	-	0/6/5/5
2	SF4	B	1102	1	-	-	0/6/5/5
4	FAD	B	1106	-	-	1/30/50/50	0/6/6/6
2	SF4	D	1101	1	-	-	0/6/5/5
2	SF4	D	1103	1	-	-	0/6/5/5

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1105	FMN	C4A-N5	5.99	1.42	1.30
4	C	1106	FAD	C10-N1	-5.77	1.21	1.33
3	C	1105	FMN	C4A-N5	5.25	1.41	1.30
5	D	1107	TDR	C2-N1	4.61	1.43	1.36
3	D	1105	FMN	C5'-C4'	4.21	1.57	1.51

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1107	TDR	CM5-C5-C4	-6.48	111.63	118.77
3	C	1105	FMN	C4A-C10-N10	5.72	124.85	116.48
3	D	1105	FMN	C4A-C10-N10	5.57	124.62	116.48
3	A	1105	FMN	C10-N1-C2	5.33	127.56	116.90
3	D	1105	FMN	C4-C4A-C10	5.23	125.58	116.79

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1105	FMN	C5'-O5'-P-O3P
3	C	1105	FMN	C2'-C3'-C4'-O4'
4	A	1106	FAD	P-O3P-PA-O5B
4	A	1106	FAD	C5B-O5B-PA-O3P
4	C	1106	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

15 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1103	SF4	2	0
4	A	1106	FAD	2	0

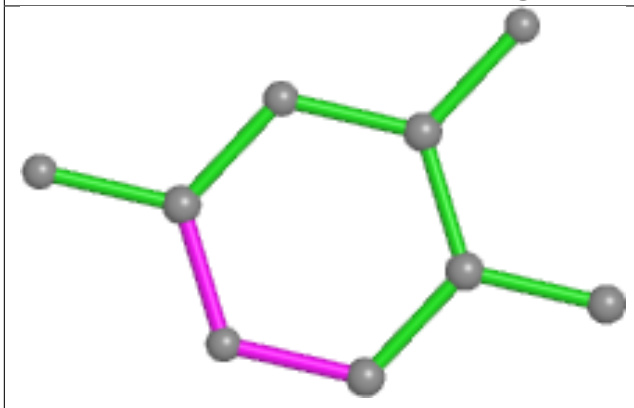
Continued on next page...

Continued from previous page...

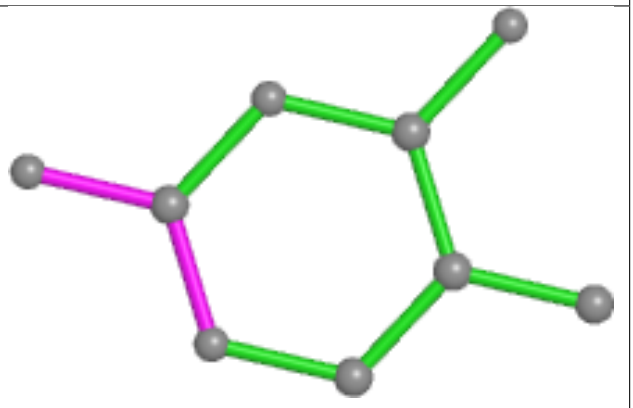
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1102	SF4	1	0
3	D	1105	FMN	1	0
2	C	1102	SF4	3	0
5	A	1107	TDR	1	0
2	B	1103	SF4	1	0
3	C	1105	FMN	1	0
4	D	1106	FAD	2	0
3	B	1105	FMN	1	0
2	B	1101	SF4	1	0
4	C	1106	FAD	1	0
3	A	1105	FMN	1	0
4	B	1106	FAD	3	0
2	D	1101	SF4	1	0

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.

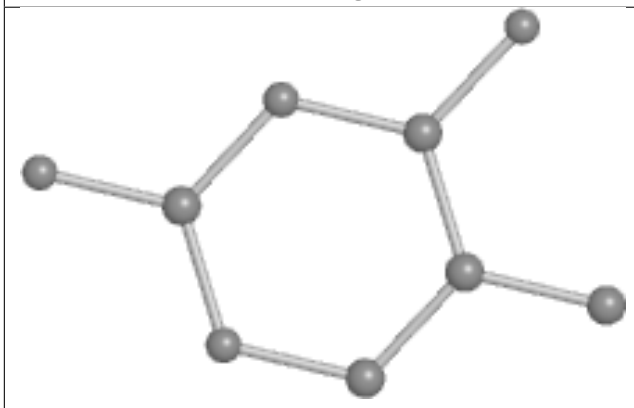
Ligand TDR B 1107



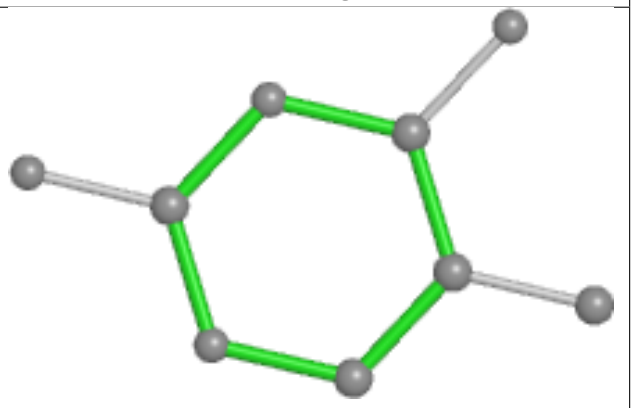
Bond lengths



Bond angles

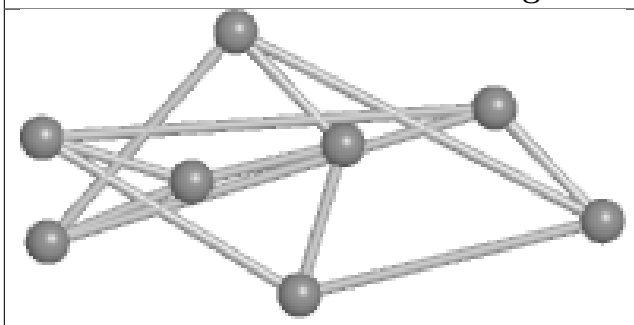


Torsions

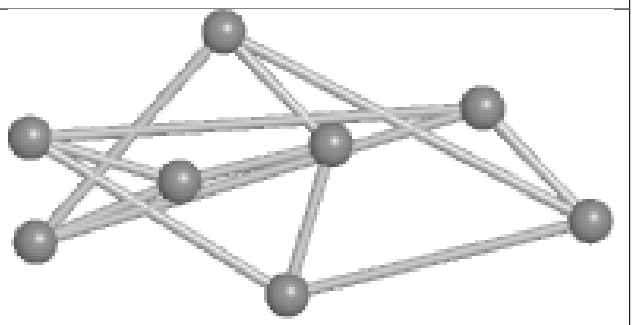


Rings

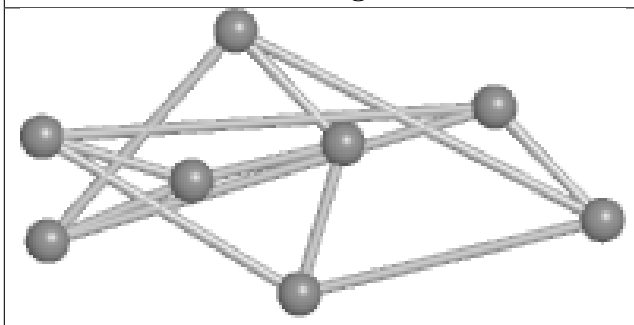
Ligand SF4 A 1103



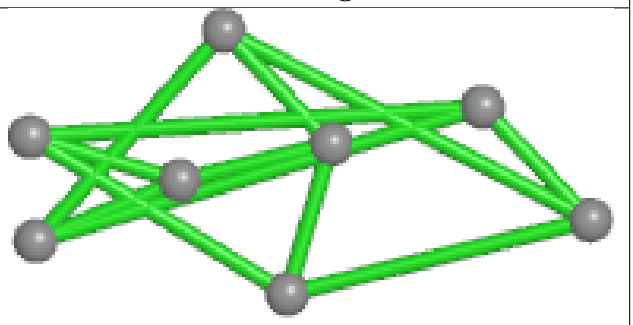
Bond lengths



Bond angles

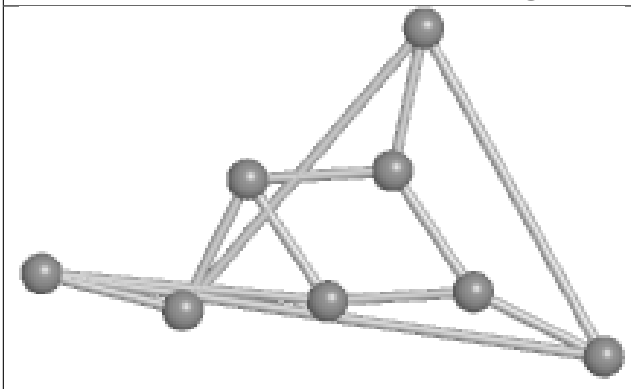


Torsions

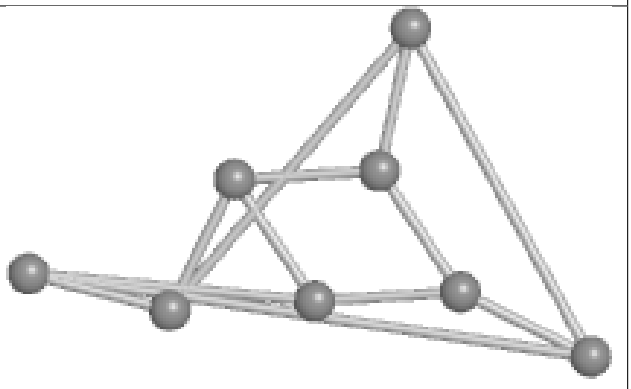


Rings

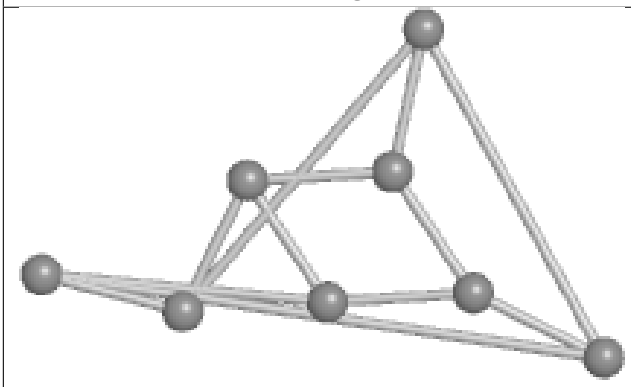
Ligand SF4 C 1103



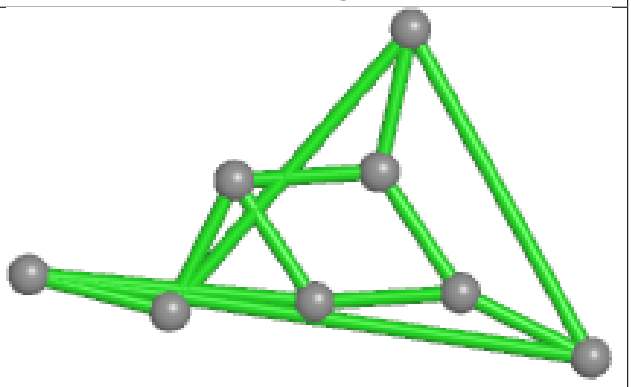
Bond lengths



Bond angles

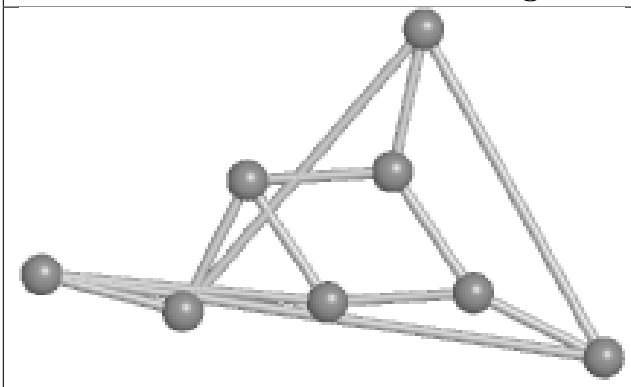


Torsions

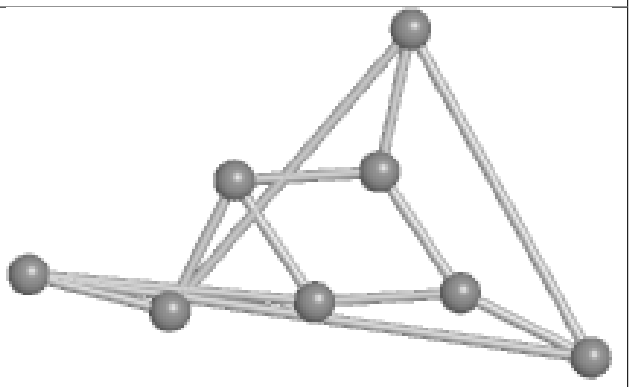


Rings

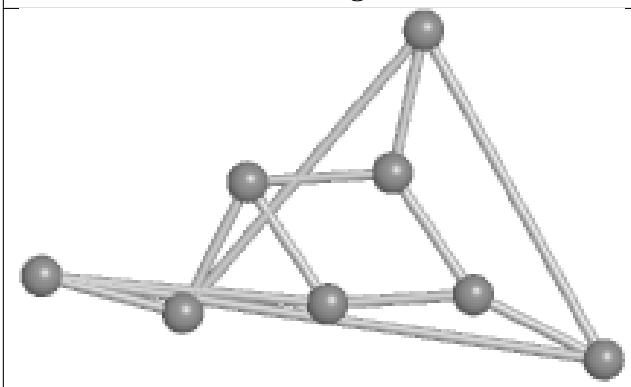
Ligand SF4 A 1104



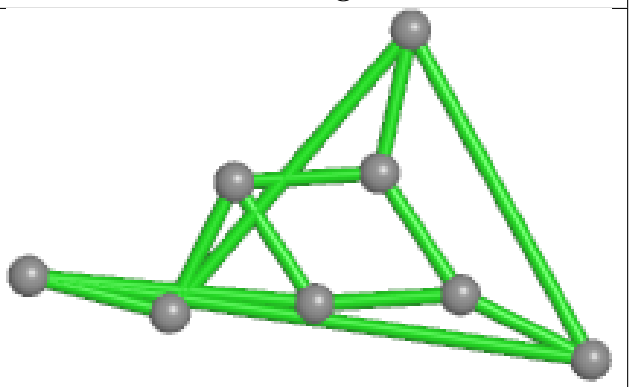
Bond lengths



Bond angles

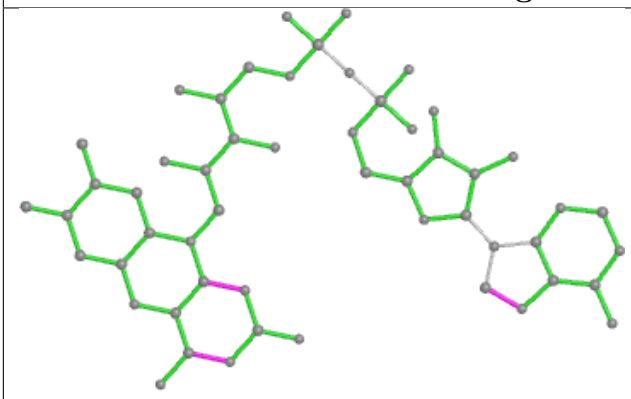


Torsions

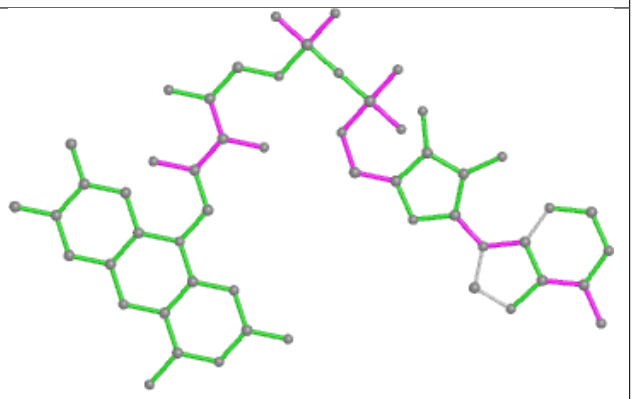


Rings

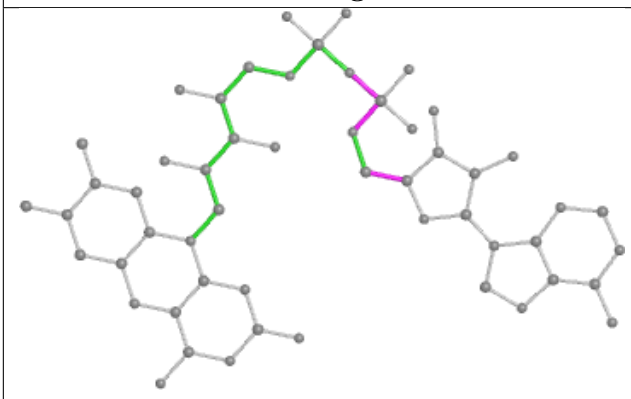
Ligand FAD A 1106



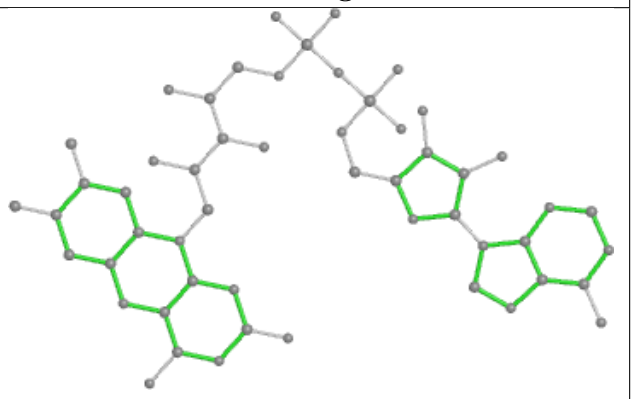
Bond lengths



Bond angles

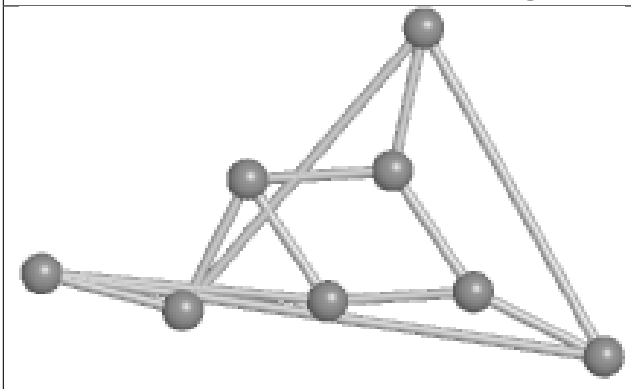


Torsions

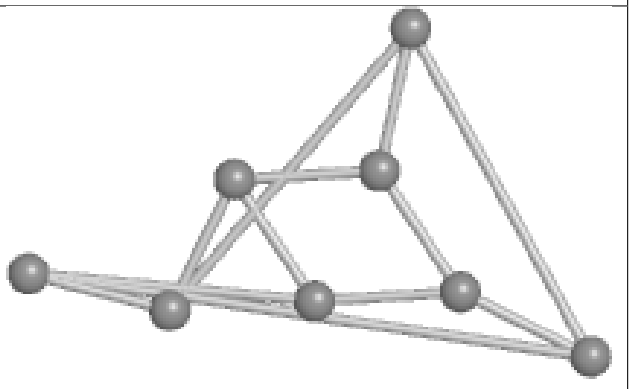


Rings

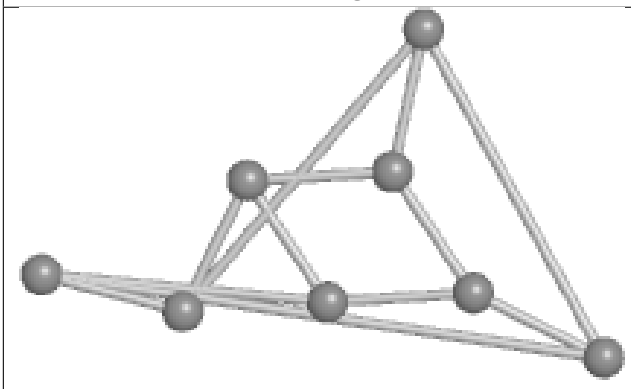
Ligand SF4 A 1102



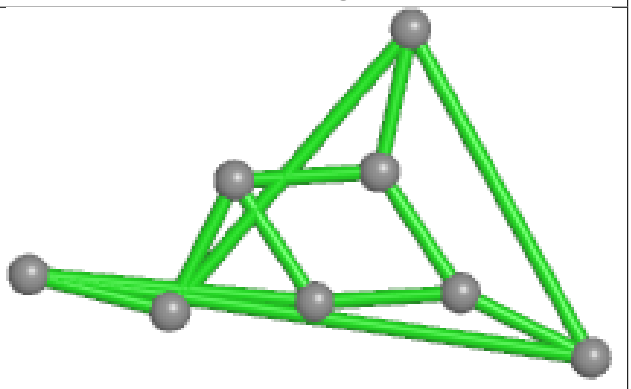
Bond lengths



Bond angles

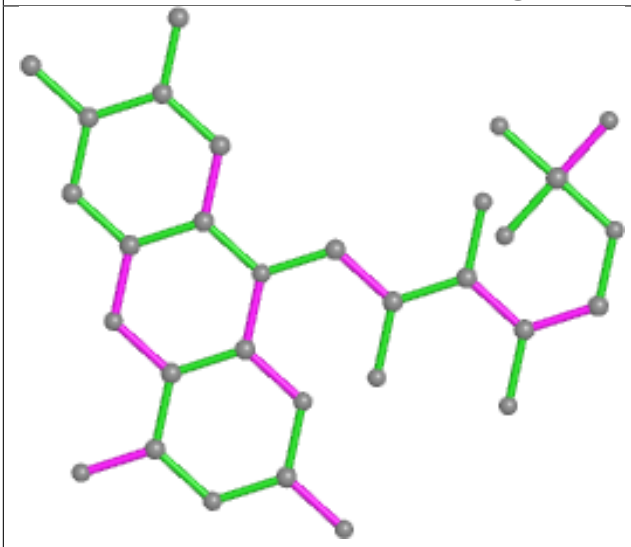


Torsions

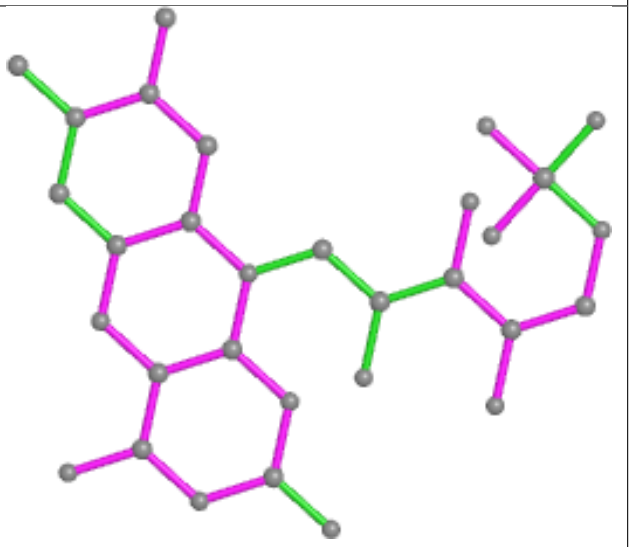


Rings

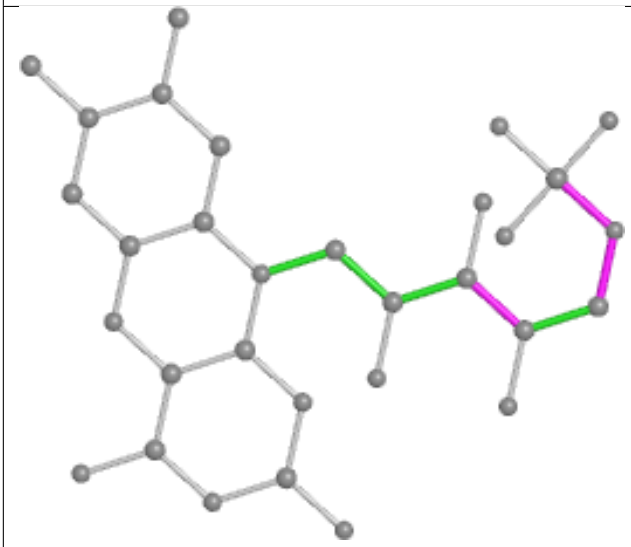
Ligand FMN D 1105



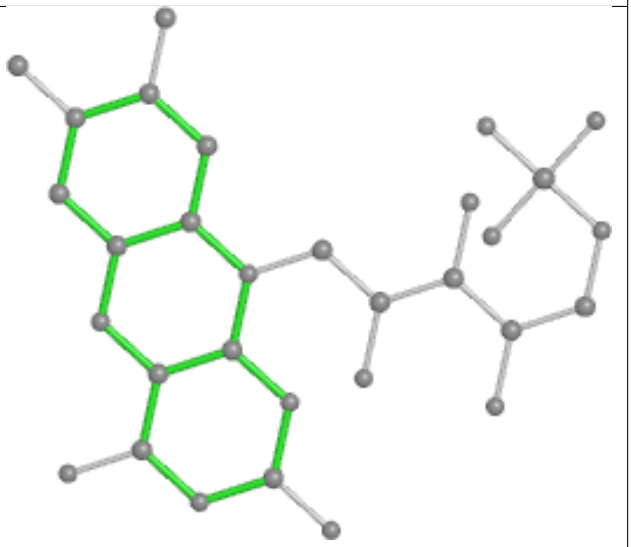
Bond lengths



Bond angles

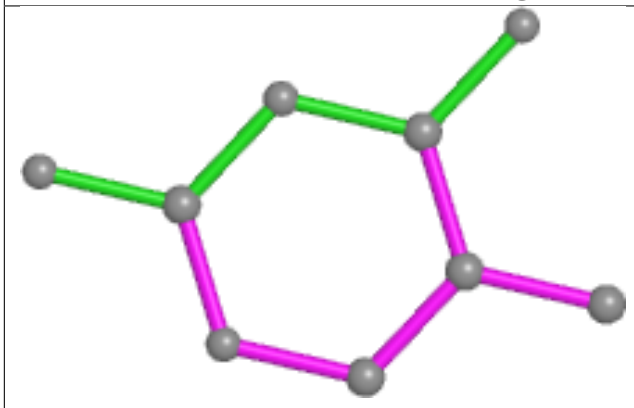


Torsions

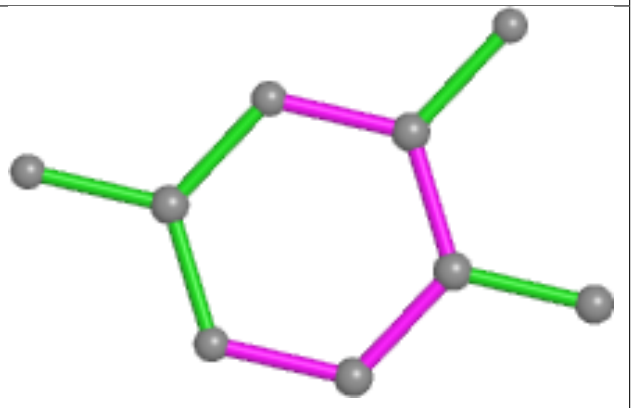


Rings

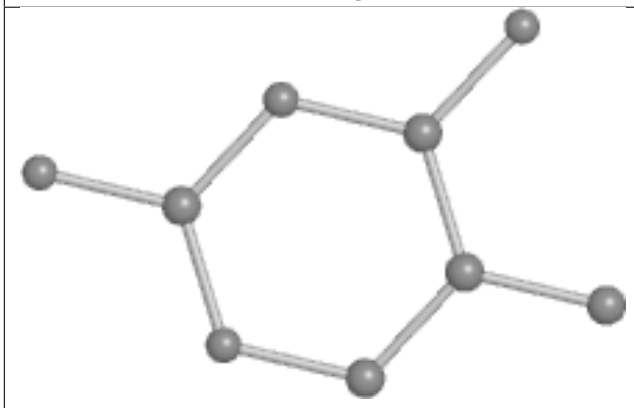
Ligand TDR D 1107



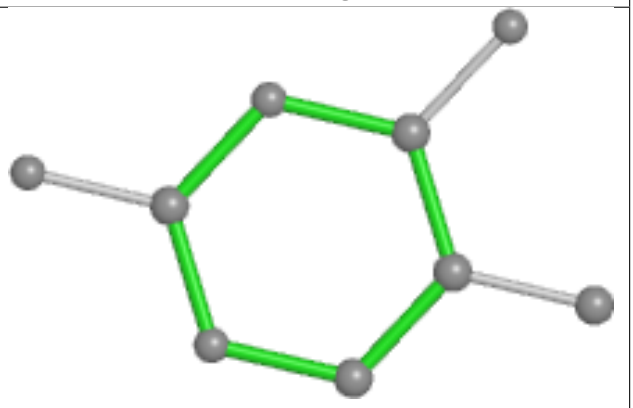
Bond lengths



Bond angles

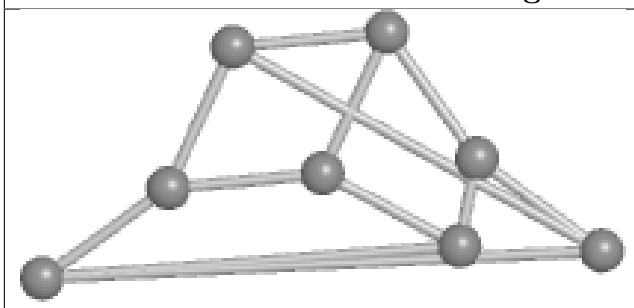


Torsions

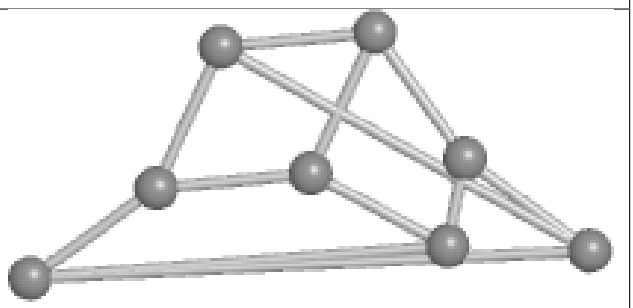


Rings

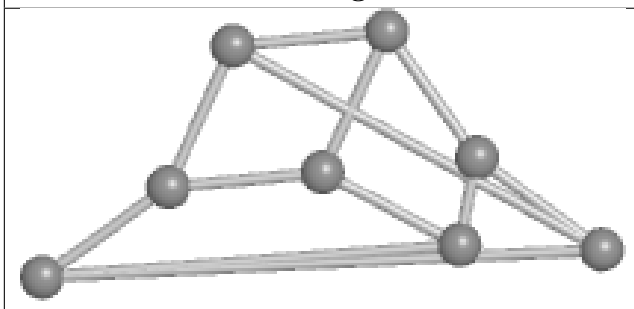
Ligand SF4 C 1102



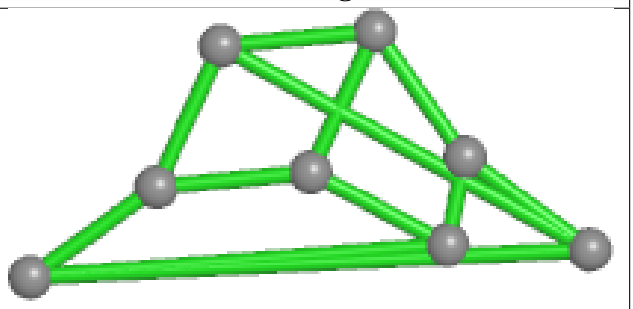
Bond lengths



Bond angles

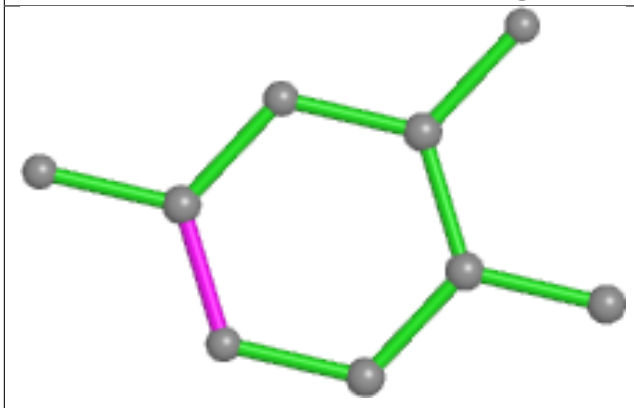


Torsions

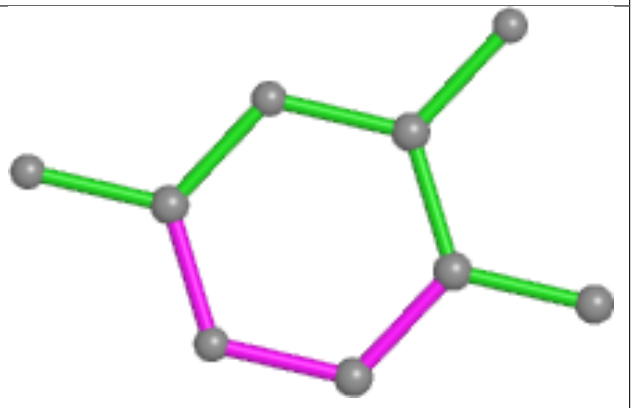


Rings

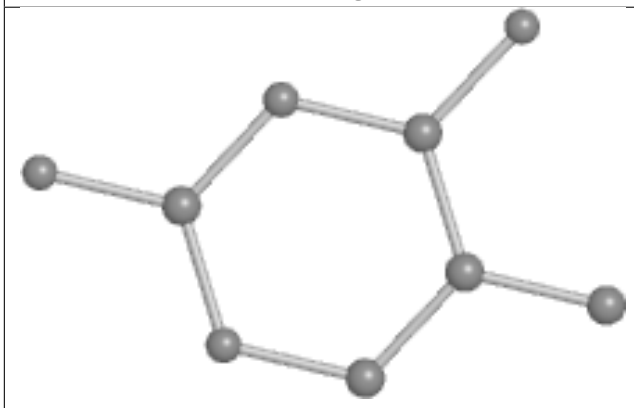
Ligand TDR A 1107



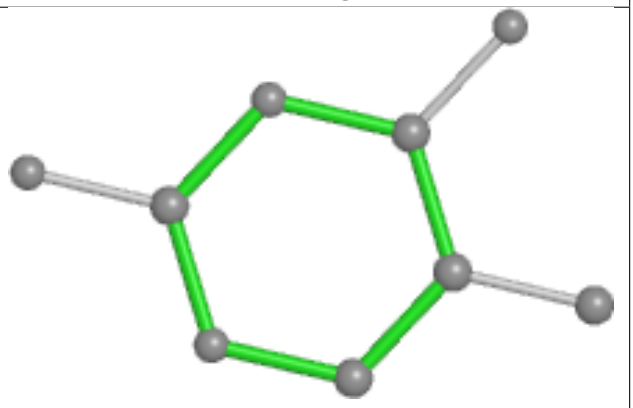
Bond lengths



Bond angles

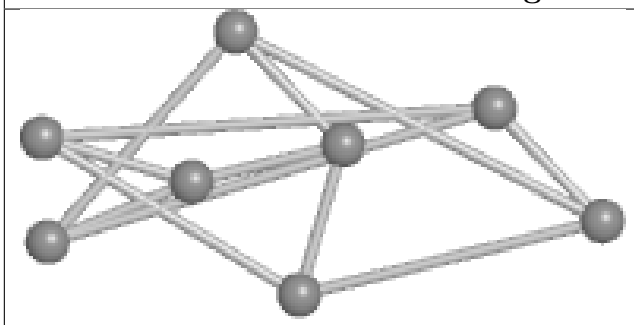


Torsions

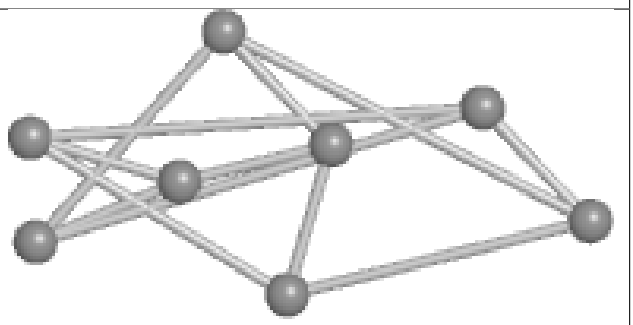


Rings

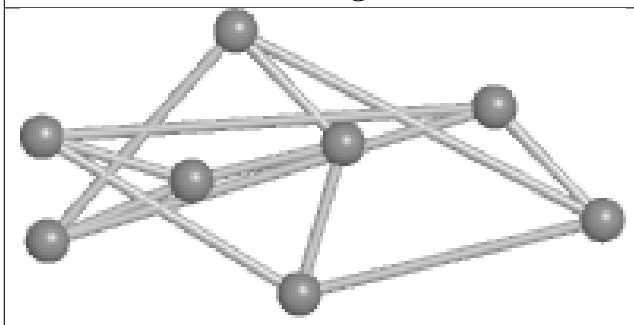
Ligand SF4 B 1103



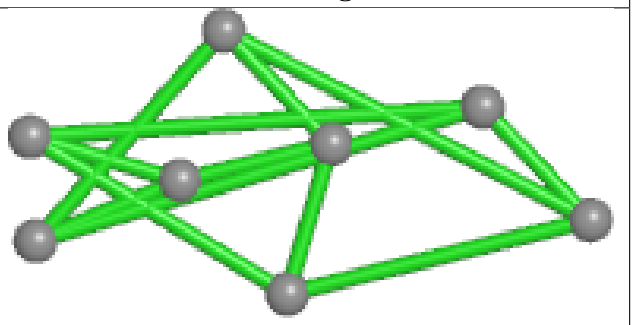
Bond lengths



Bond angles

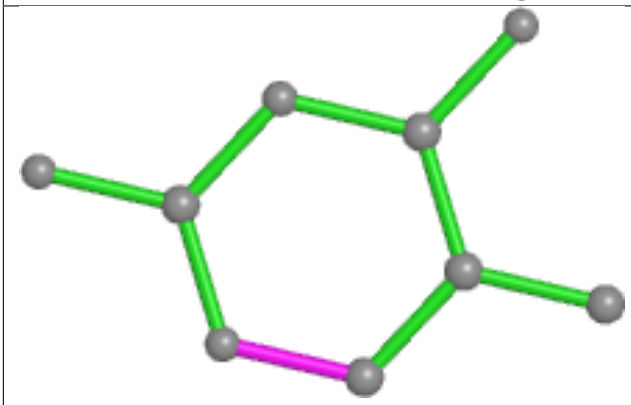


Torsions

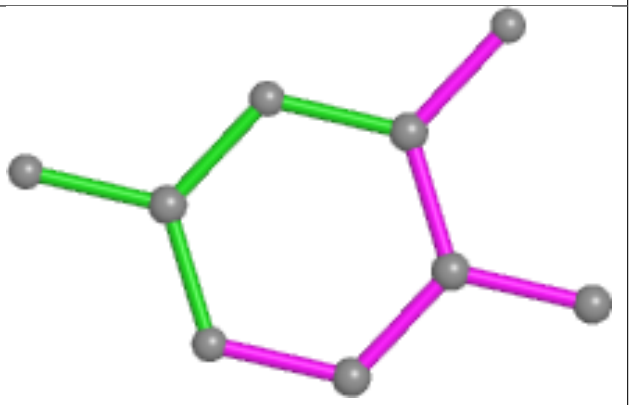


Rings

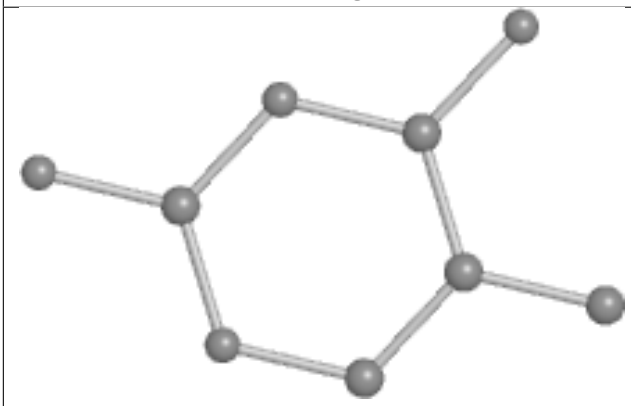
Ligand TDR C 1107



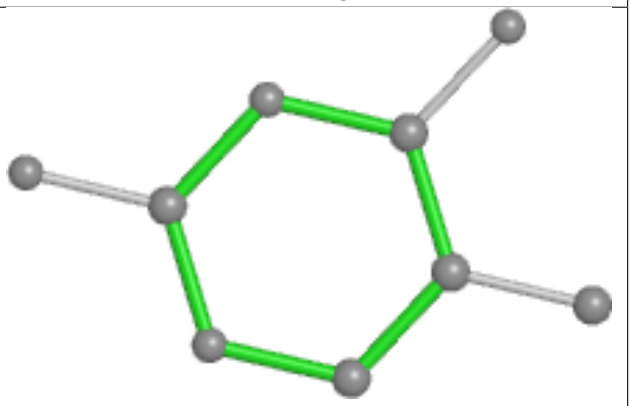
Bond lengths



Bond angles

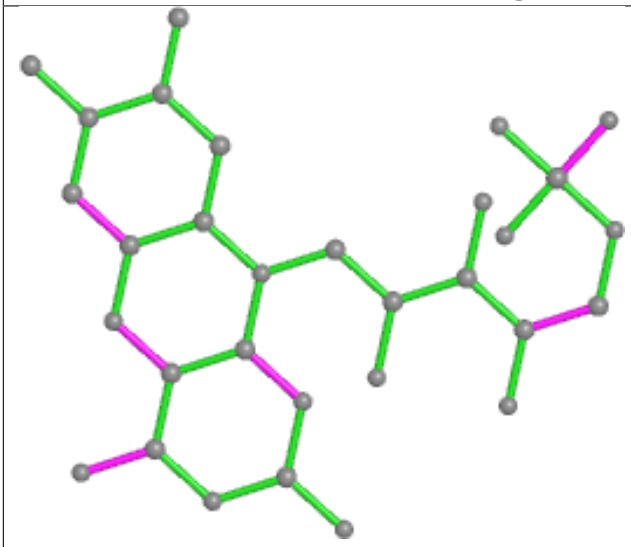


Torsions

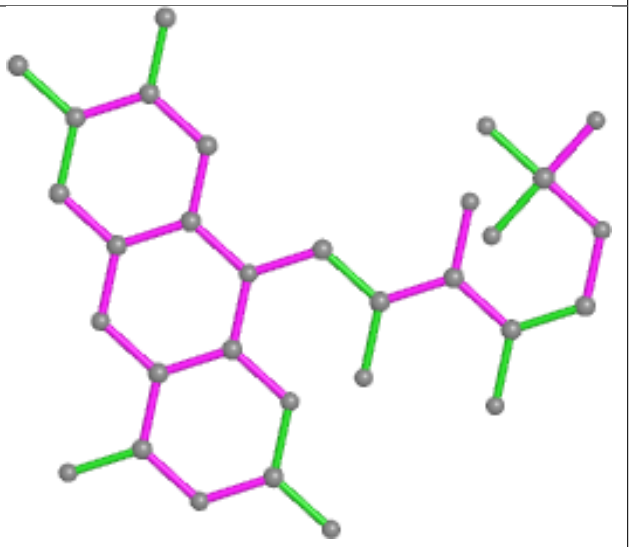


Rings

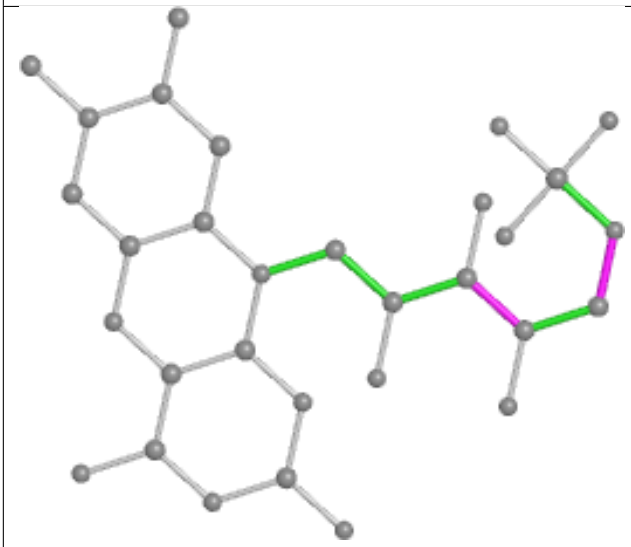
Ligand FMN C 1105



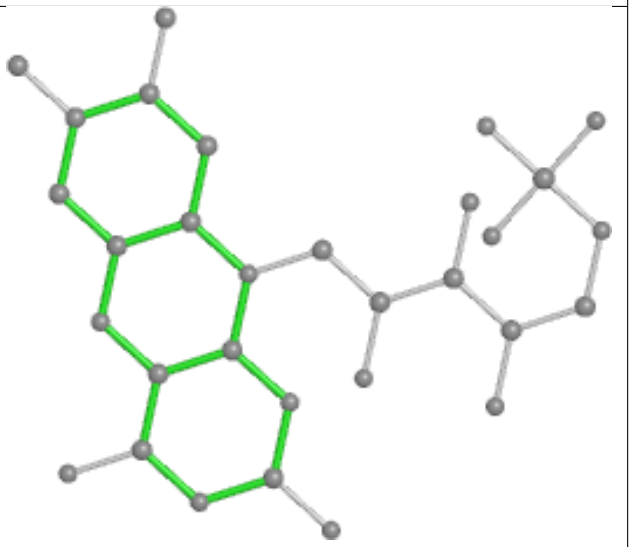
Bond lengths



Bond angles

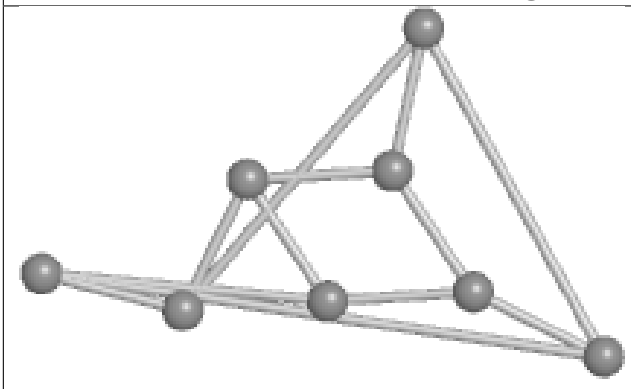


Torsions

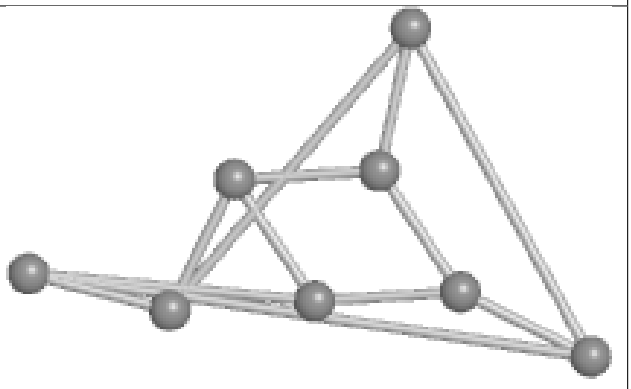


Rings

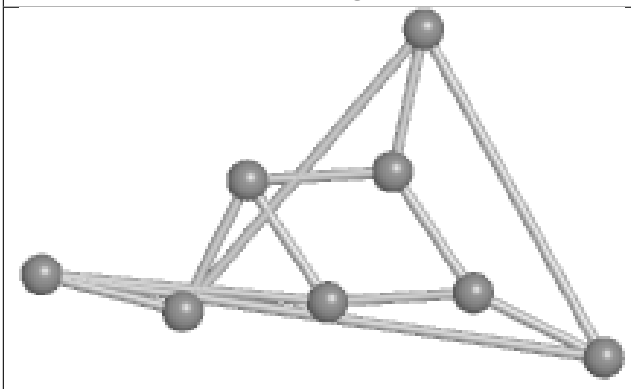
Ligand SF4 B 1104



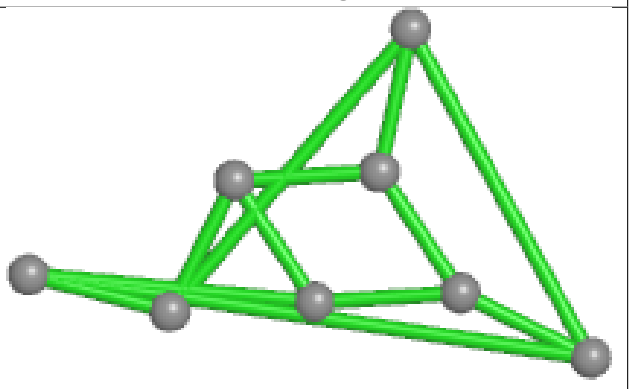
Bond lengths



Bond angles

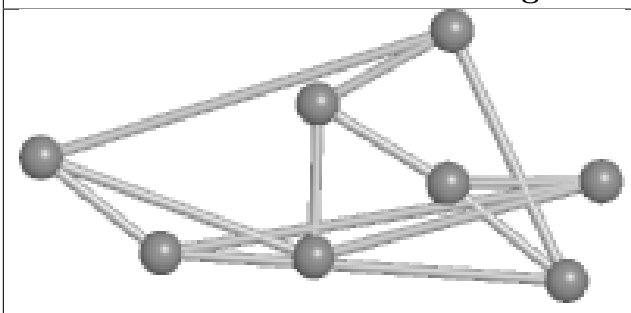


Torsions

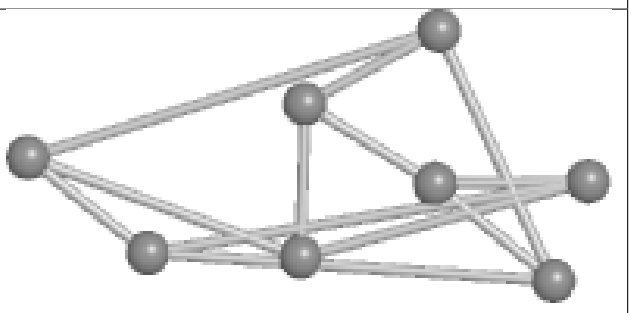


Rings

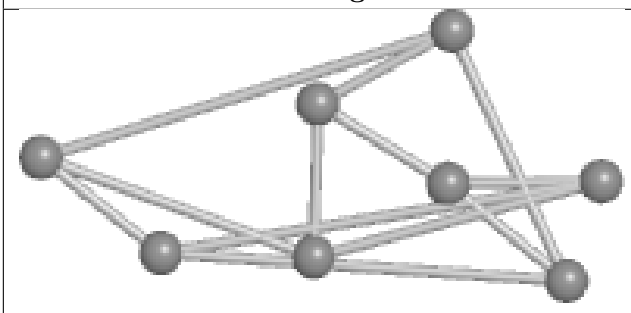
Ligand SF4 D 1102



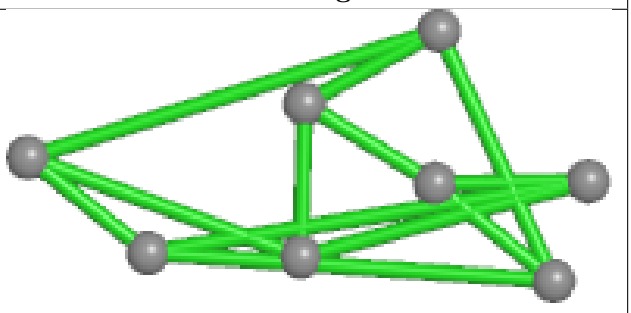
Bond lengths



Bond angles

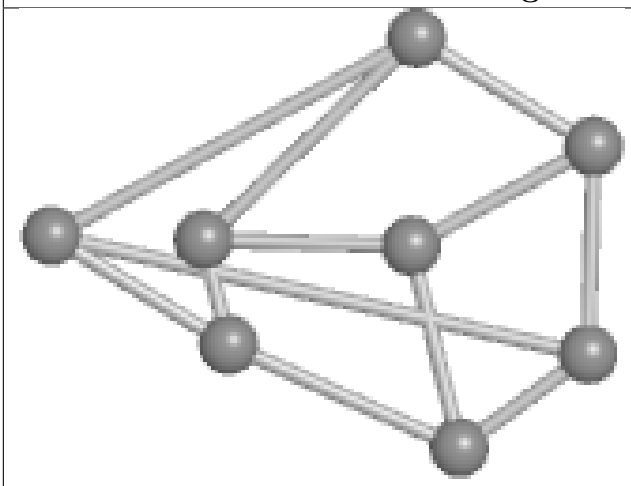


Torsions

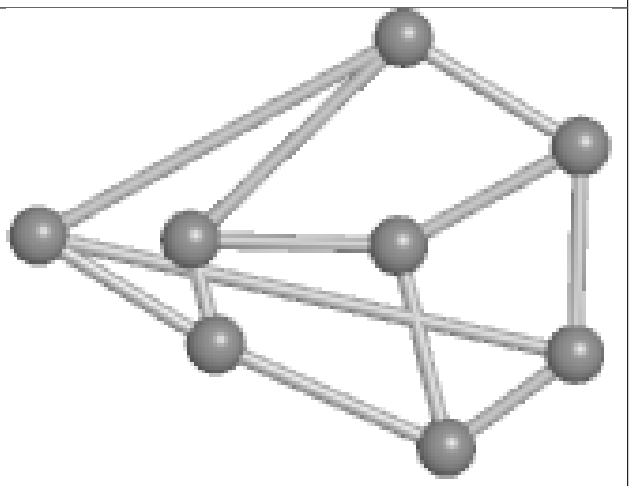


Rings

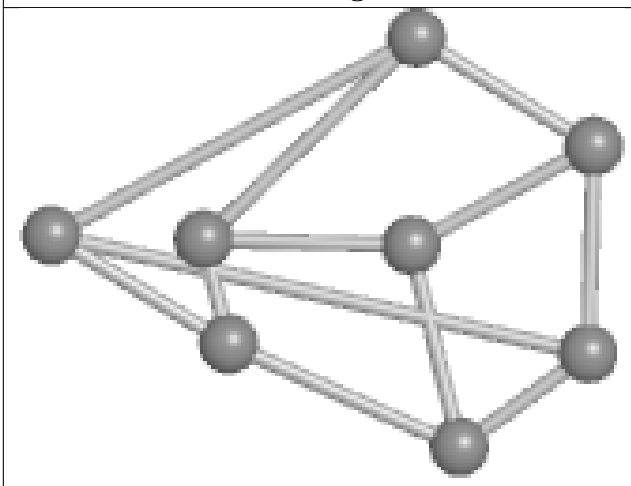
Ligand SF4 D 1104



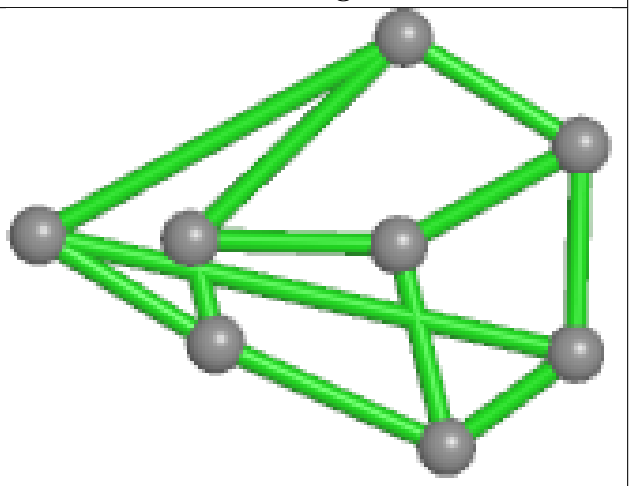
Bond lengths



Bond angles

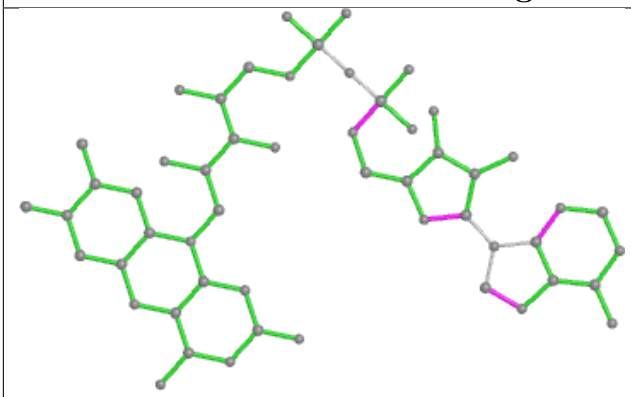


Torsions

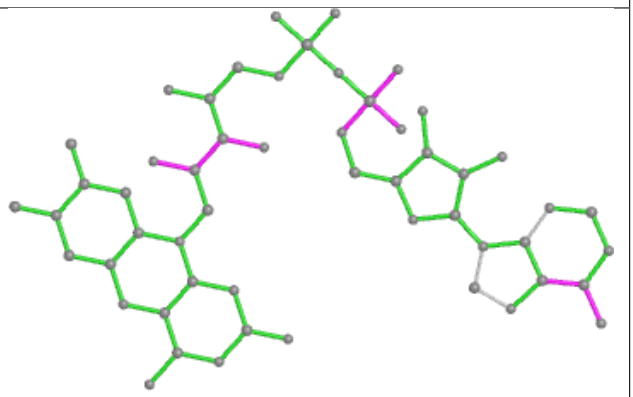


Rings

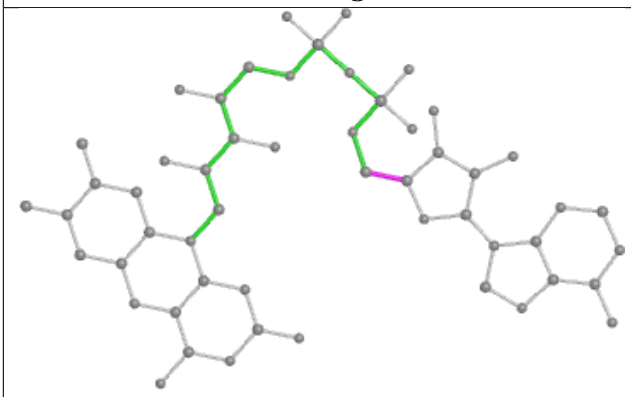
Ligand FAD D 1106



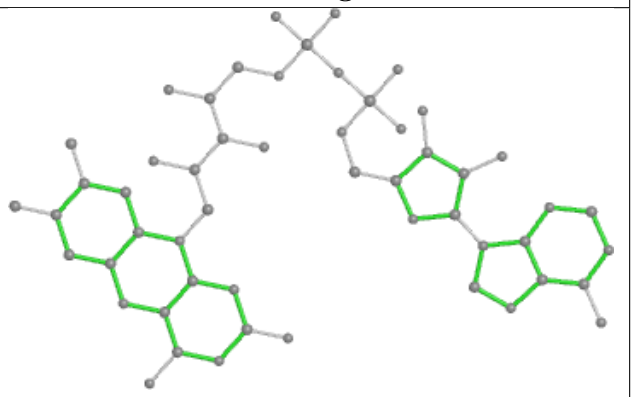
Bond lengths



Bond angles

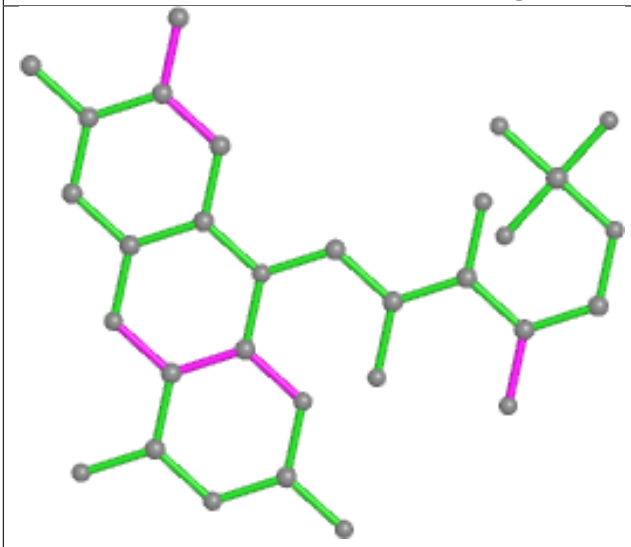


Torsions

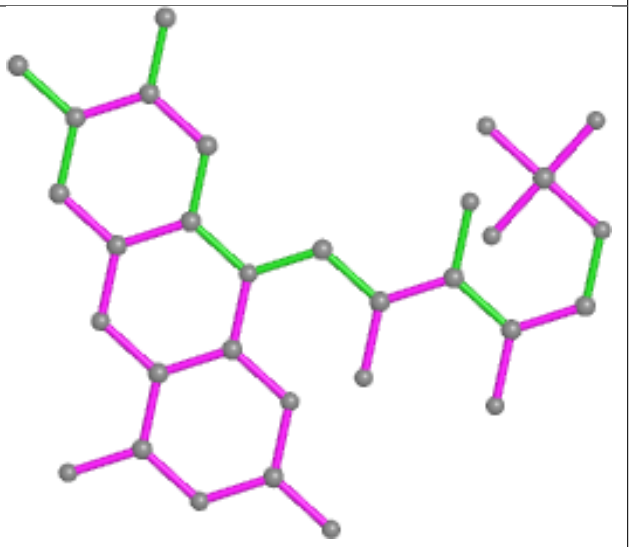


Rings

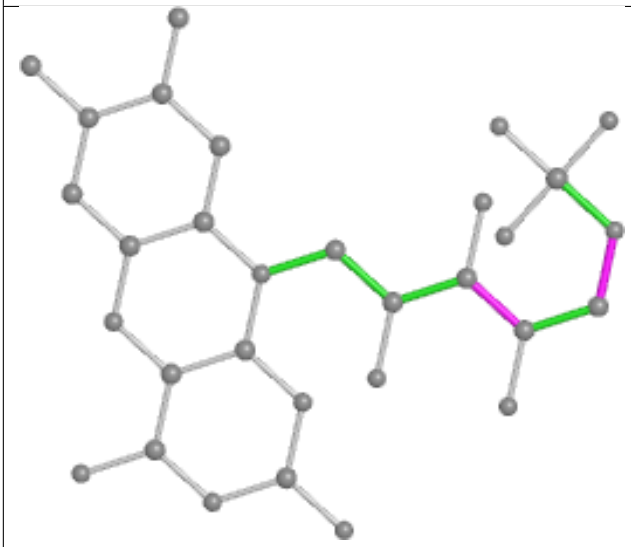
Ligand FMN B 1105



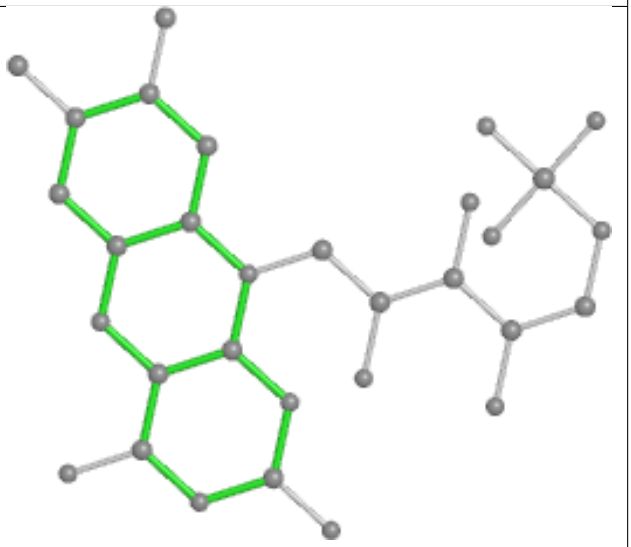
Bond lengths



Bond angles

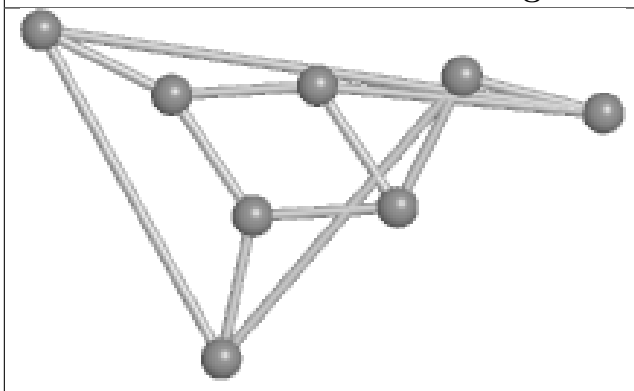


Torsions

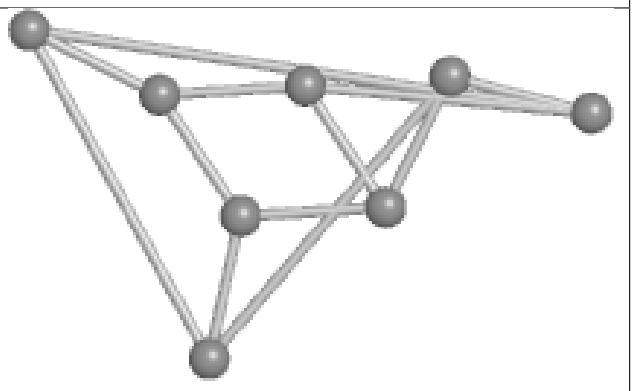


Rings

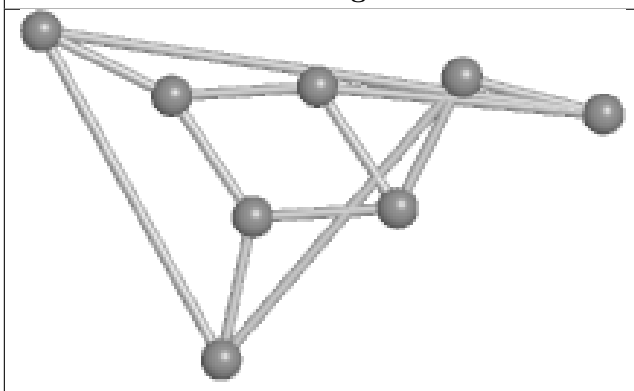
Ligand SF4 C 1101



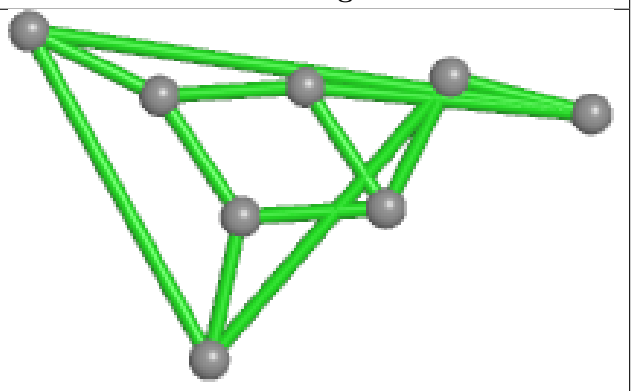
Bond lengths



Bond angles

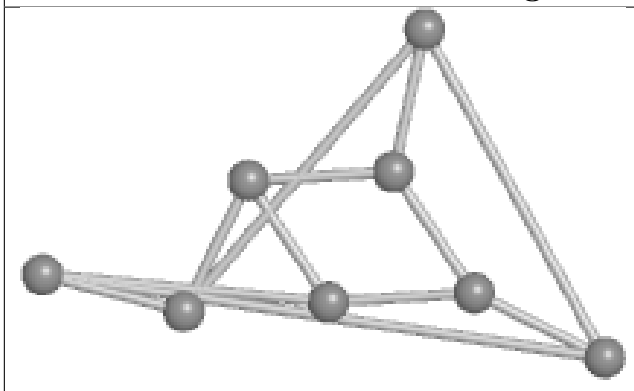


Torsions

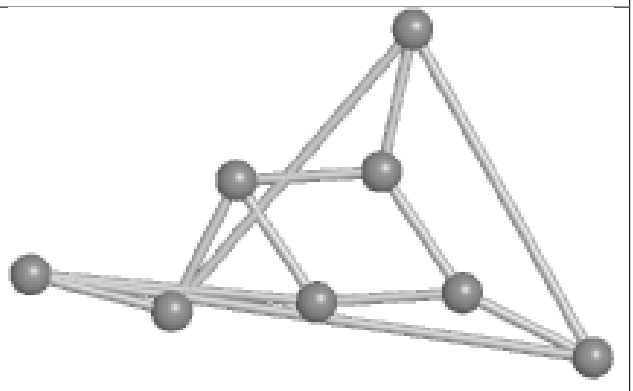


Rings

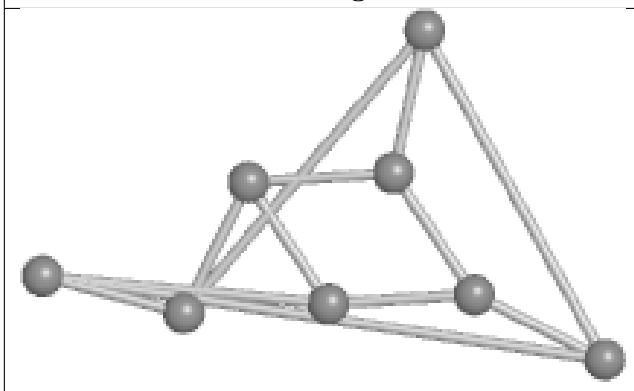
Ligand SF4 B 1101



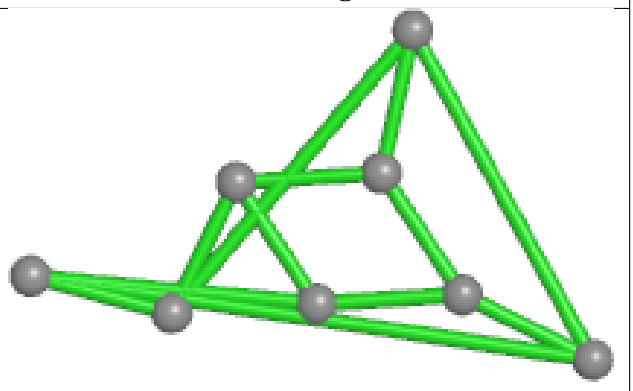
Bond lengths



Bond angles

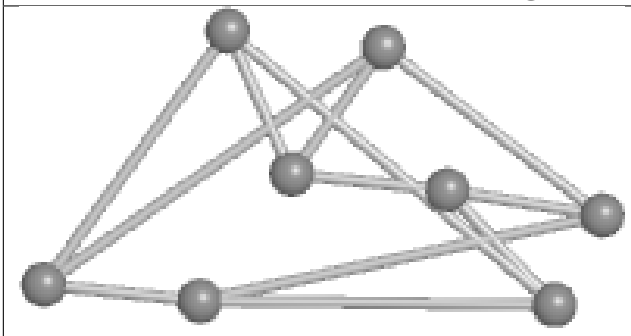


Torsions

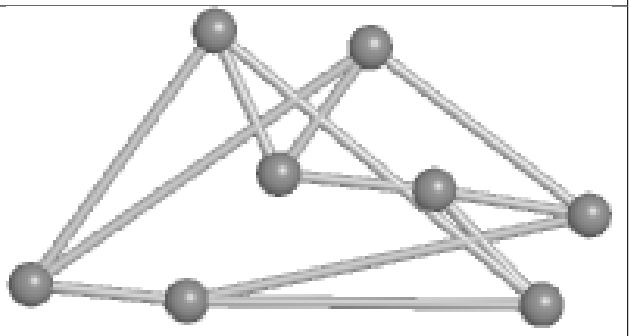


Rings

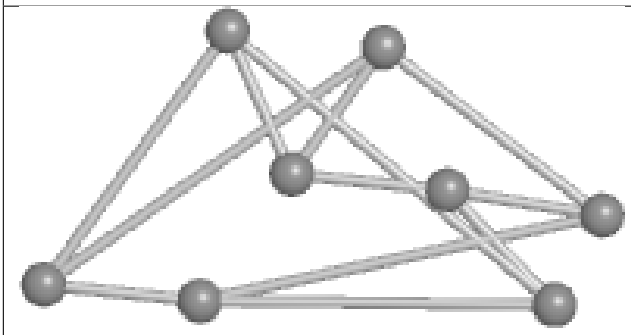
Ligand SF4 C 1104



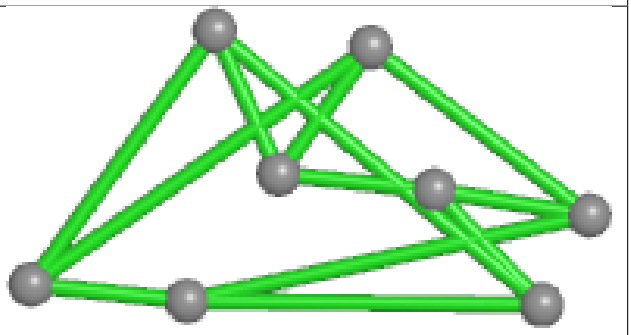
Bond lengths



Bond angles

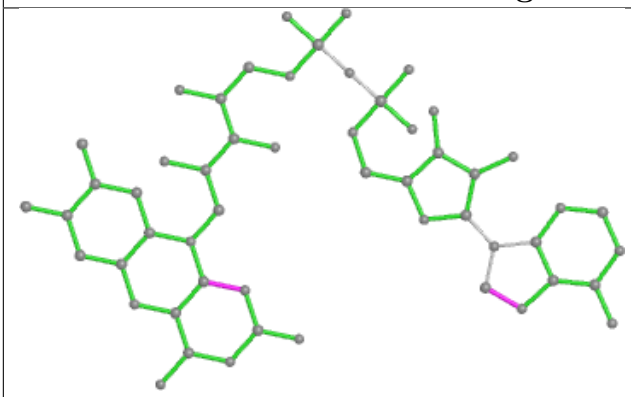


Torsions

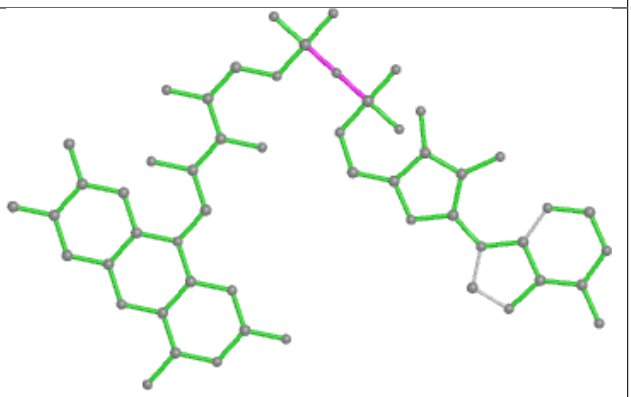


Rings

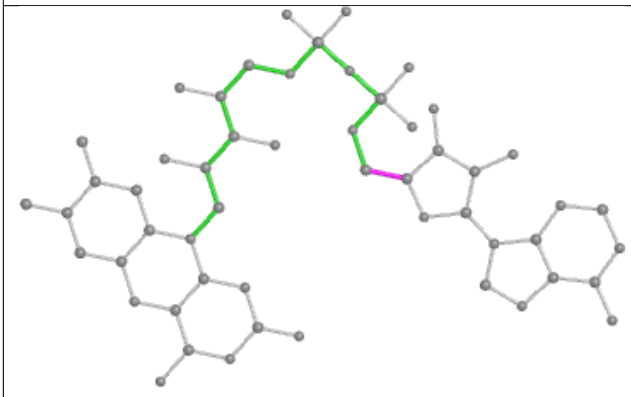
Ligand FAD C 1106



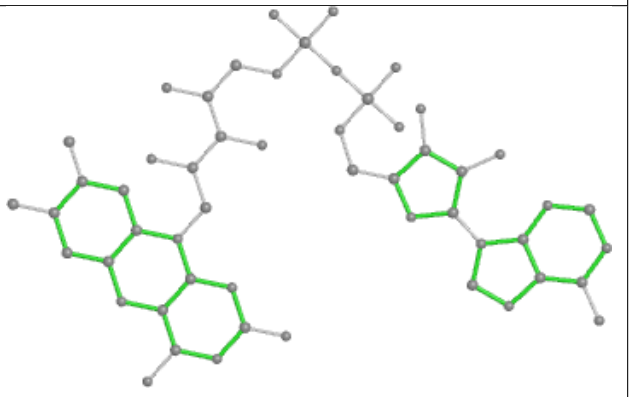
Bond lengths



Bond angles

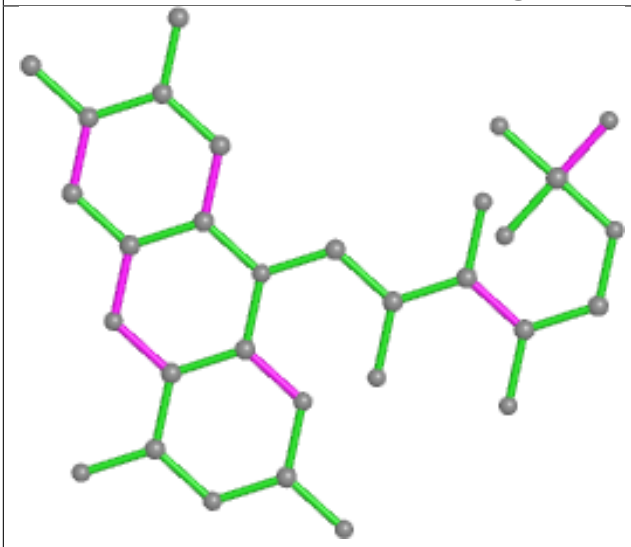


Torsions

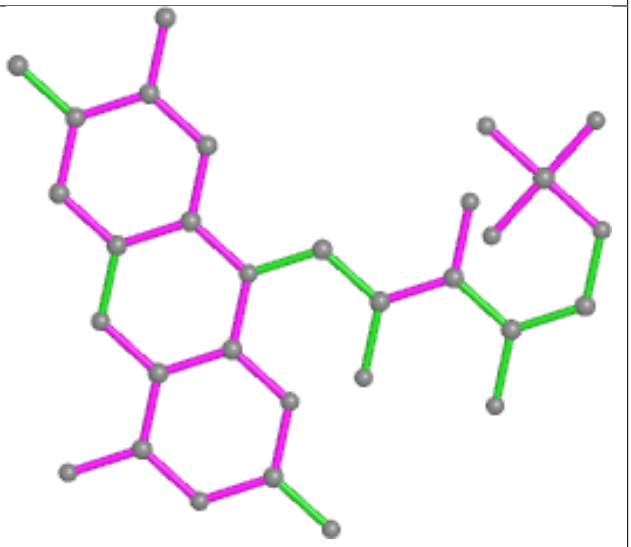


Rings

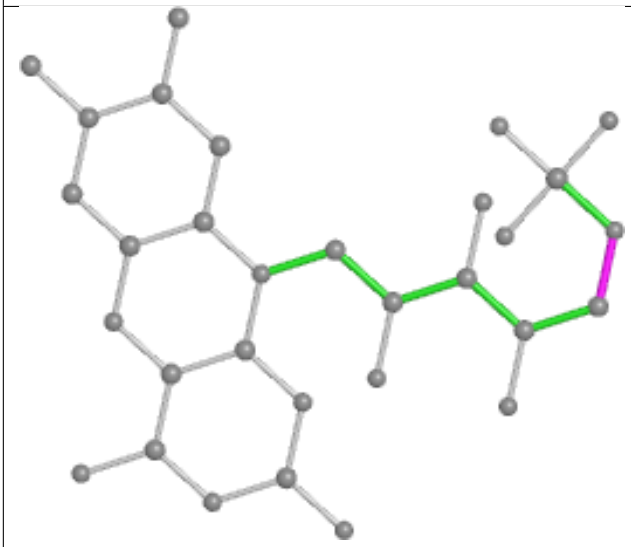
Ligand FMN A 1105



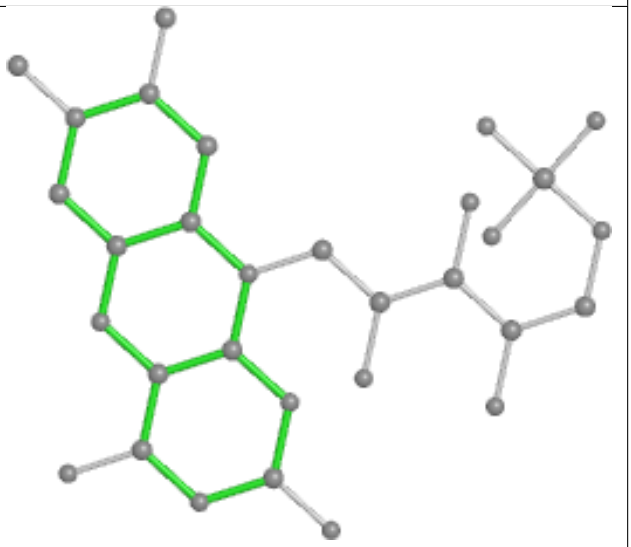
Bond lengths



Bond angles

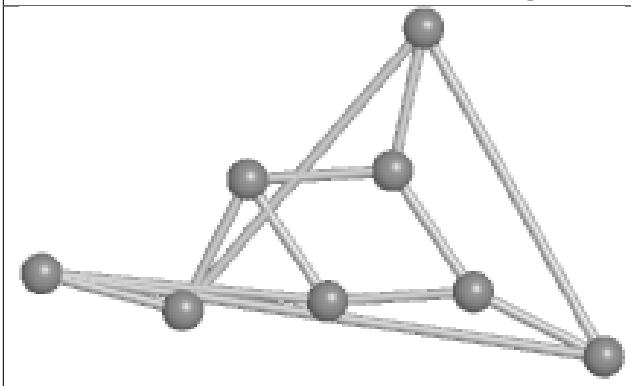


Torsions

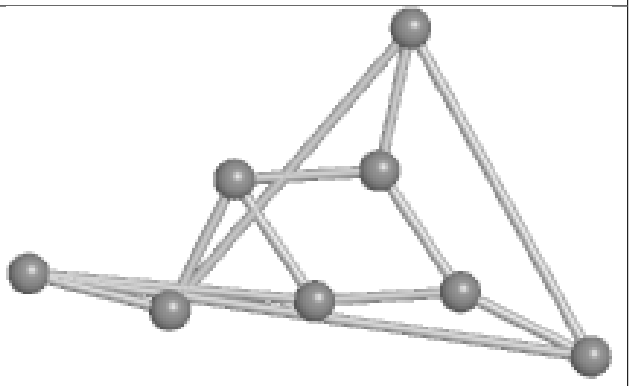


Rings

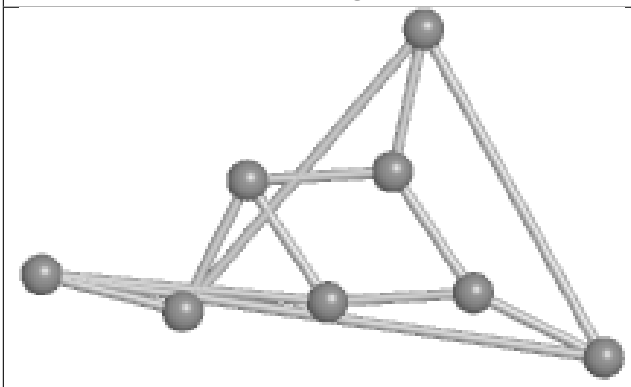
Ligand SF4 A 1101



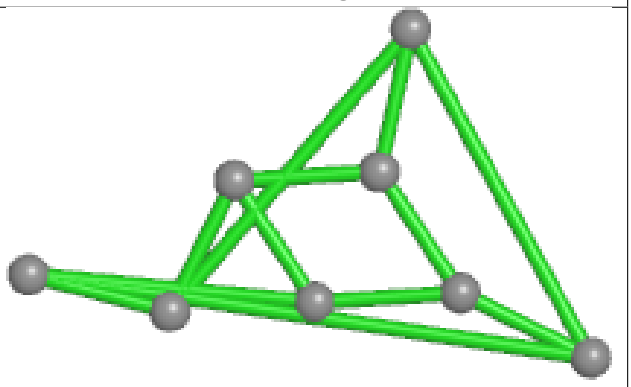
Bond lengths



Bond angles

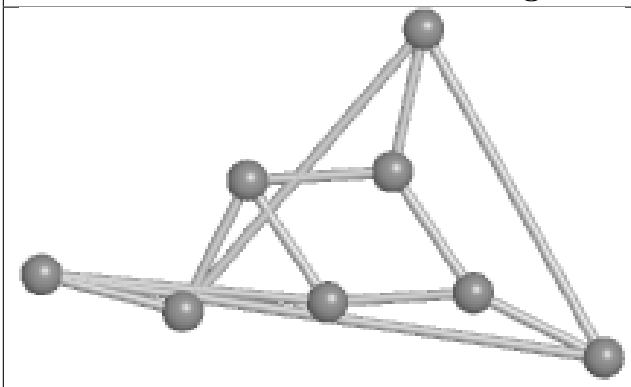


Torsions

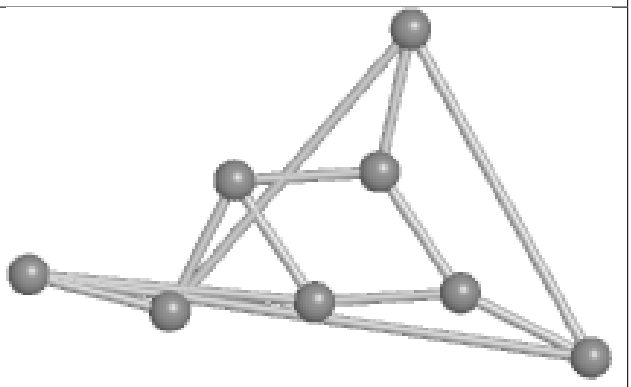


Rings

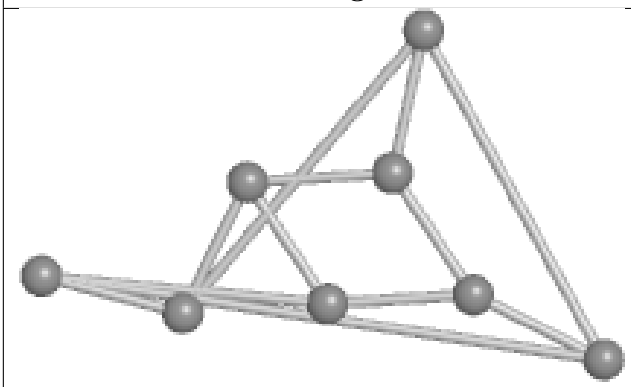
Ligand SF4 B 1102



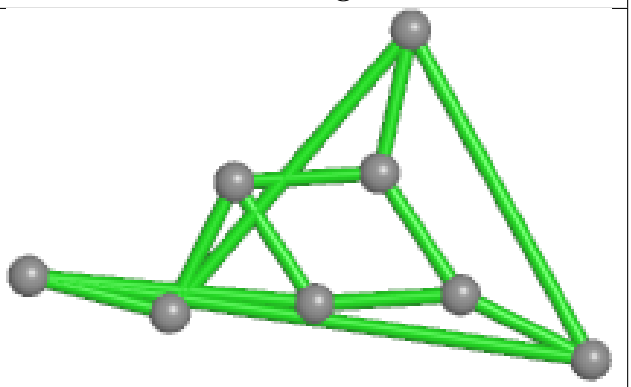
Bond lengths



Bond angles

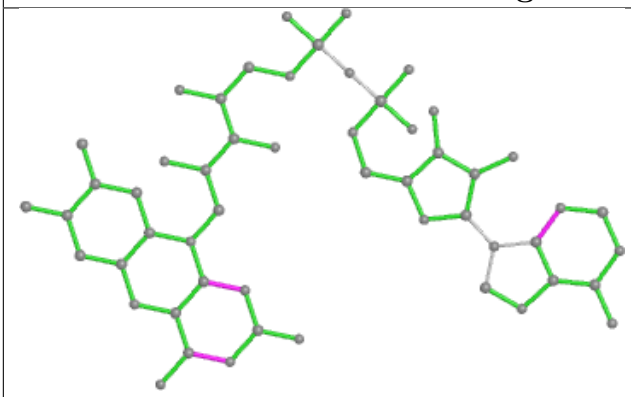


Torsions

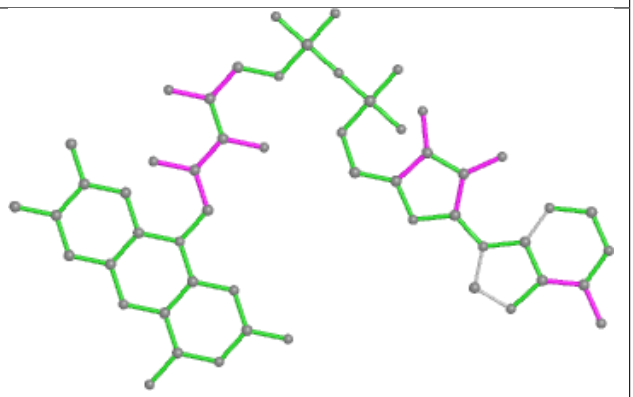


Rings

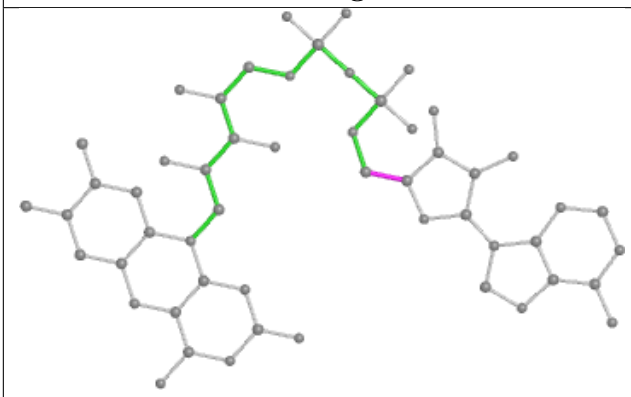
Ligand FAD B 1106



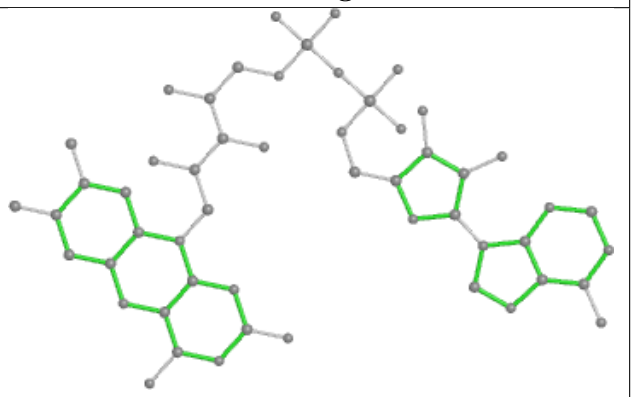
Bond lengths



Bond angles

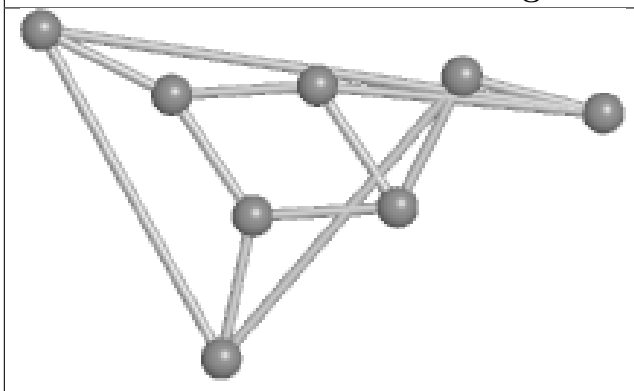


Torsions

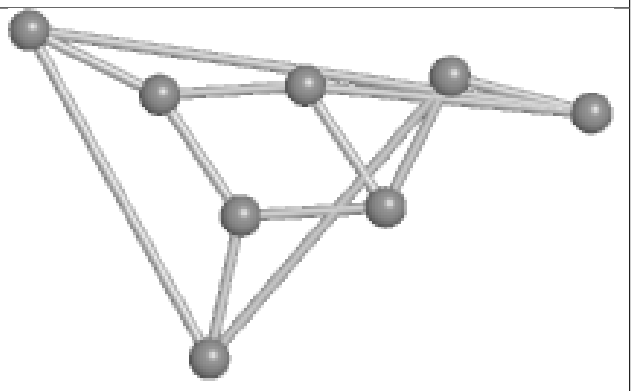


Rings

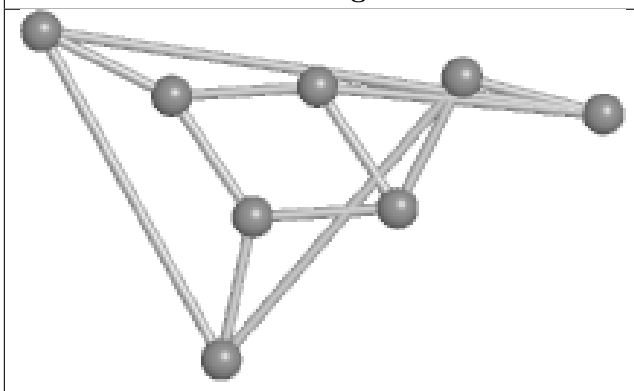
Ligand SF4 D 1101



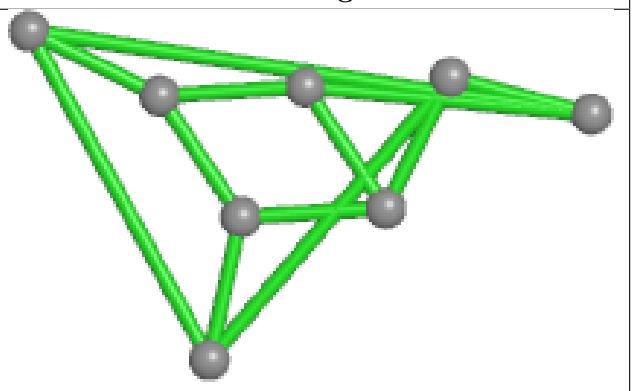
Bond lengths



Bond angles

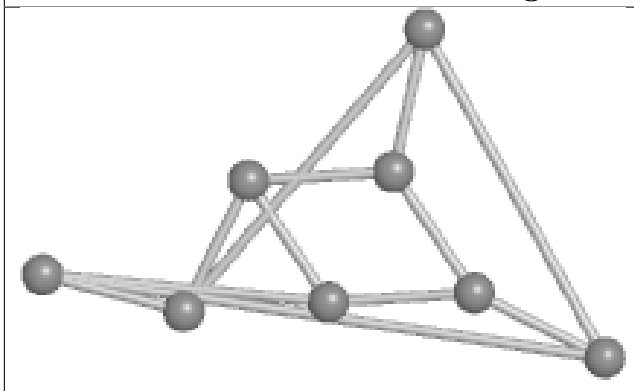


Torsions

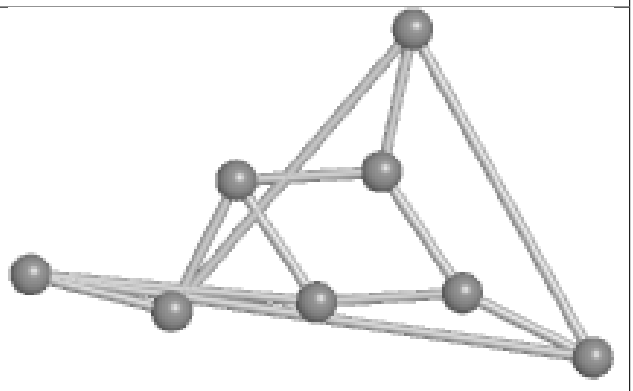


Rings

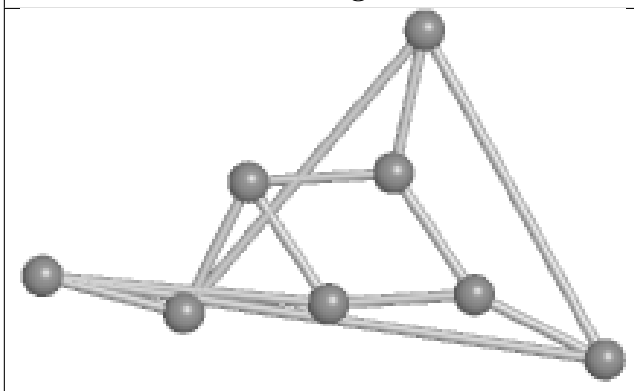
Ligand SF4 D 1103



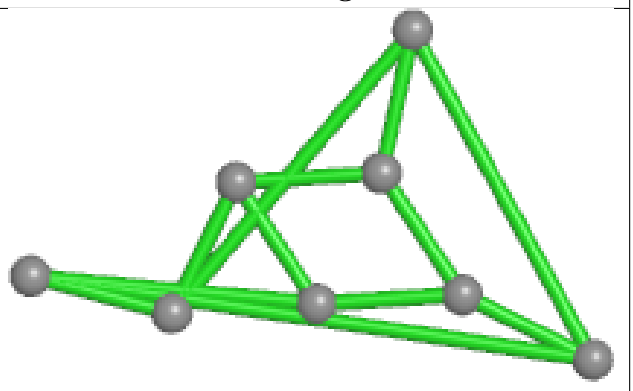
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2
1	B	2
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	670:SER	C	671:SER	N	1.13
1	B	671:SER	C	672:PRO	N	1.11
1	D	670:SER	C	671:SER	N	1.07
1	B	670:SER	C	671:SER	N	1.03
1	C	671:SER	C	672:PRO	N	0.96

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	996/1025 (97%)	0.32	79 (7%) 12 16	11, 30, 88, 160	0
1	B	1001/1025 (97%)	0.43	101 (10%) 7 8	13, 31, 89, 187	0
1	C	1002/1025 (97%)	0.39	103 (10%) 6 8	14, 32, 89, 164	0
1	D	992/1025 (96%)	0.56	107 (10%) 5 7	15, 34, 100, 192	0
All	All	3991/4100 (97%)	0.42	390 (9%) 7 9	11, 32, 91, 192	0

The worst 5 of 390 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	868	ILE	23.0
1	D	864	PRO	21.2
1	D	52	CYS	20.1
1	A	868	ILE	18.1
1	D	868	ILE	17.6

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

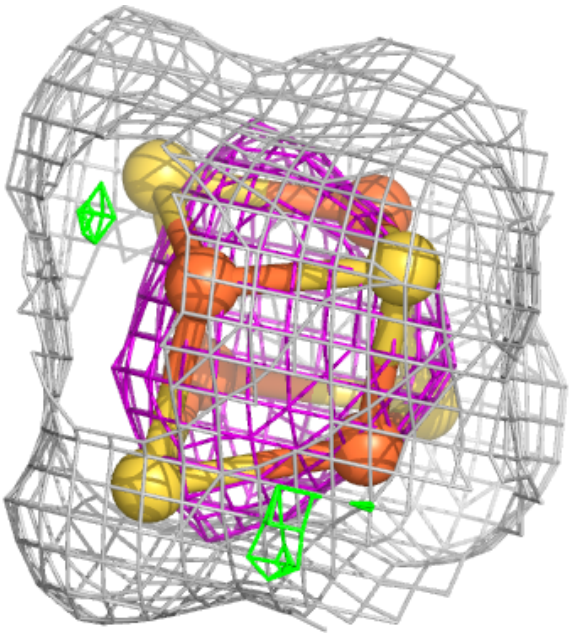
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

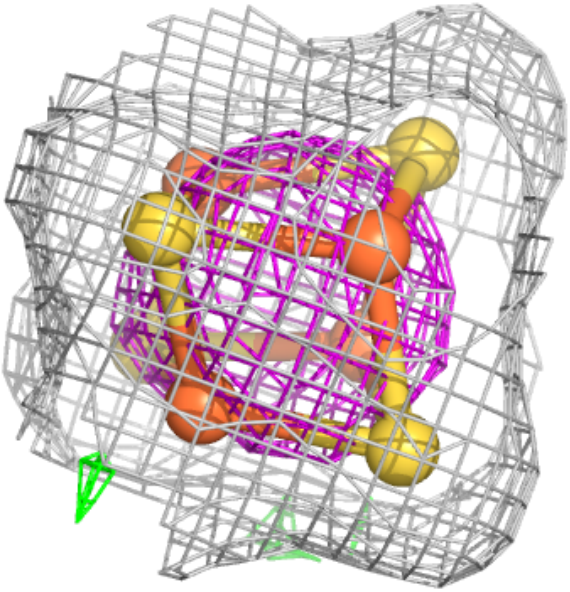
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SF4	A	1104	8/8	0.92	0.07	20,23,24,24	0
2	SF4	B	1101	8/8	0.92	0.07	19,21,21,22	0
2	SF4	B	1103	8/8	0.92	0.07	18,19,21,21	0
2	SF4	B	1104	8/8	0.92	0.07	19,21,23,23	0
2	SF4	A	1103	8/8	0.93	0.07	19,22,24,24	0
2	SF4	B	1102	8/8	0.93	0.07	20,21,23,23	0
2	SF4	C	1104	8/8	0.93	0.07	21,22,23,23	0
2	SF4	D	1103	8/8	0.93	0.08	17,22,24,25	0
2	SF4	D	1104	8/8	0.93	0.06	21,23,25,25	0
2	SF4	C	1103	8/8	0.94	0.07	17,20,21,21	0
2	SF4	A	1101	8/8	0.94	0.07	18,21,22,23	0
2	SF4	D	1101	8/8	0.94	0.07	22,24,27,27	0
2	SF4	C	1101	8/8	0.94	0.07	19,21,22,23	0
2	SF4	C	1102	8/8	0.94	0.07	21,22,23,24	0
2	SF4	A	1102	8/8	0.95	0.06	15,16,19,20	0
2	SF4	D	1102	8/8	0.95	0.06	19,20,21,21	0
3	FMN	C	1105	31/31	0.97	0.16	17,23,26,33	0
4	FAD	A	1106	53/53	0.97	0.12	20,27,31,38	0
4	FAD	B	1106	53/53	0.97	0.12	23,31,37,43	0
4	FAD	C	1106	53/53	0.97	0.12	20,32,37,39	0
4	FAD	D	1106	53/53	0.97	0.12	25,34,41,41	0
5	TDR	B	1107	9/9	0.97	0.13	22,25,27,28	0
5	TDR	D	1107	9/9	0.97	0.12	22,25,27,27	0
3	FMN	B	1105	31/31	0.98	0.14	16,24,29,33	0
5	TDR	A	1107	9/9	0.98	0.13	21,21,25,27	0
3	FMN	A	1105	31/31	0.98	0.17	19,28,36,37	0
3	FMN	D	1105	31/31	0.98	0.15	19,23,28,31	0
5	TDR	C	1107	9/9	0.99	0.14	18,20,23,25	0

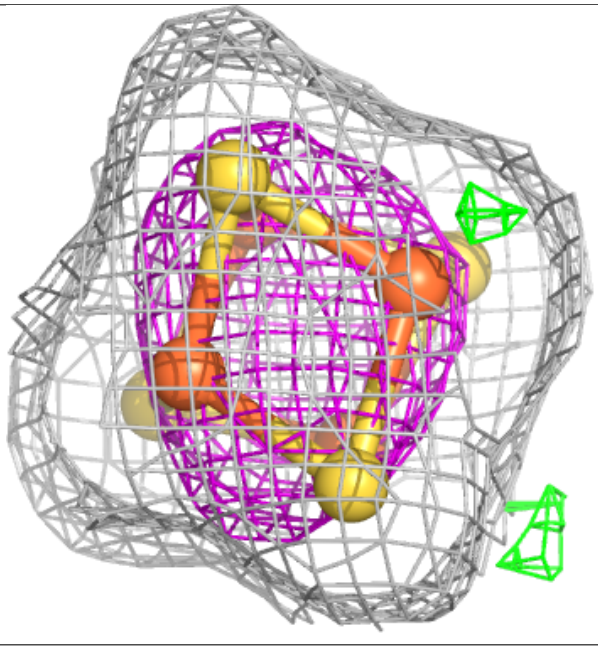
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

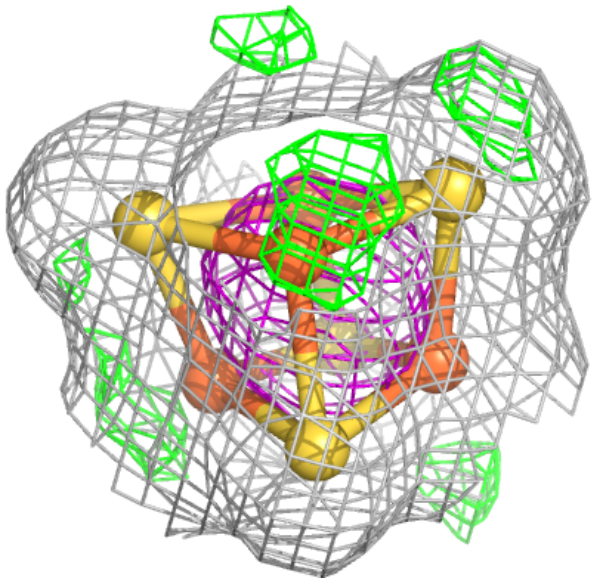


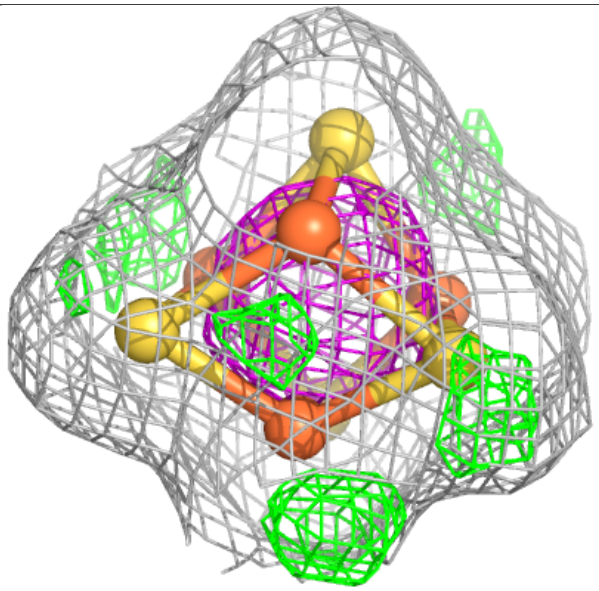


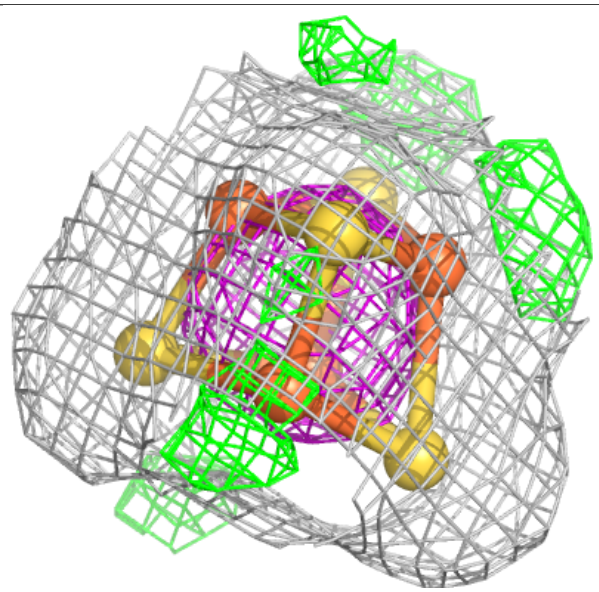


Electron density around SF4 B 1101:

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

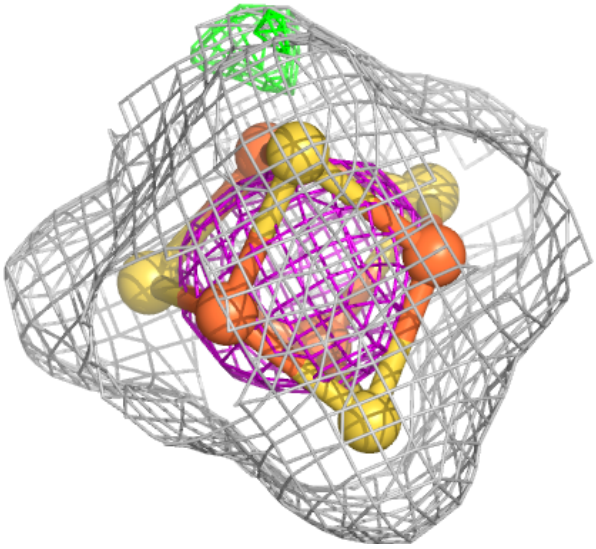


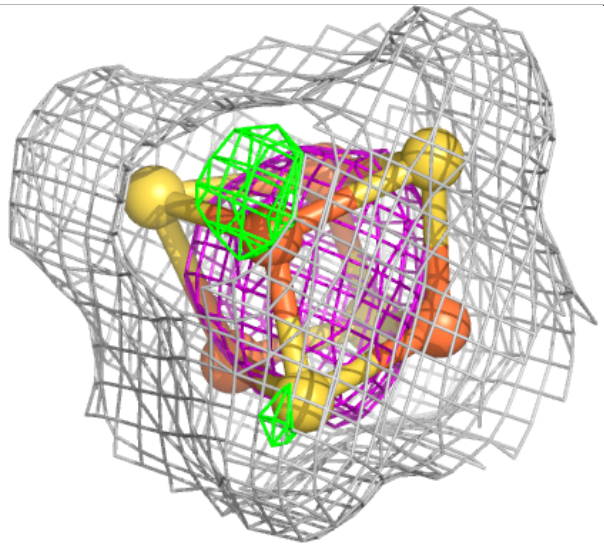


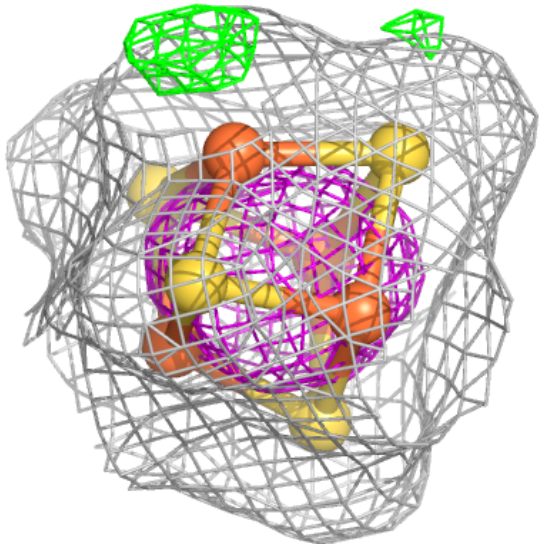


Electron density around SF4 B 1103:

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

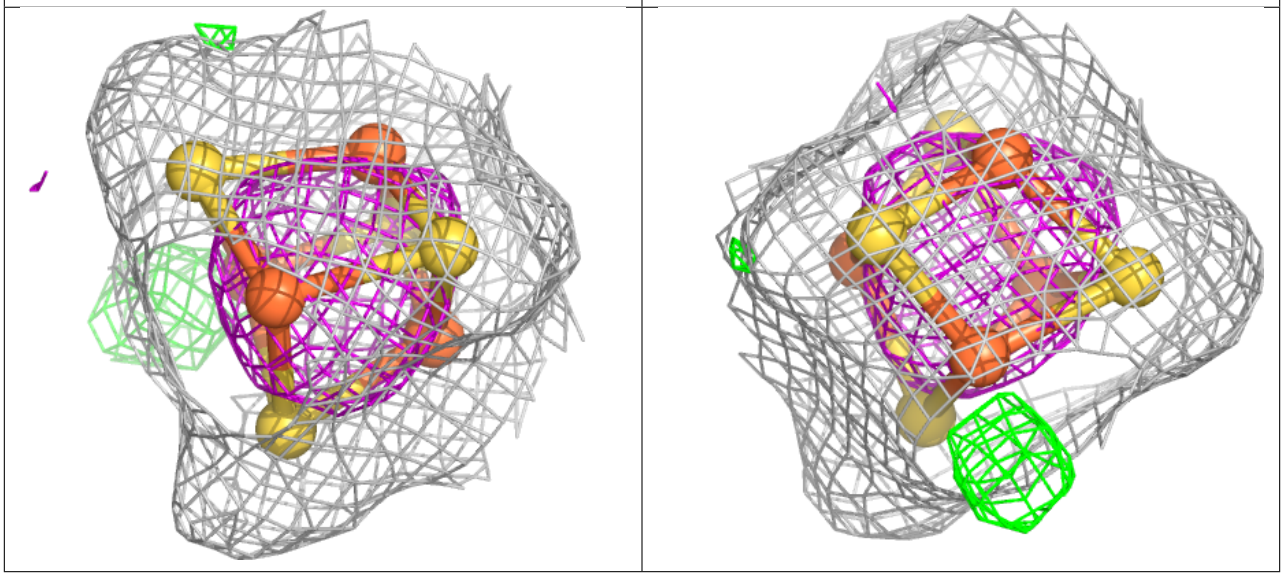






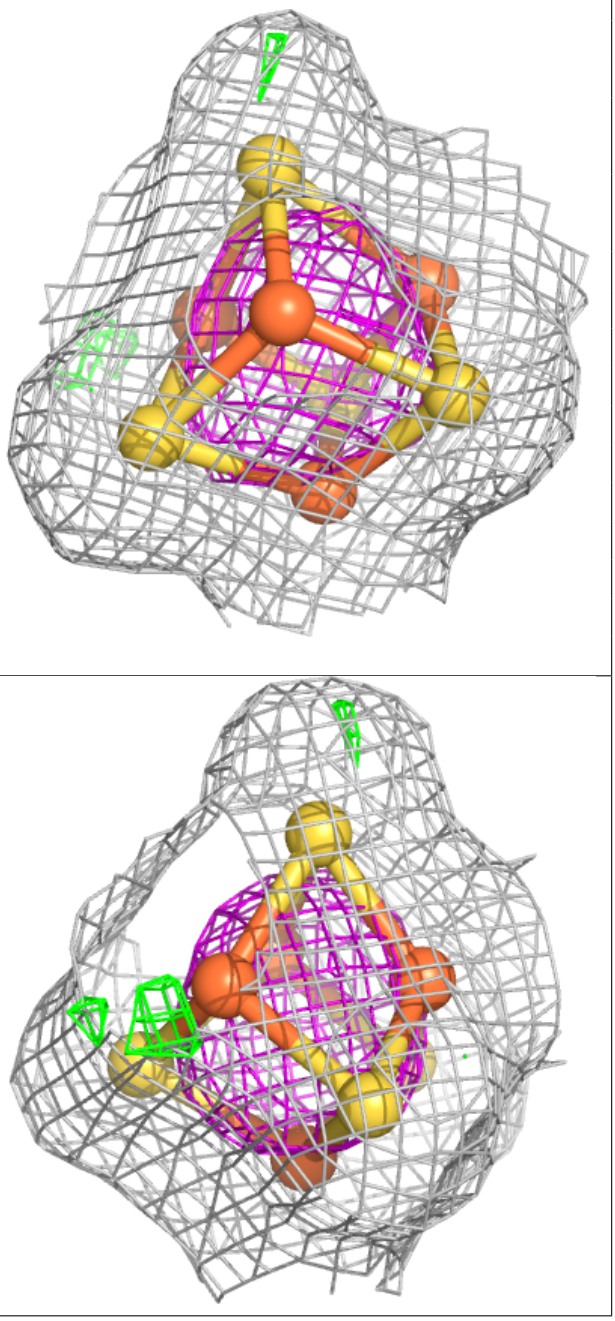
Electron density around SF4 B 1104:

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



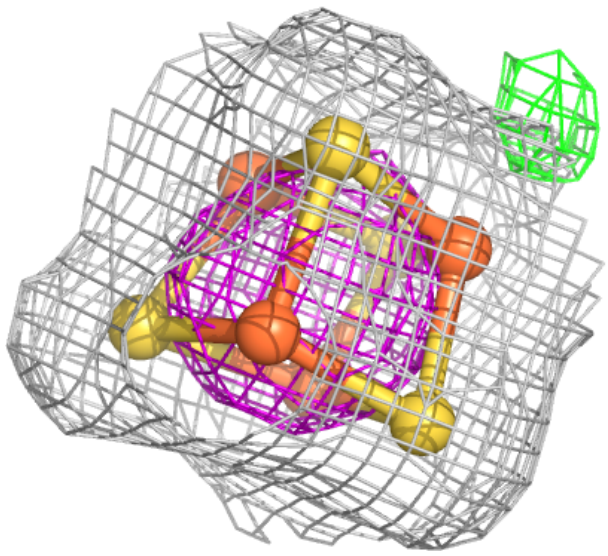
Electron density around SF4 A 1103:

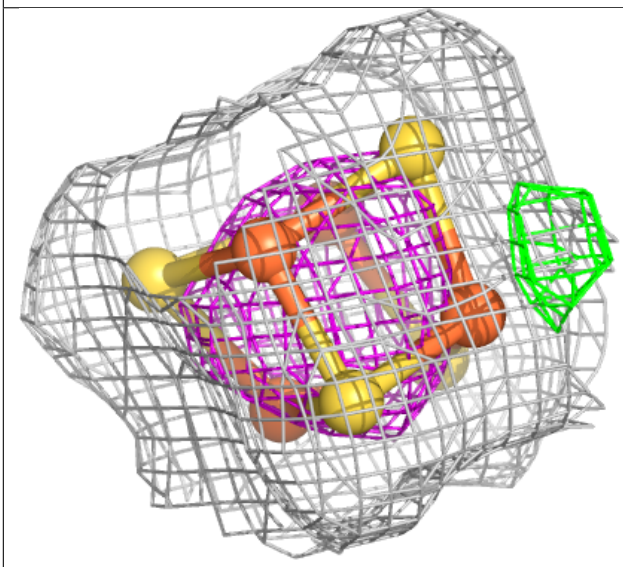
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

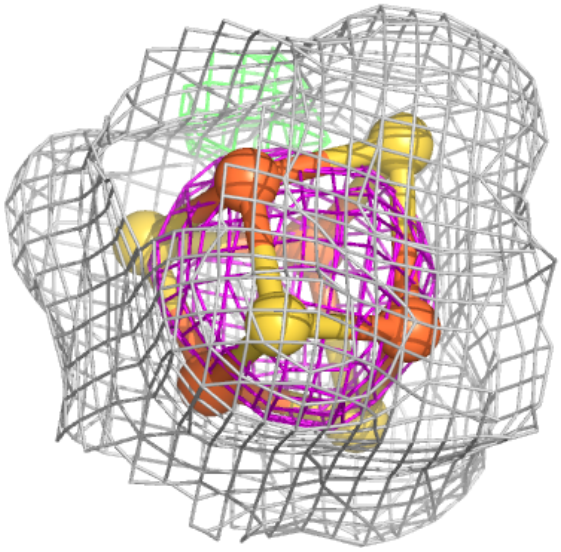


Electron density around SF4 B 1102:

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

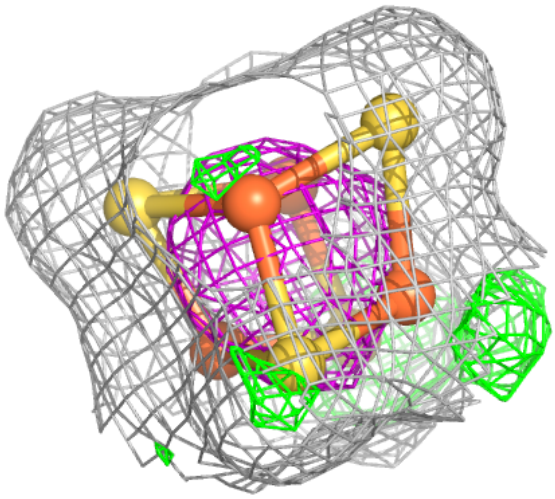


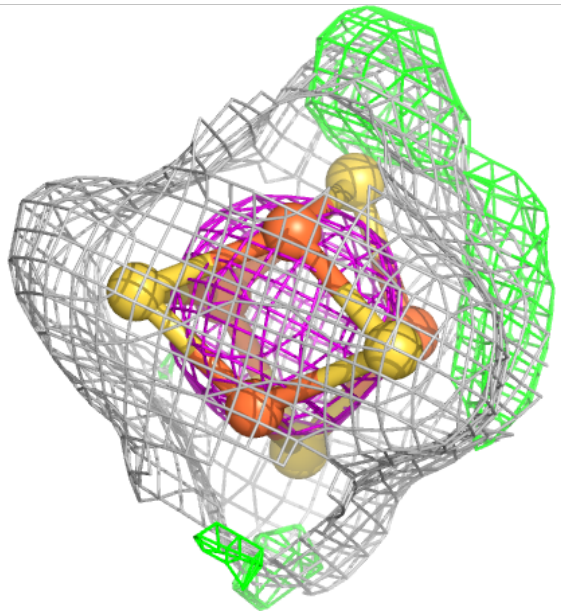


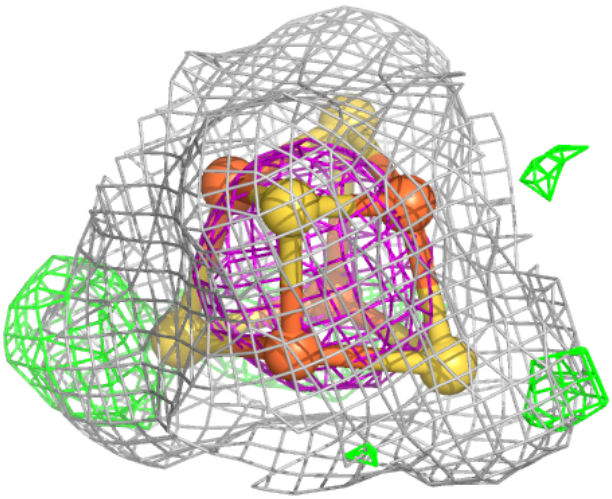


Electron density around SF4 C 1104:

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

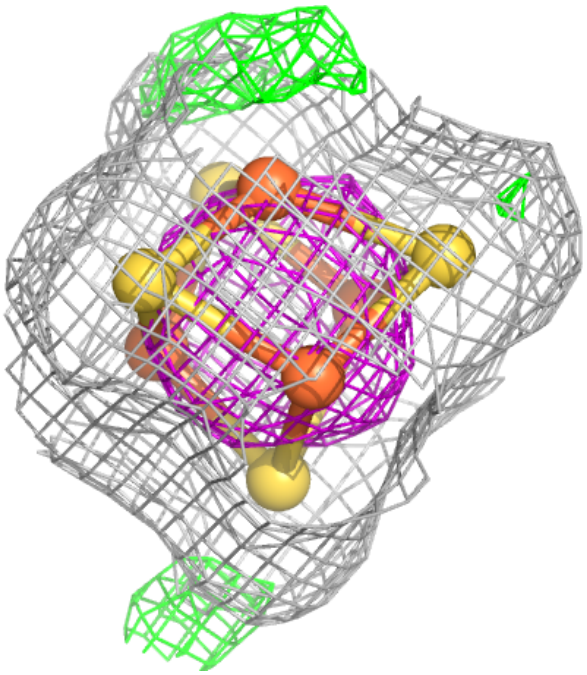


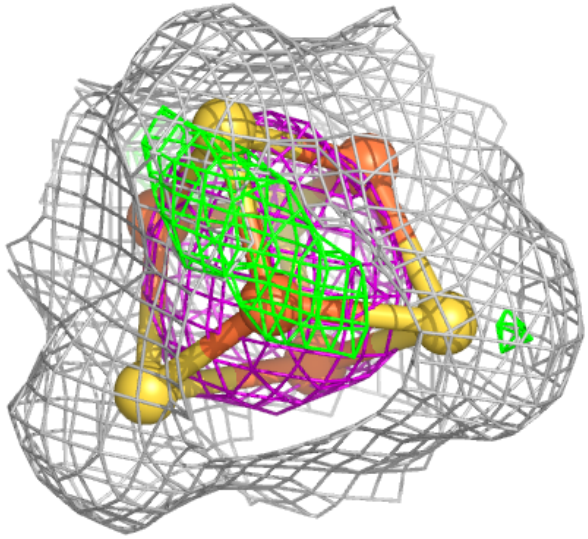


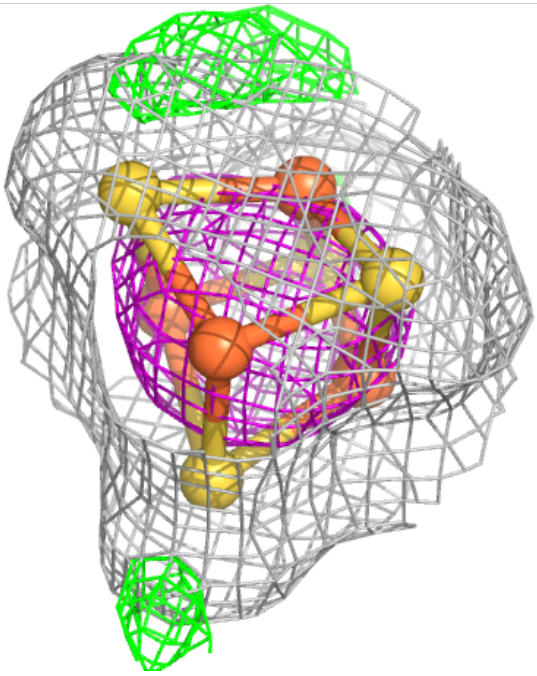


Electron density around SF4 D 1103:

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

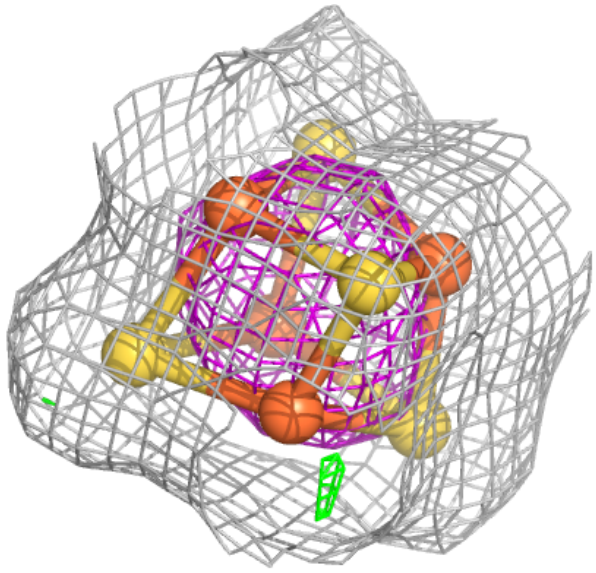


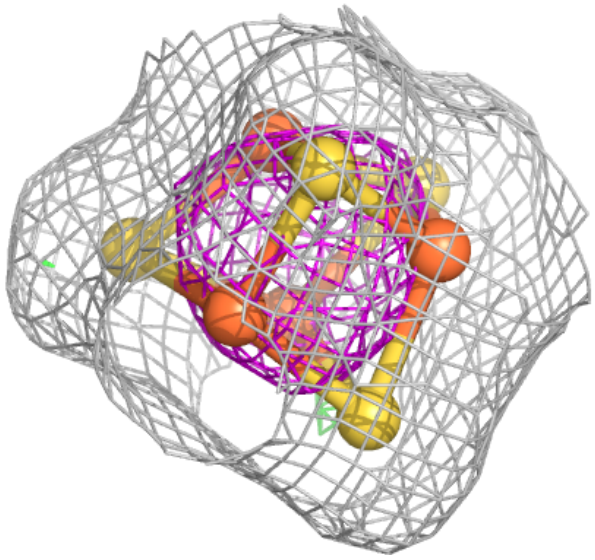


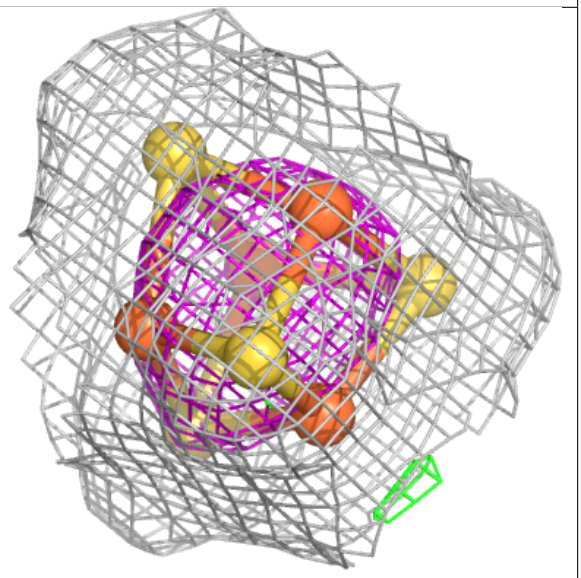


Electron density around SF4 D 1104:

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

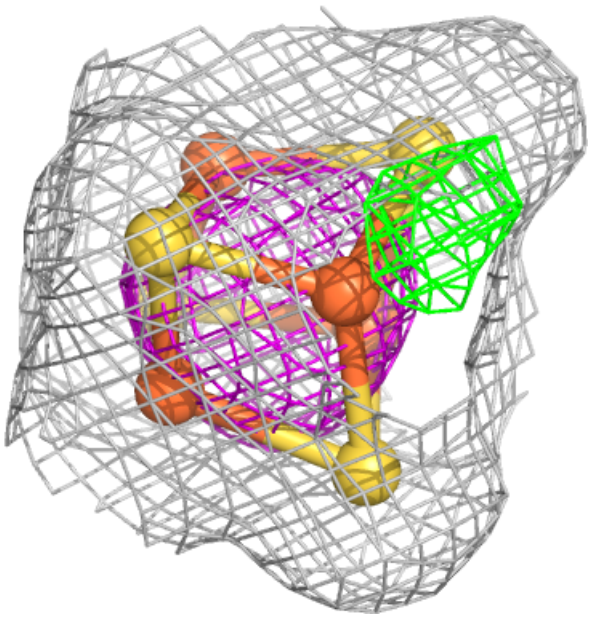


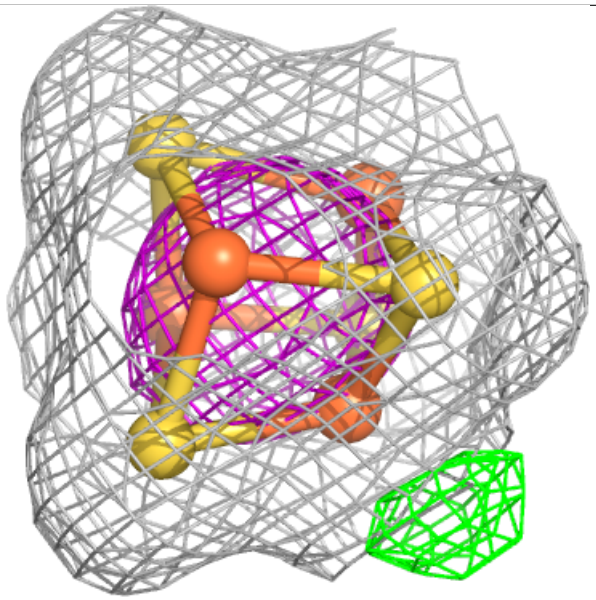


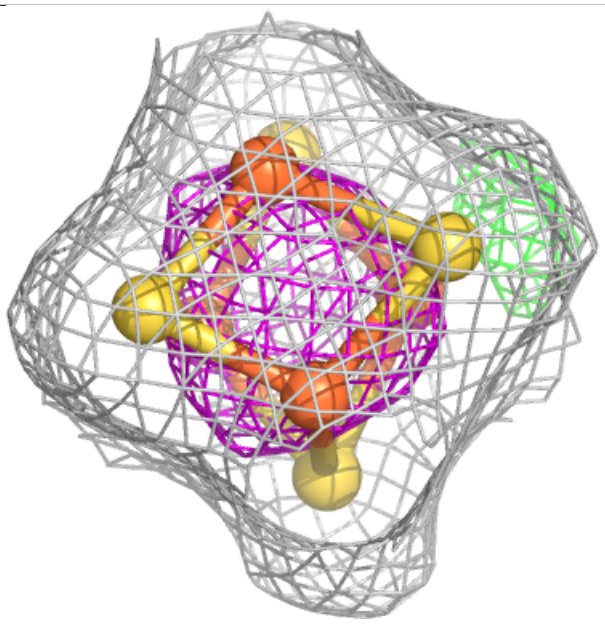


Electron density around SF4 C 1103:

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

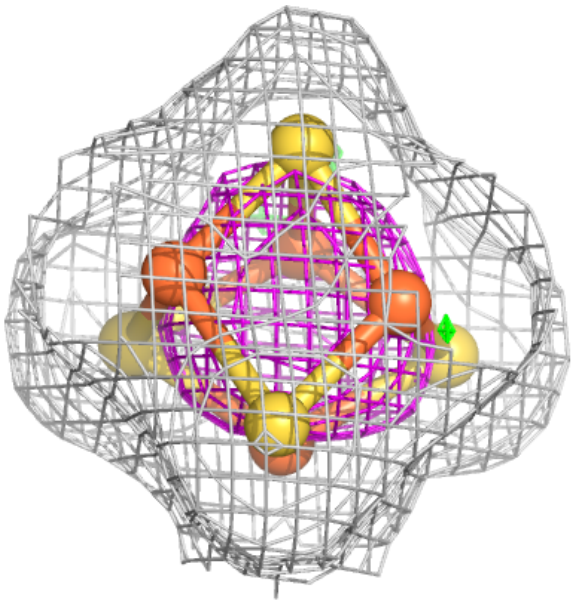


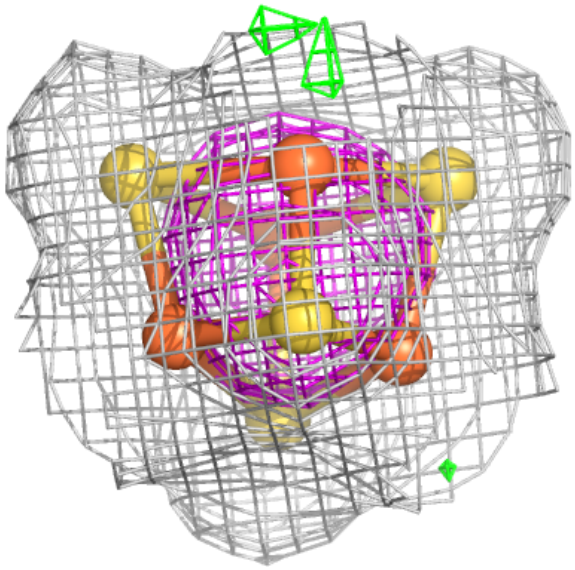


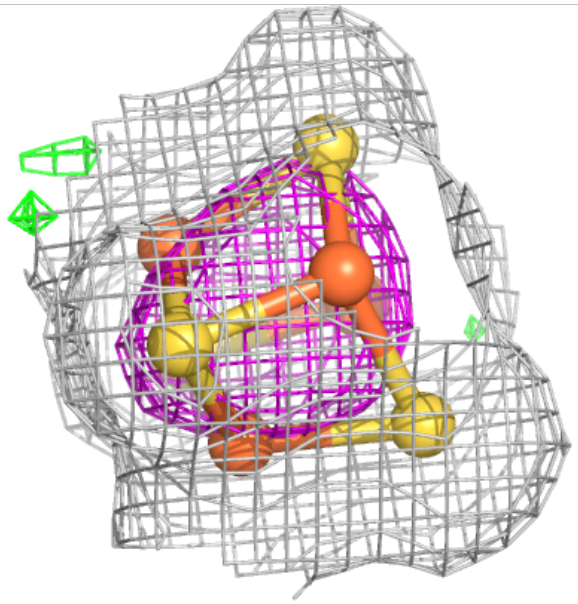


Electron density around SF4 A 1101:

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

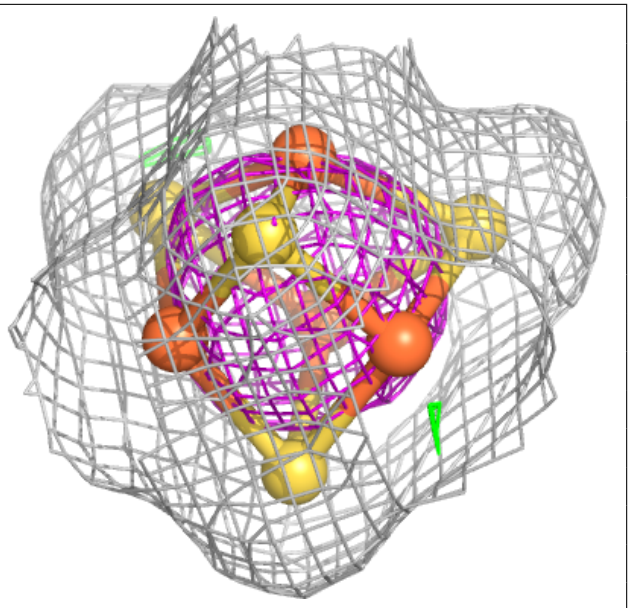


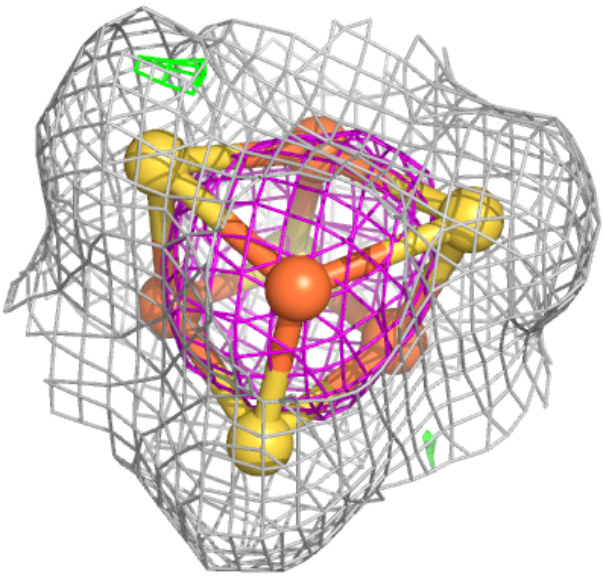


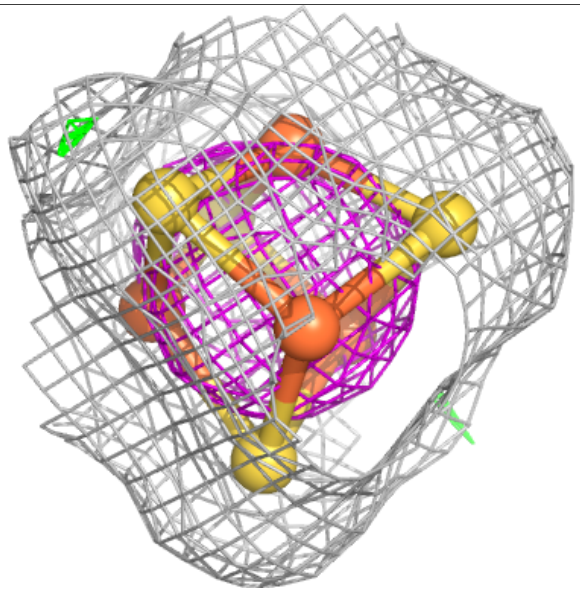


Electron density around SF4 D 1101:

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

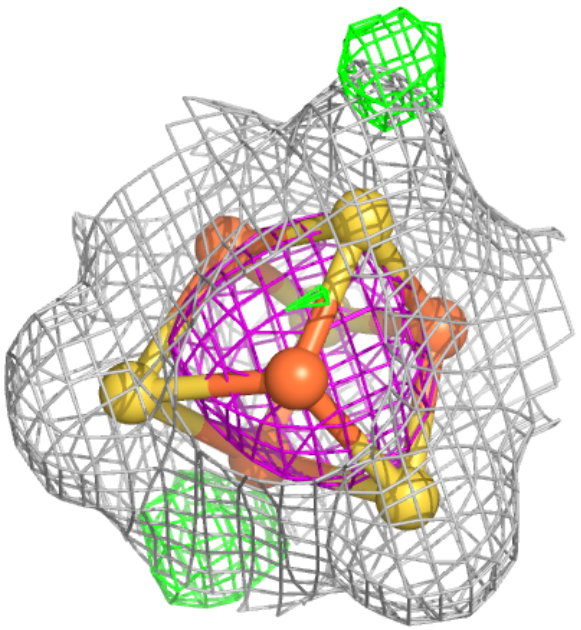


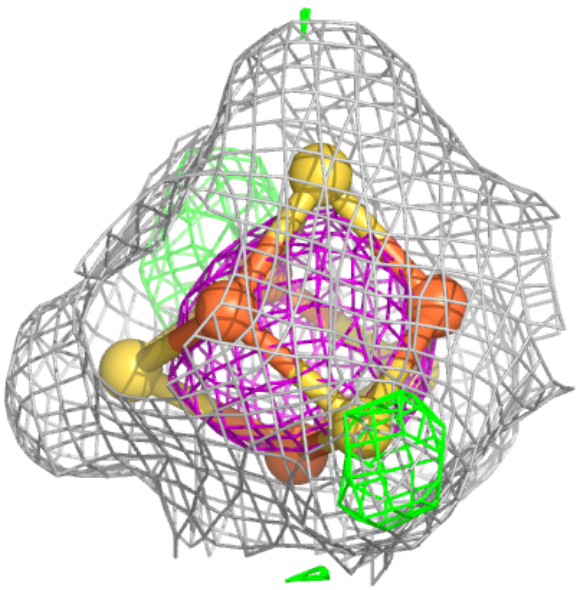


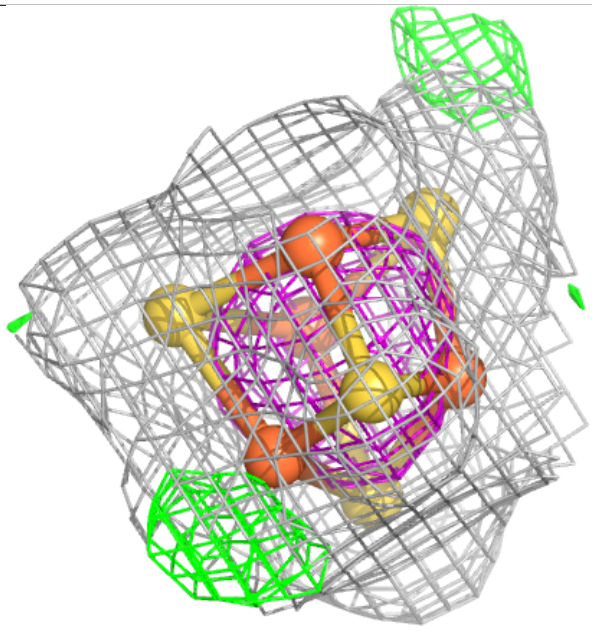


Electron density around SF4 C 1101:

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

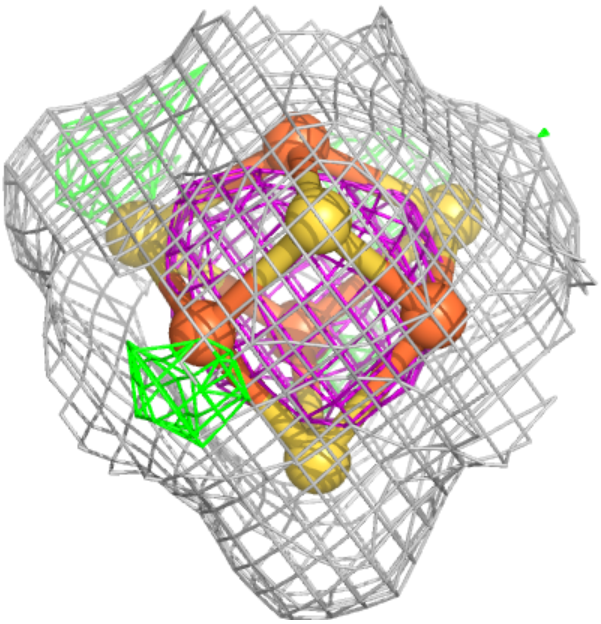


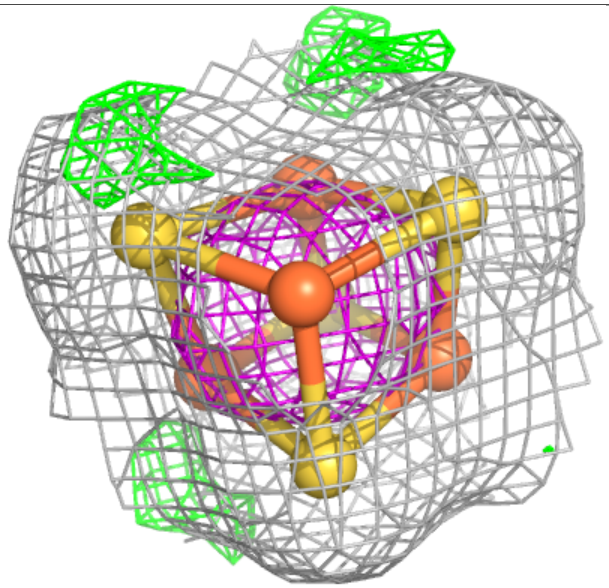


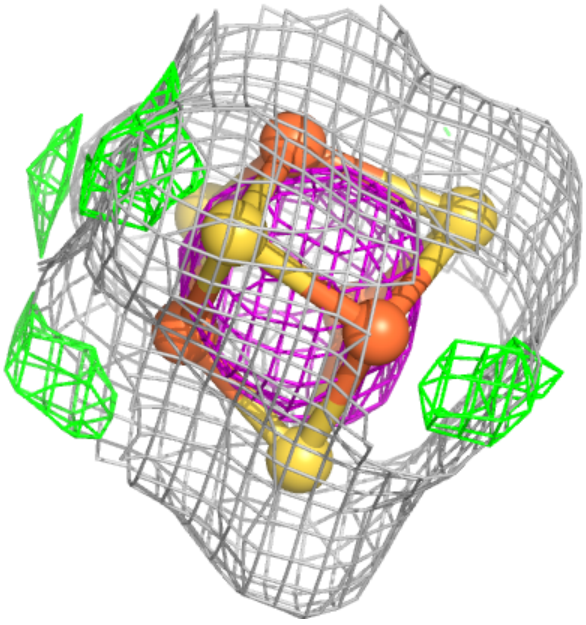


Electron density around SF4 C 1102:

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

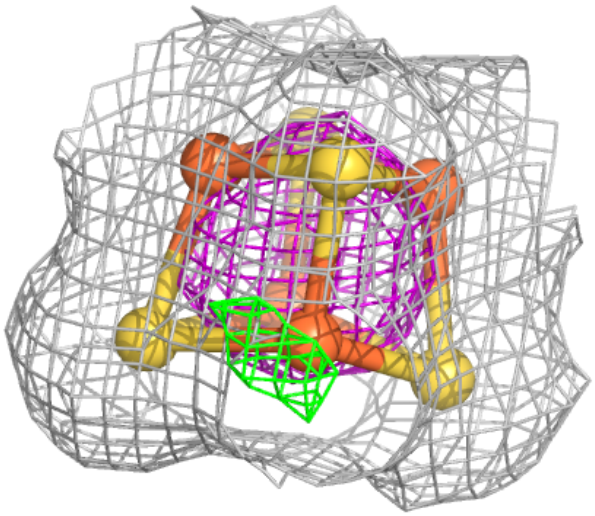


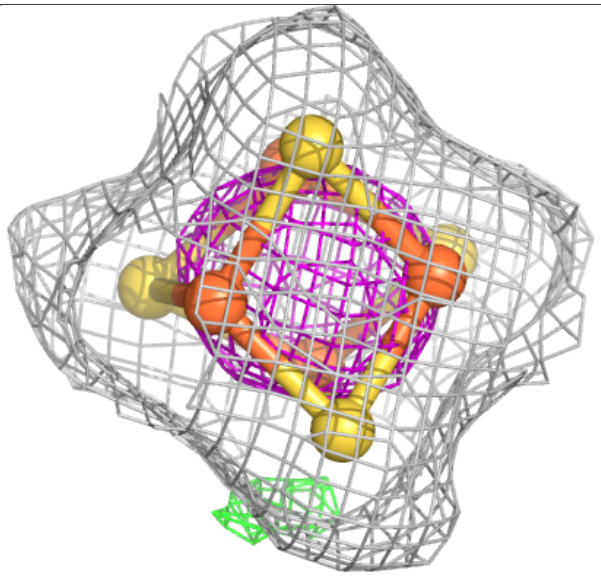


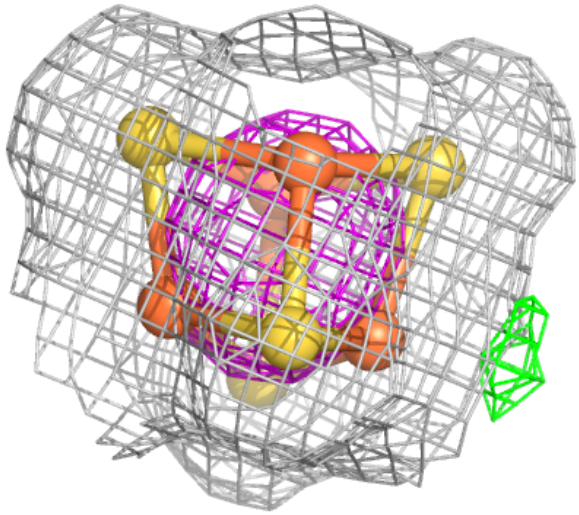


Electron density around SF4 A 1102:

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

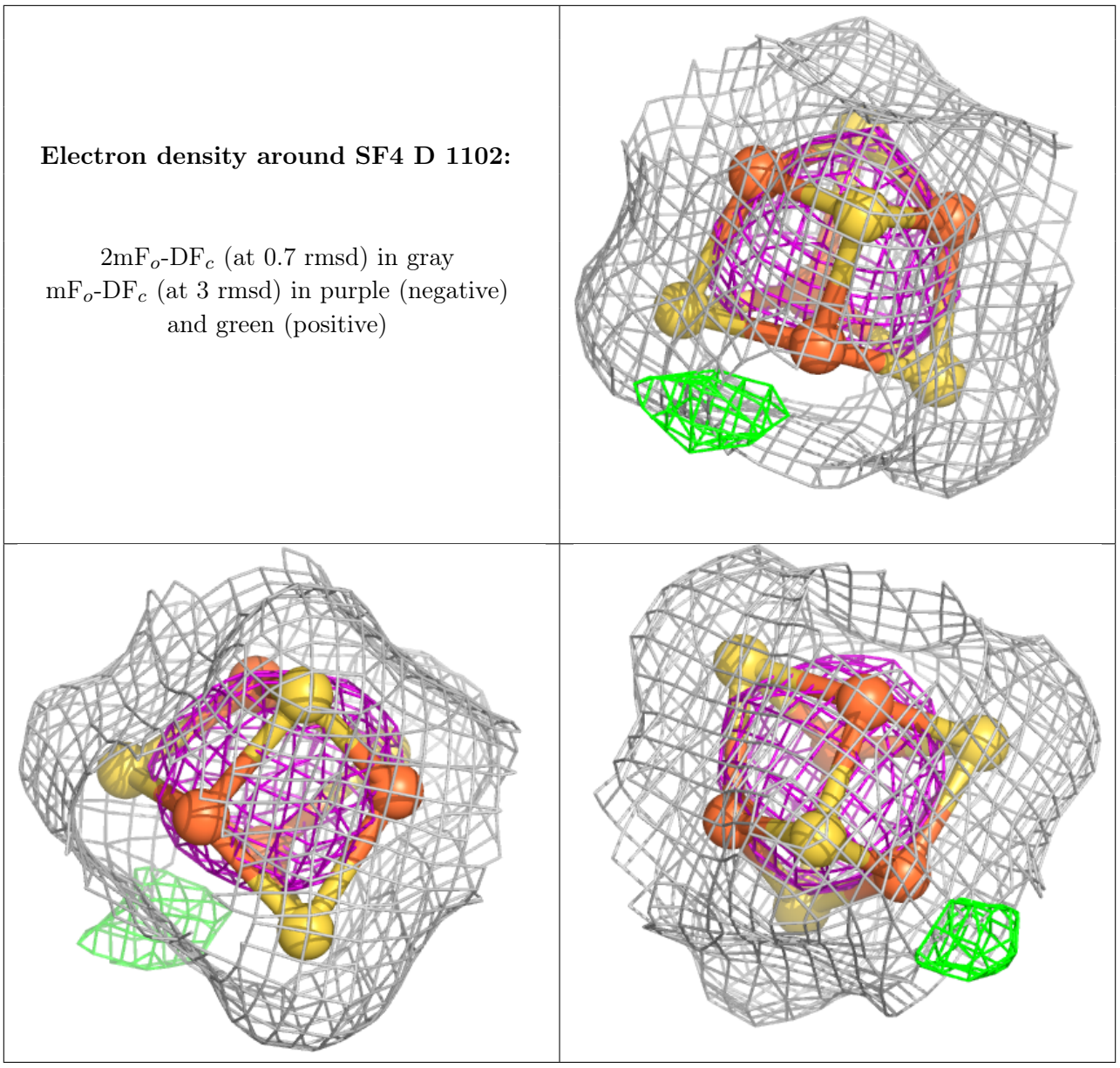






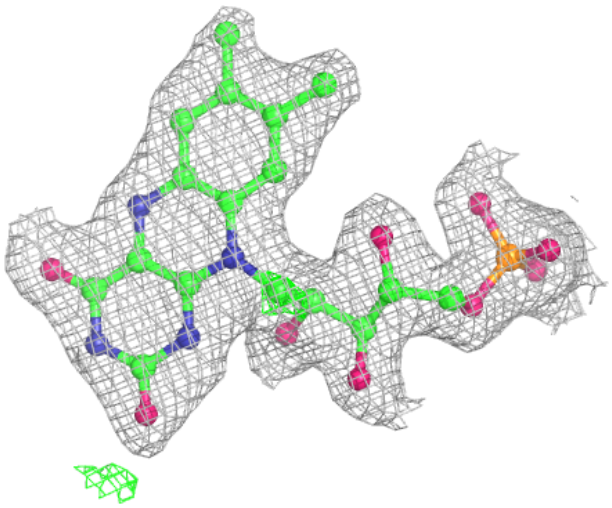
Electron density around SF4 D 1102:

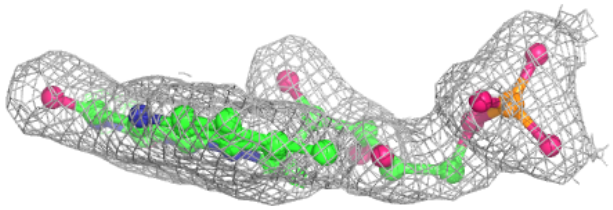
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

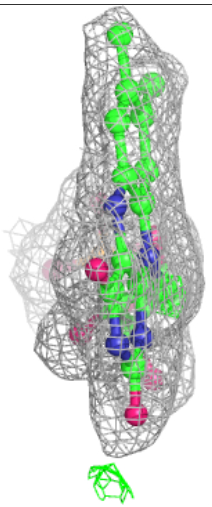


Electron density around FMN C 1105:

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

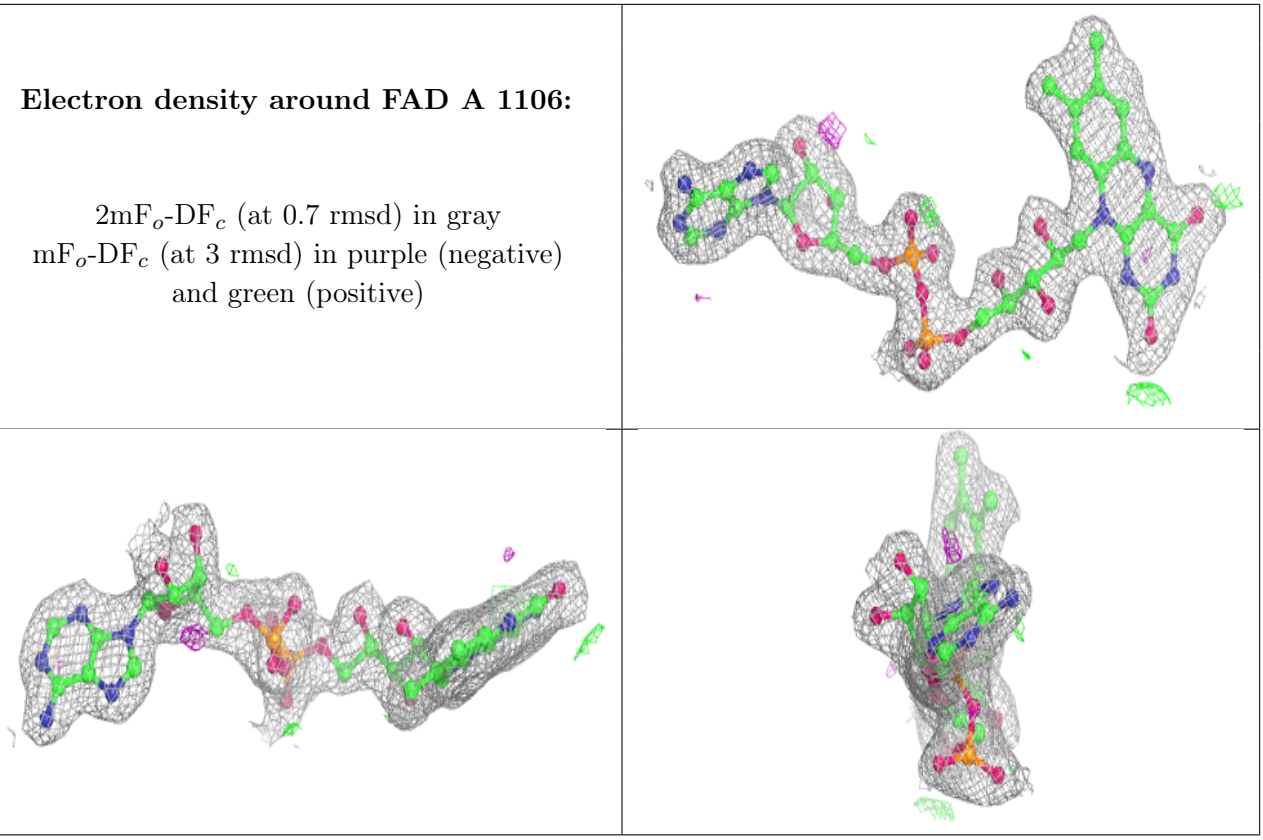






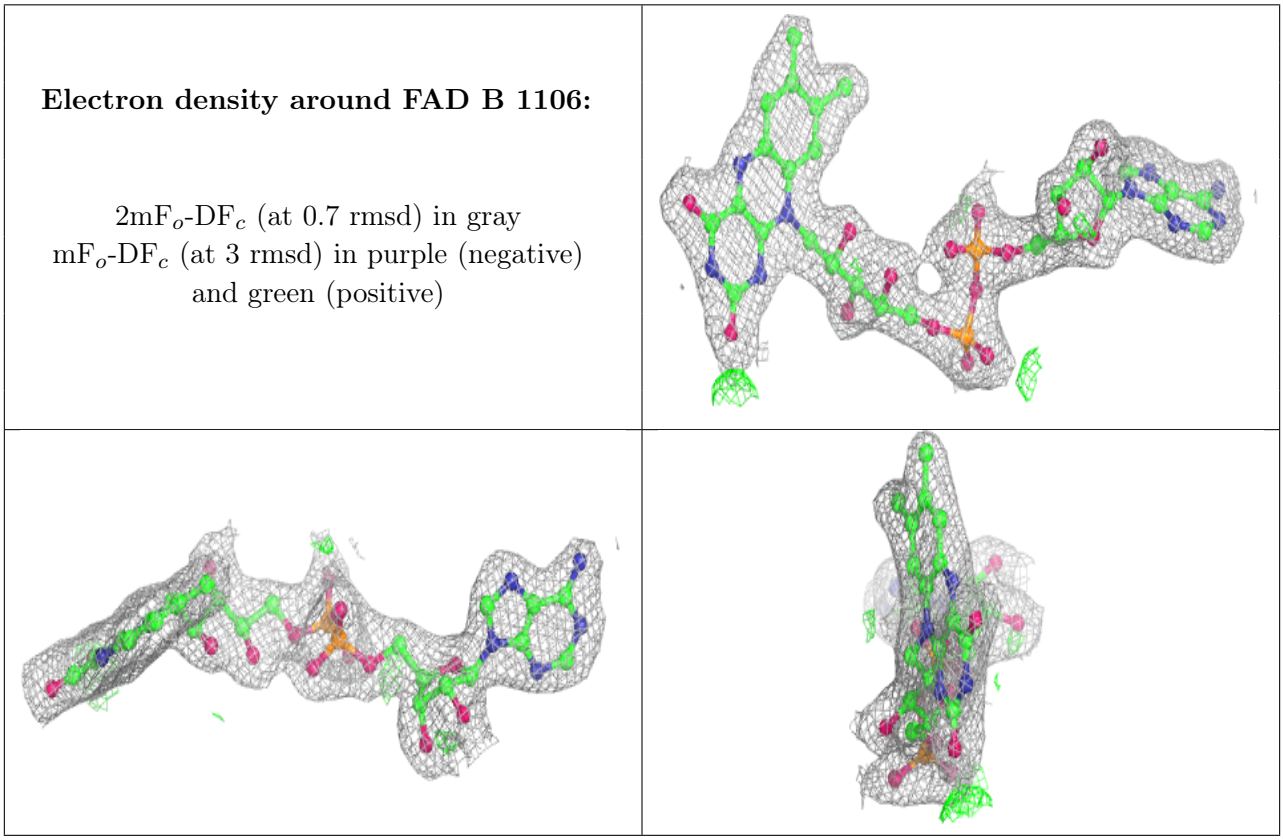
Electron density around FAD A 1106:

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



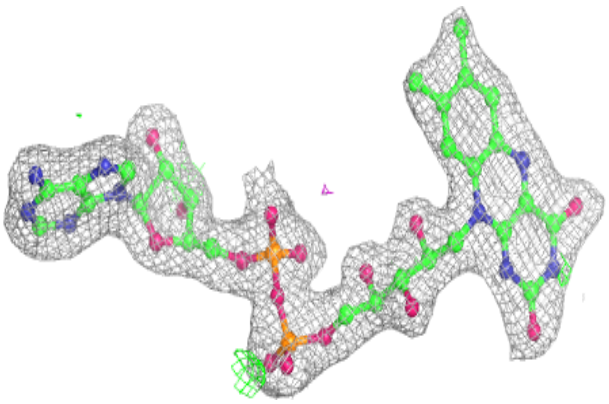
Electron density around FAD B 1106:

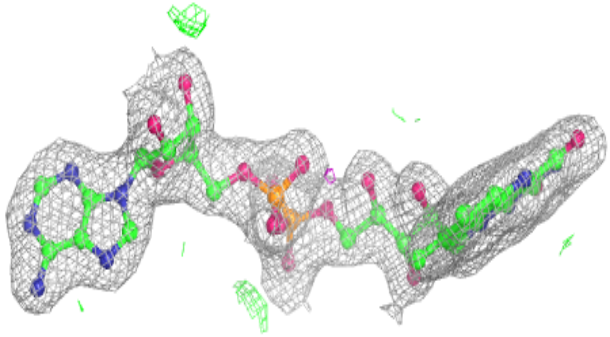
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

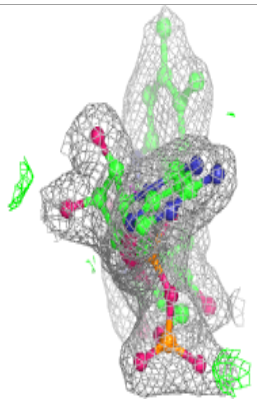


Electron density around FAD C 1106:

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

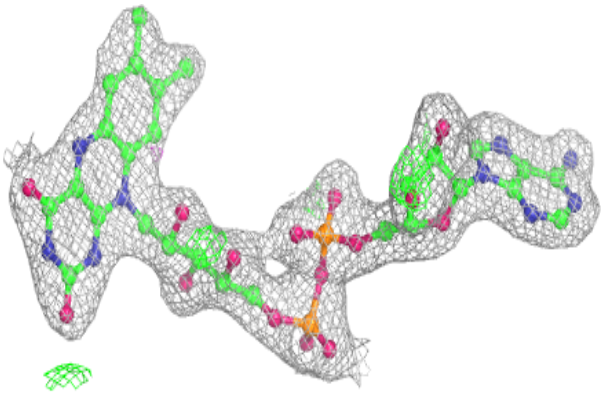


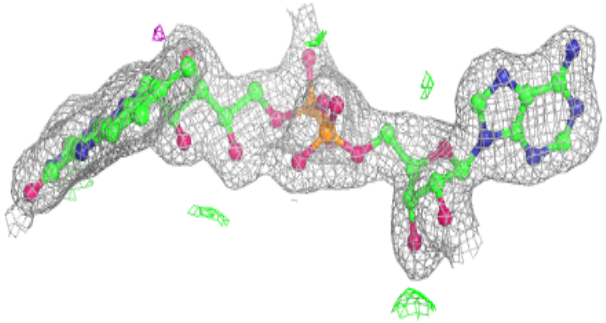


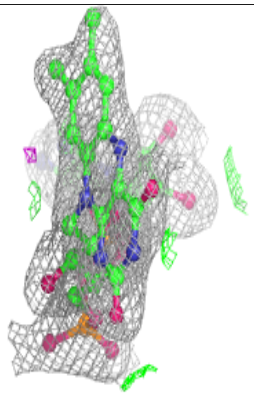


Electron density around FAD D 1106:

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

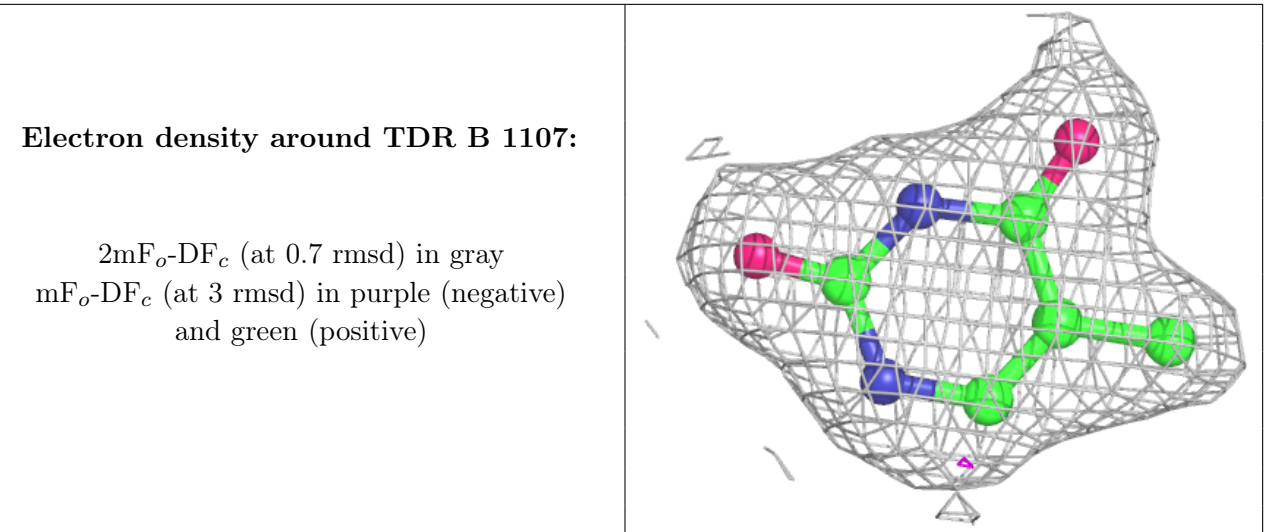


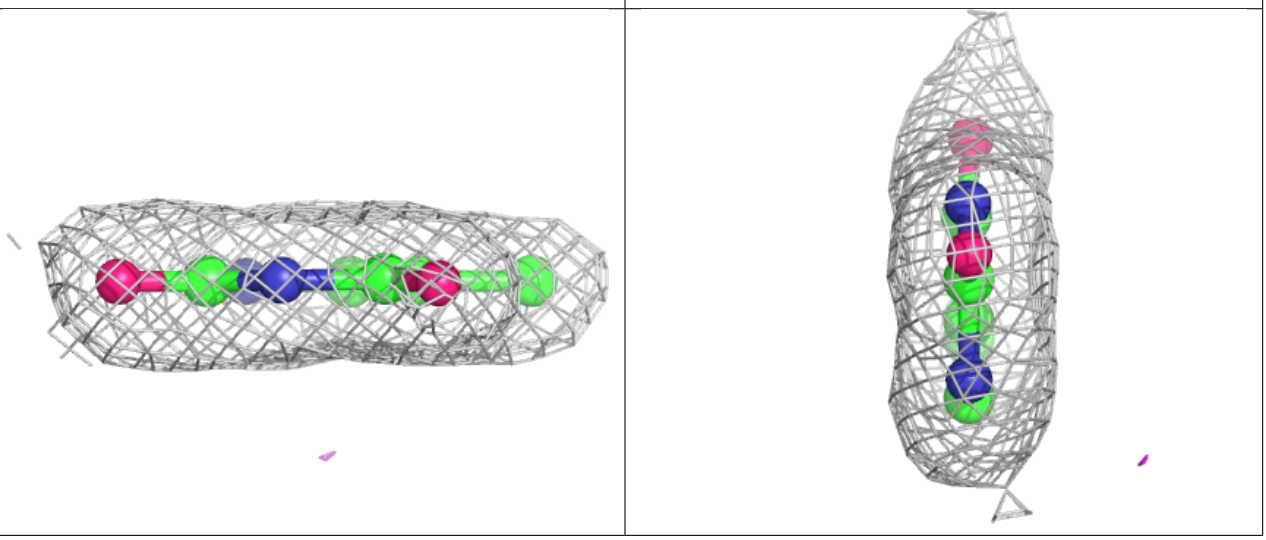




Electron density around TDR B 1107:

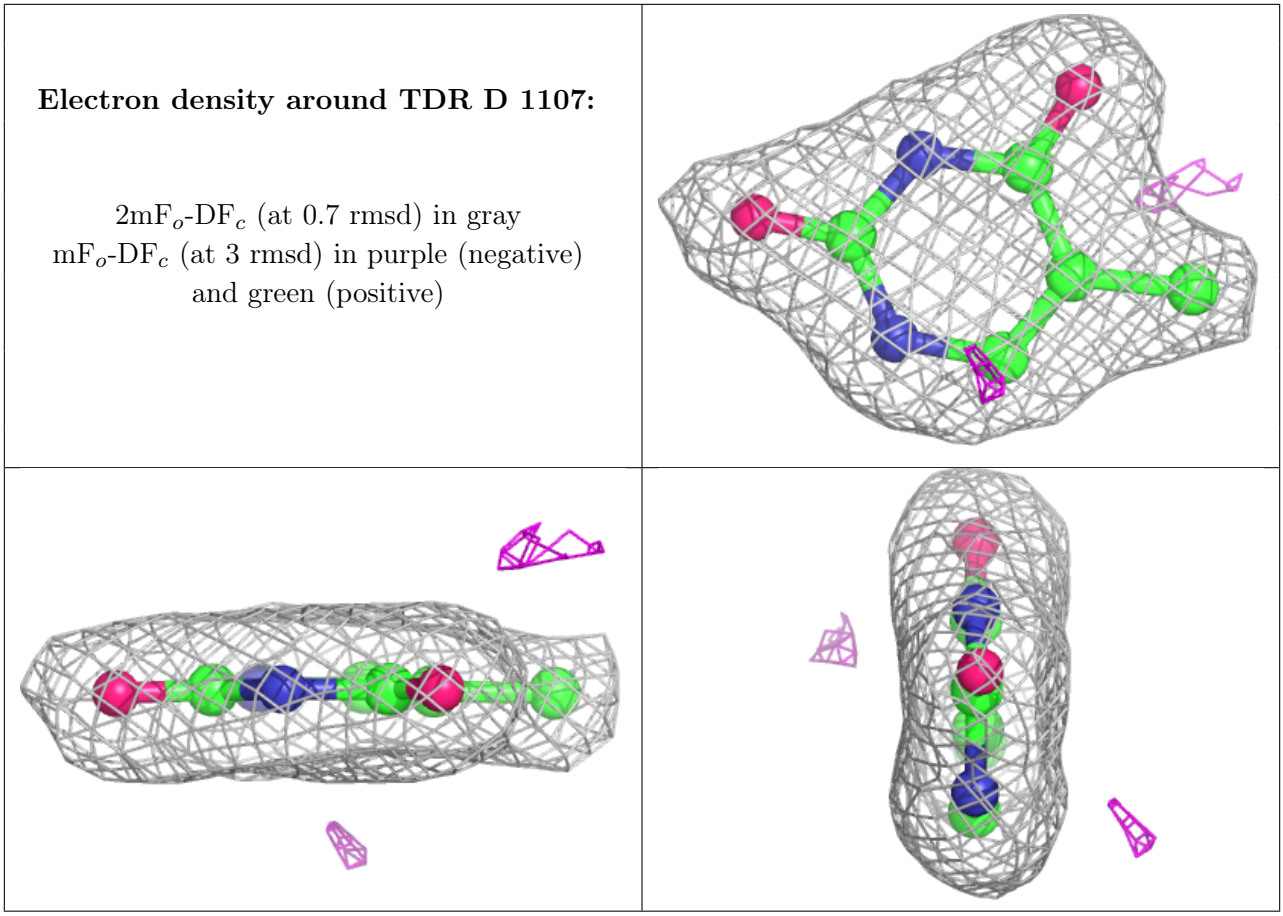
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





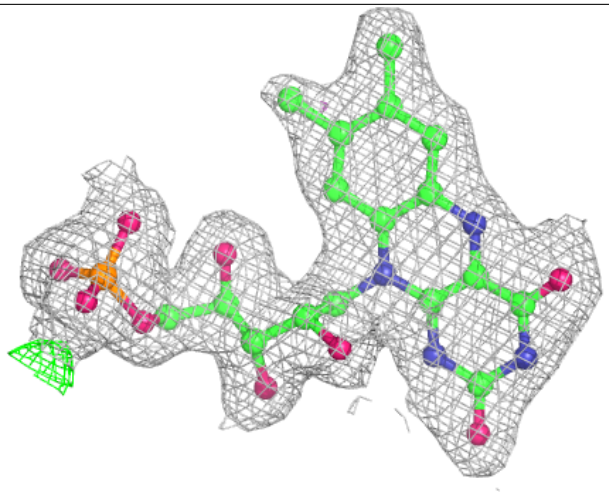
Electron density around TDR D 1107:

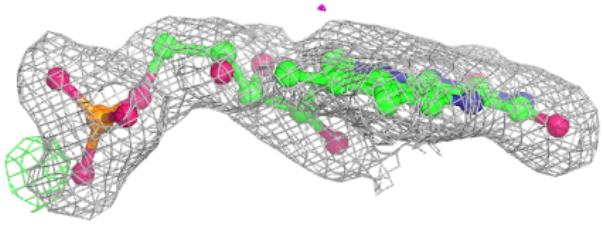
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

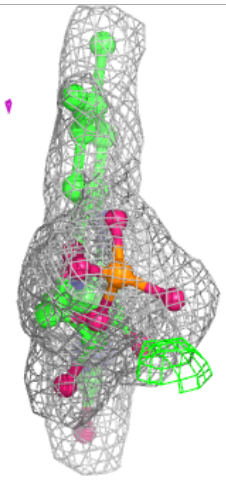


Electron density around FMN B 1105:

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

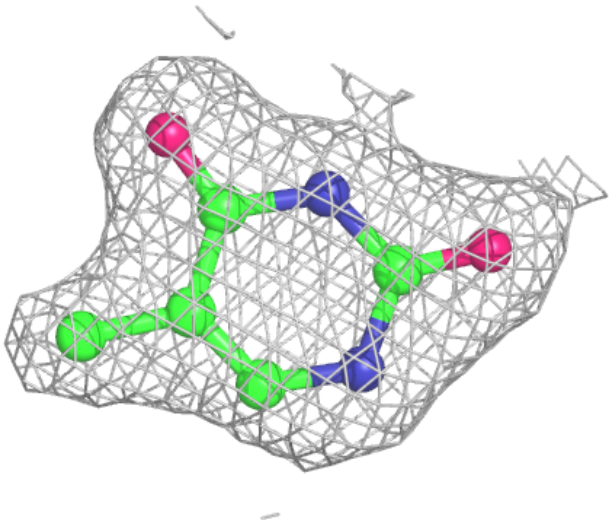


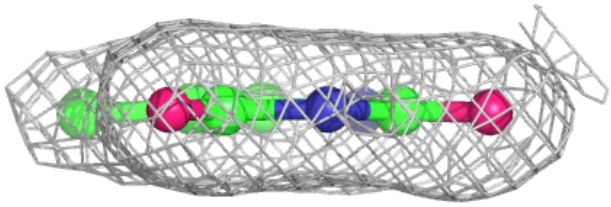


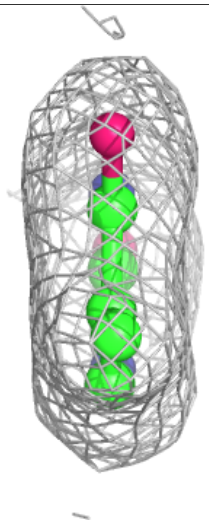


Electron density around TDR A 1107:

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

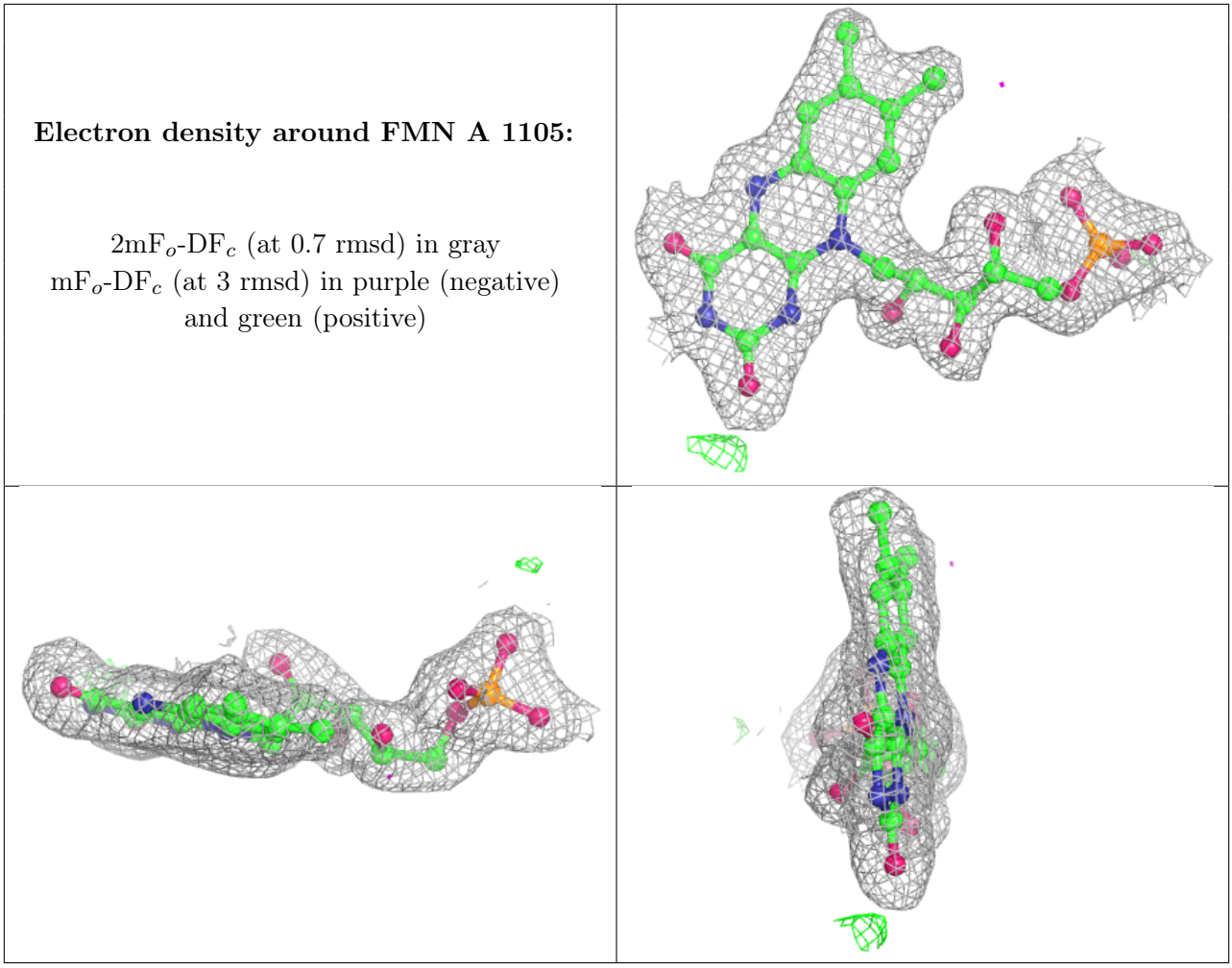






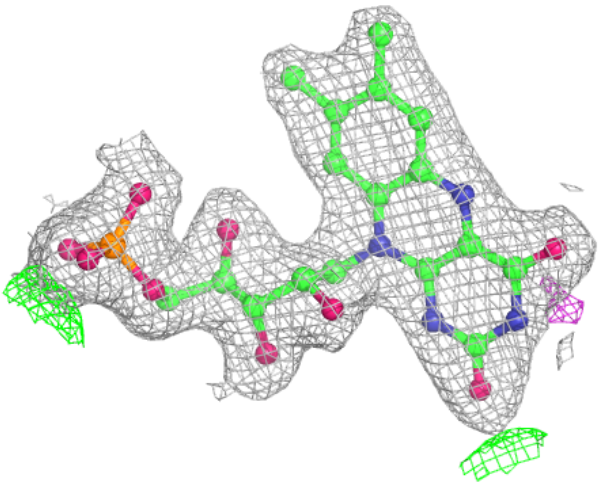
Electron density around FMN A 1105:

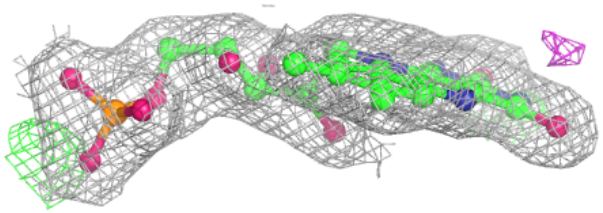
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

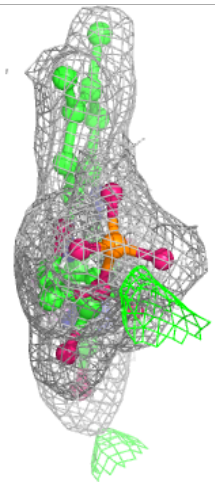


Electron density around FMN D 1105:

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

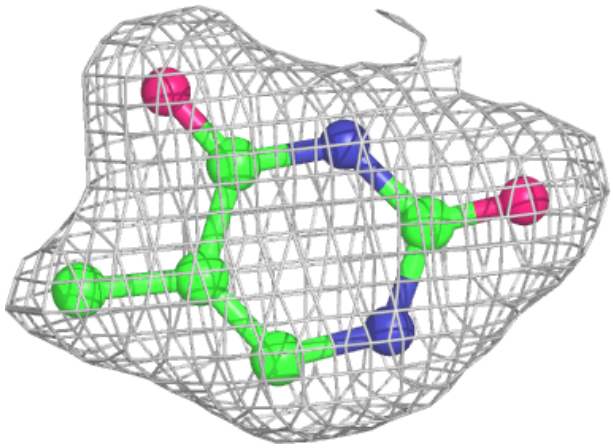


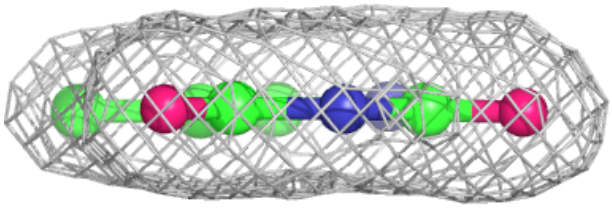


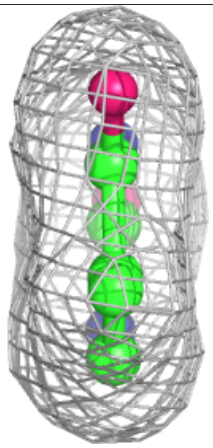


Electron density around TDR C 1107:

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







6.5 Other polymers

There are no such residues in this entry.