Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 07:29 AM EDT

PDB ID	:	7M32
Title	:	Dihydropyrimidine Dehydrogenase (DPD) C671A Mutant Soaked with Uracil and NADPH Anaerobically
Authors	:	Butrin, A.; Beaupre, B.; Forouzesh, D.; Liu, D.; Moran, G.
Deposited on	:	2021-03-18
Resolution	:	1.82 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

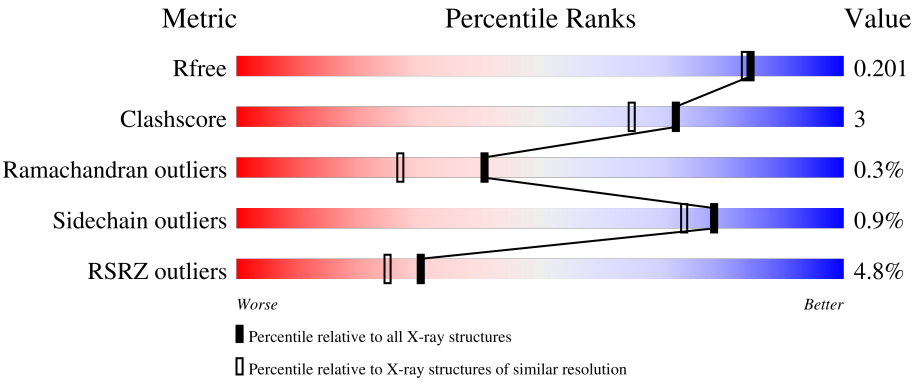
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	5% 91% 8% ·
1	B	1025	5% 91% 8% ·
1	C	1025	5% 91% 7% ·
1	D	1025	4% 90% 8% ·

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	URA	A	1106	-	X	-	-
4	URA	B	1107	-	X	-	-
4	URA	C	1107	-	X	-	-
4	URA	D	1108	-	X	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 33840 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.

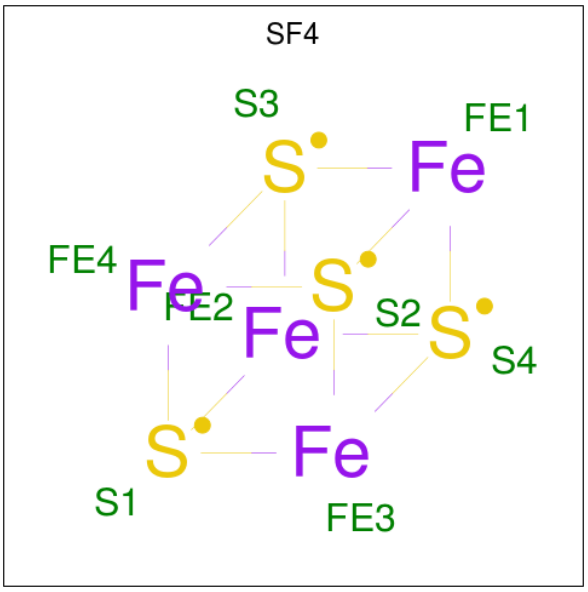
- Molecule 1 is a protein called Dihydropyrimidine dehydrogenase [NADP(+)].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	30	0	0
			7639	4855	1284	1447	53			
1	B	1010	Total	C	N	O	S	30	0	0
			7689	4882	1300	1453	54			
1	C	1007	Total	C	N	O	S	0	2	0
			7659	4862	1296	1450	51			
1	D	1012	Total	C	N	O	S	30	1	0
			7694	4886	1304	1451	53			

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	ALA	CYS	engineered mutation	UNP Q28943
B	60	ASP	GLY	conflict	UNP Q28943
B	671	ALA	CYS	engineered mutation	UNP Q28943
C	60	ASP	GLY	conflict	UNP Q28943
C	671	ALA	CYS	engineered mutation	UNP Q28943
D	60	ASP	GLY	conflict	UNP Q28943
D	671	ALA	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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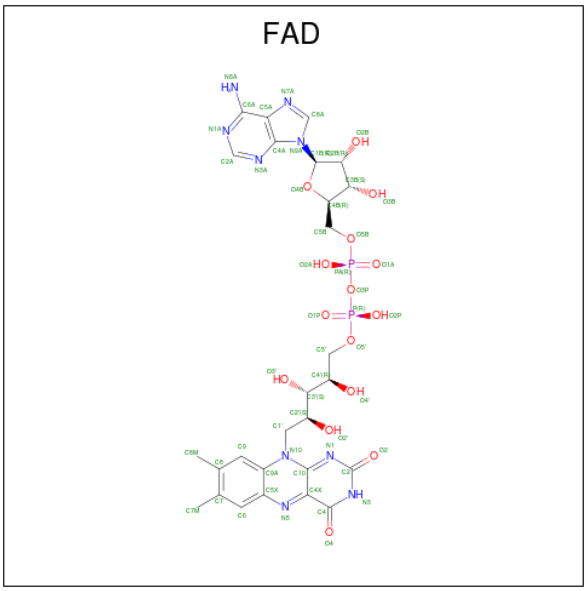
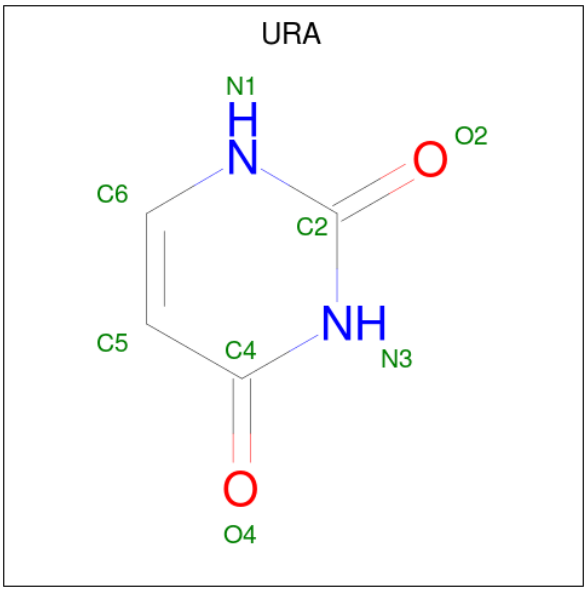
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0

- 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).



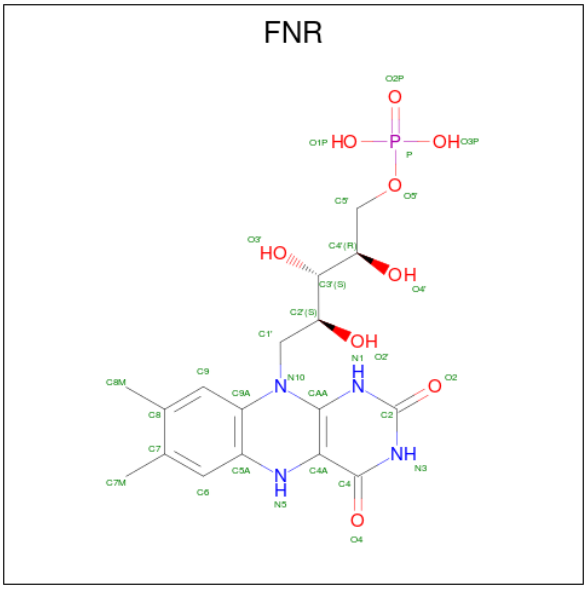
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 53 27 9 15 2	0	0
3	B	1	Total C N O P 53 27 9 15 2	0	0
3	C	1	Total C N O P 53 27 9 15 2	0	0
3	D	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 4 is URACIL (three-letter code: URA) (formula: $C_4H_4N_2O_2$) (labeled as "Ligand of Interest" by depositor).



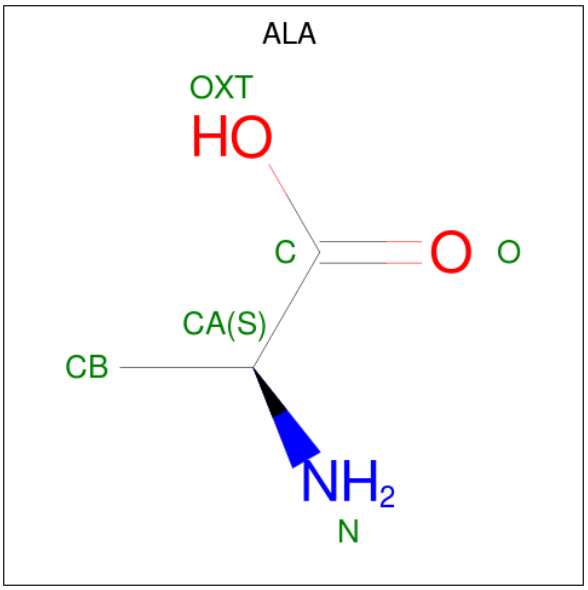
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 8 4 2 2	0	0
4	B	1	Total C N O 8 4 2 2	0	0
4	C	1	Total C N O 8 4 2 2	0	0
4	D	1	Total C N O 8 4 2 2	0	0

- Molecule 5 is 1-DEOXY-1-(7,8-DIMETHYL-2,4-DIOXO-3,4-DIHYDRO-2H-BENZO[G]PTERIDIN-1-ID-10(5H)-YL)-5-O-PHOSPHONATO-D-RIBITOL (three-letter code: FNR) (formula: $C_{17}H_{23}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



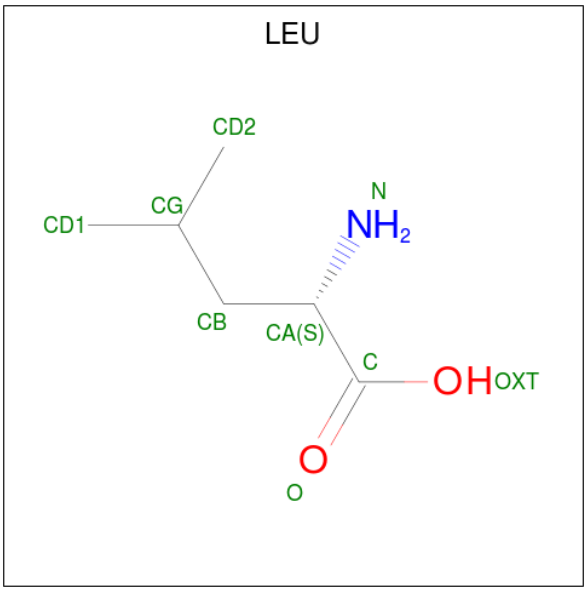
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
5	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
5	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
5	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 6 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$) (labeled as "Ligand of Interest" by depositor).



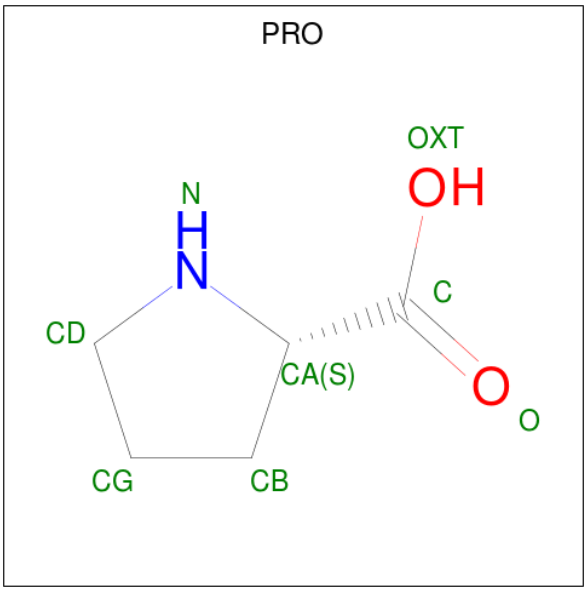
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			5	3	1	1		
6	D	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 7 is LEUCINE (three-letter code: LEU) (formula: $C_6H_{13}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O 8 6 1 1	0	0
7	D	1	Total C N O 8 6 1 1	0	0

- Molecule 8 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is water.

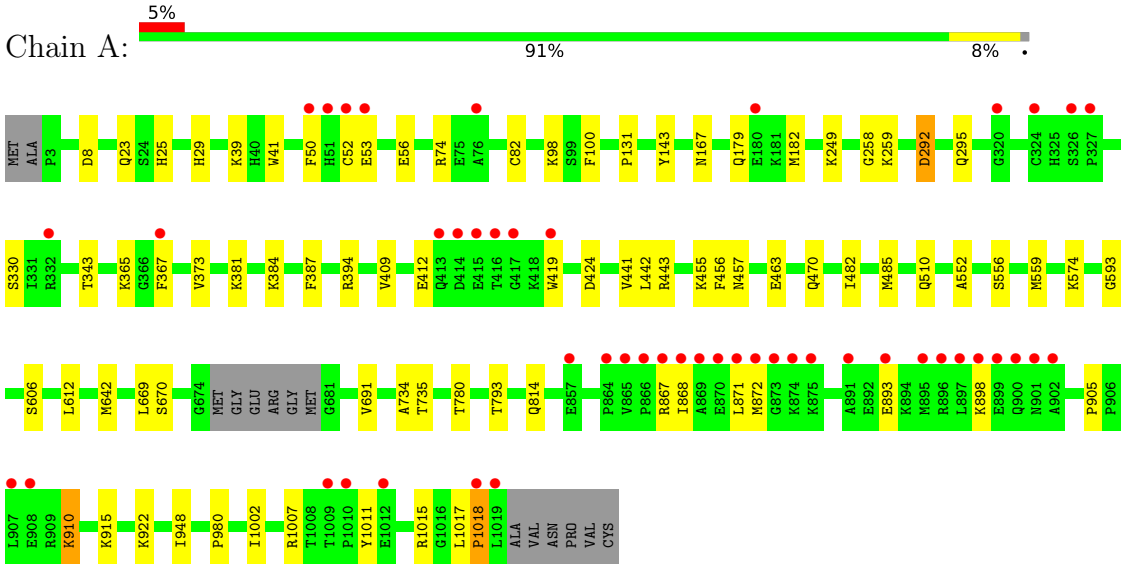
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	676	Total O 676 676	0	0
9	B	606	Total O 606 606	0	0
9	C	688	Total O 688 688	0	0
9	D	660	Total O 660 660	0	0

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.

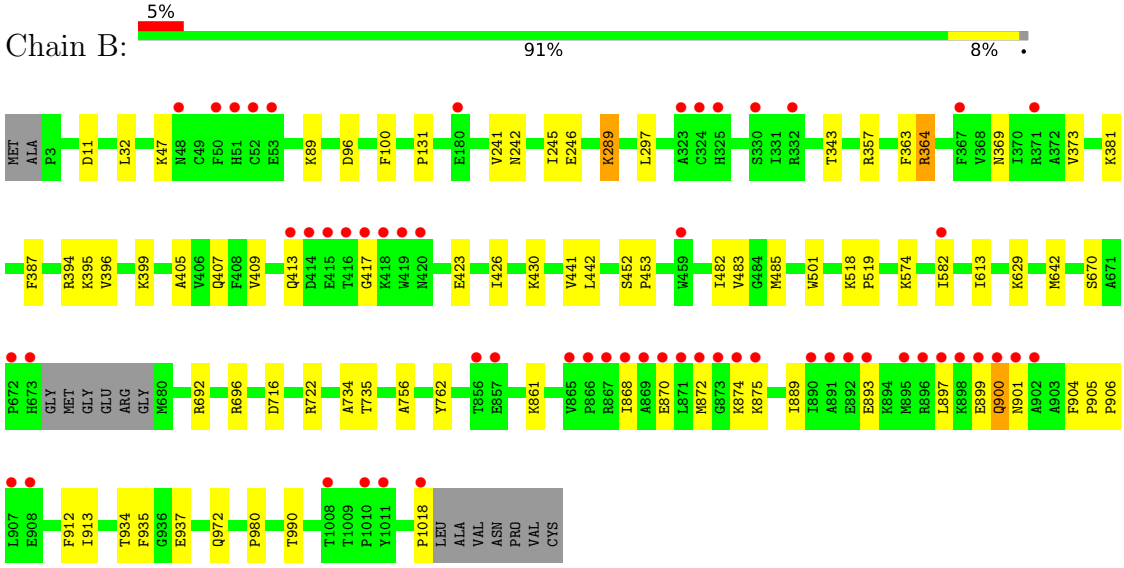
• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]

Chain A:



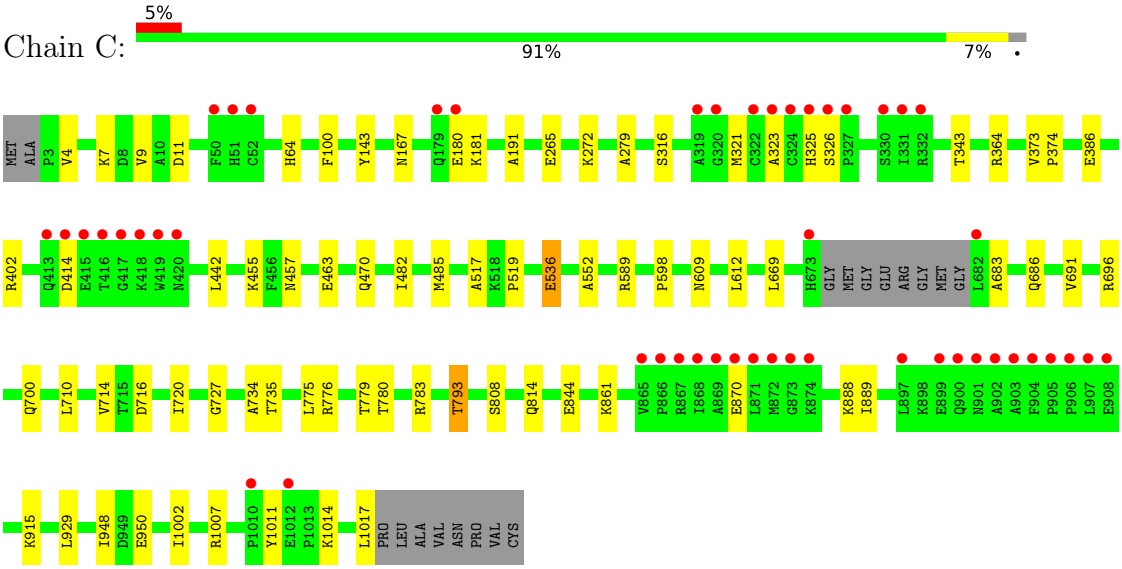
• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]

Chain B:



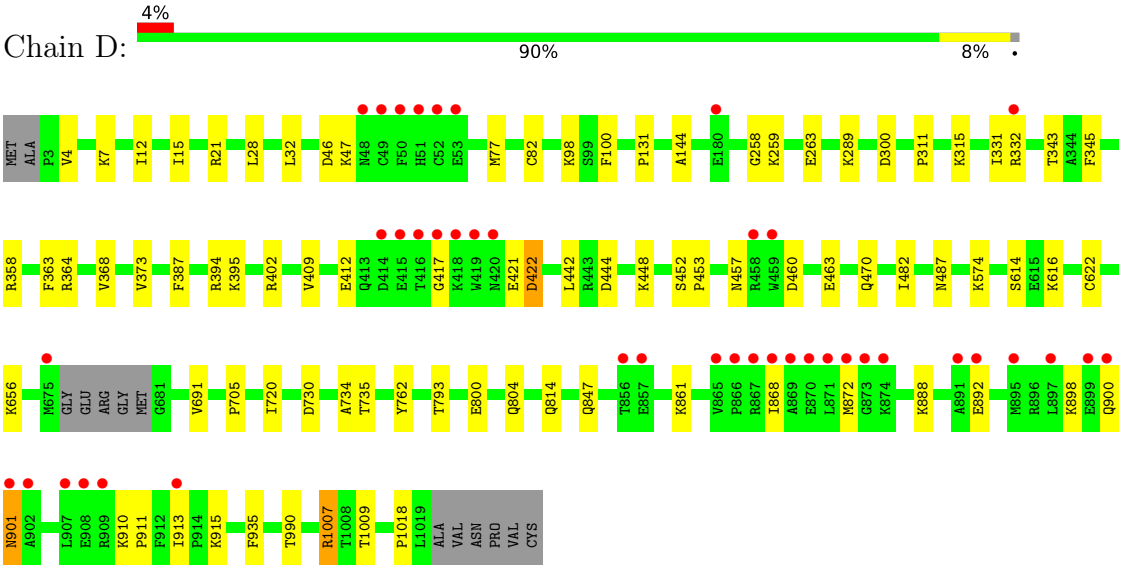
• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]

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	81.87Å 158.73Å 162.70Å 90.00° 95.89° 90.00°	Depositor
Resolution (Å)	47.26 – 1.82 51.69 – 1.82	Depositor EDS
% Data completeness (in resolution range)	96.3 (47.26-1.82) 96.3 (51.69-1.82)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.169 , 0.202 0.168 , 0.201	Depositor DCC
R_{free} test set	17915 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	33840	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: SF4, URA, FAD, FNR

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	0.36	0/7798	0.57	0/10580
1	B	0.35	0/7849	0.57	1/10641 (0.0%)
1	C	0.36	0/7819	0.71	4/10602 (0.0%)
1	D	0.35	0/7854	0.86	3/10650 (0.0%)
All	All	0.35	0/31320	0.69	8/42473 (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	C	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	422	ASP	CB-CG-OD1	45.13	158.92	118.30
1	D	422	ASP	CB-CG-OD2	-40.92	81.47	118.30
1	C	536	GLU	OE1-CD-OE2	-29.43	87.98	123.30
1	D	422	ASP	OD1-CG-OD2	-22.94	79.72	123.30
1	C	536	GLU	CG-CD-OE1	19.02	156.35	118.30
1	C	536	GLU	CG-CD-OE2	-15.15	87.99	118.30
1	C	517	ALA	C-N-CA	-7.23	103.63	121.70
1	B	1018	PRO	CA-N-CD	-6.22	102.78	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	536	GLU	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	7639	0	7622	68	0
1	B	7689	0	7714	60	0
1	C	7659	0	7666	49	0
1	D	7694	0	7709	54	0
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	1	0
4	A	8	0	3	0	0
4	B	8	0	3	0	0
4	C	8	0	3	0	0
4	D	8	0	3	0	0
5	A	31	0	22	3	0
5	B	31	0	21	2	0
5	C	31	0	21	1	0
5	D	31	0	21	1	0
6	A	5	0	4	2	0
6	D	5	0	4	1	0
7	B	8	0	10	0	0
7	D	8	0	10	0	0
8	C	7	0	7	1	0
9	A	676	0	0	18	0
9	B	606	0	0	9	1
9	C	688	0	0	8	1
9	D	660	0	0	10	2
All	All	33840	0	30967	213	2

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 3.

All (213) 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:B:357:ARG:NH2	9:B:1201:HOH:O	1.84	1.09
1:A:52:CYS:SG	9:A:1753:HOH:O	2.24	0.93
1:A:898:LYS:NZ	9:A:1202:HOH:O	2.03	0.92
1:D:402:ARG:NH2	9:D:1201:HOH:O	2.09	0.85
1:B:394:ARG:NH2	1:B:423:GLU:OE2	2.09	0.85
1:B:716:ASP:OD1	9:B:1202:HOH:O	1.94	0.84
1:B:874:LYS:NZ	9:B:1203:HOH:O	2.15	0.80
1:B:574:LYS:HZ2	5:B:1108:FNR:H5	1.33	0.76
1:C:870:GLU:HG3	1:C:889:ILE:HD13	1.65	0.76
1:D:7:LYS:NZ	9:D:1205:HOH:O	2.18	0.74
1:C:716:ASP:OD1	9:C:1201:HOH:O	2.04	0.74
1:D:343:THR:HA	3:D:1107:FAD:HM73	1.68	0.74
1:B:343:THR:HA	3:B:1106:FAD:HM73	1.70	0.73
1:B:289:LYS:HD3	1:B:441:VAL:HG21	1.71	0.73
1:C:950:GLU:OE2	9:C:1202:HOH:O	2.06	0.71
1:A:868:ILE:HG12	1:A:893:GLU:OE1	1.90	0.70
1:B:868:ILE:HG21	1:B:893:GLU:HG3	1.73	0.70
1:A:793:THR:HG22	1:A:814:GLN:HB2	1.74	0.69
1:C:343:THR:HA	3:C:1106:FAD:HM73	1.74	0.68
1:D:394:ARG:NH2	1:D:421:GLU:OE1	2.27	0.68
1:A:868:ILE:HD12	1:A:871:LEU:HD22	1.76	0.66
1:A:470:GLN:OE1	9:A:1203:HOH:O	2.12	0.66
1:C:265:GLU:OE1	9:C:1203:HOH:O	2.14	0.66
1:D:915:LYS:HG2	9:D:1202:HOH:O	1.95	0.66
1:D:913:ILE:O	9:D:1202:HOH:O	2.14	0.66
1:C:844:GLU:HG3	1:C:915:LYS:HG3	1.78	0.65
1:D:793:THR:HG22	1:D:814:GLN:HB2	1.78	0.65
1:B:297:LEU:HD11	1:B:396:VAL:HG11	1.79	0.65
1:C:485:MET:HE3	1:D:32:LEU:HB2	1.79	0.65
1:A:343:THR:HA	3:A:1105:FAD:HM73	1.80	0.64
1:D:898:LYS:NZ	9:D:1210:HOH:O	2.29	0.64
1:C:180:GLU:HG3	1:C:181:LYS:HG3	1.80	0.64
1:A:23:GLN:HB2	9:A:1818:HOH:O	1.99	0.63
1:D:470:GLN:OE1	9:D:1203:HOH:O	2.15	0.63
1:A:1017:LEU:HB3	1:A:1018:PRO:HD2	1.79	0.63
1:A:556:SER:O	1:A:559:MET:HB2	1.98	0.63
1:D:46:ASP:OD2	9:D:1204:HOH:O	2.15	0.62
1:A:56:GLU:OE2	1:A:898:LYS:NZ	2.33	0.62
1:A:52:CYS:HB3	1:A:384:LYS:HB2	1.82	0.61
1:C:316:SER:OG	1:C:326:SER:O	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:MET:SD	9:C:1846:HOH:O	2.56	0.61
1:C:844:GLU:CG	1:C:915:LYS:HG3	2.29	0.61
1:A:249:LYS:NZ	9:A:1212:HOH:O	2.30	0.60
1:D:442:LEU:HD22	1:D:482:ILE:HD11	1.82	0.60
1:D:448:LYS:NZ	1:D:460:ASP:OD1	2.31	0.60
1:A:442:LEU:HD22	1:A:482:ILE:HD11	1.81	0.60
1:C:776:ARG:O	1:C:780:THR:HG23	2.01	0.60
1:D:394:ARG:HG3	1:D:409:VAL:HG13	1.85	0.58
1:A:131:PRO:HB2	1:A:373:VAL:HG11	1.84	0.58
1:B:430:LYS:NZ	9:B:1214:HOH:O	2.36	0.58
1:B:399:LYS:HE2	9:B:1719:HOH:O	2.04	0.57
1:B:405:ALA:HB2	1:B:430:LYS:HD2	1.86	0.57
1:B:483:VAL:HG12	1:B:485:MET:HG3	1.85	0.57
1:B:900:GLN:OE1	1:B:900:GLN:N	2.37	0.57
1:B:131:PRO:HB2	1:B:373:VAL:HG11	1.85	0.57
1:A:915:LYS:HG2	9:A:1399:HOH:O	2.03	0.56
1:B:574:LYS:NZ	5:B:1108:FNR:H5	2.02	0.56
1:B:868:ILE:O	1:B:872:MET:HG3	2.06	0.56
1:B:696:ARG:HH11	1:B:696:ARG:HG2	1.71	0.56
1:D:800:GLU:OE1	1:D:804:GLN:NE2	2.38	0.56
1:B:692:ARG:O	1:B:696:ARG:HG3	2.06	0.56
6:A:1108:ALA:N	9:A:1220:HOH:O	2.38	0.56
1:A:50:PHE:HD2	1:B:369:ASN:HD22	1.55	0.55
1:C:143:TYR:O	1:D:861:LYS:HE2	2.04	0.55
1:D:847:GLN:HG3	9:D:1502:HOH:O	2.06	0.55
1:B:364:ARG:NH2	9:B:1215:HOH:O	2.40	0.55
1:C:793:THR:HB	1:C:814:GLN:HB2	1.89	0.55
1:D:910:LYS:HE2	1:D:911:PRO:HD2	1.88	0.54
1:A:258:GLY:C	1:A:259:LYS:HD2	2.28	0.54
1:C:373:VAL:HG22	1:C:374:PRO:HD2	1.88	0.54
1:D:412:GLU:HG2	1:D:422:ASP:OD1	2.08	0.53
1:A:457:ASN:HB3	1:A:463:GLU:HG2	1.91	0.53
1:D:131:PRO:HB2	1:D:373:VAL:HG11	1.90	0.53
1:D:21:ARG:NH1	9:D:1220:HOH:O	2.41	0.53
1:A:552:ALA:HB2	5:A:1107:FNR:H7M3	1.90	0.53
1:A:23:GLN:CB	9:A:1818:HOH:O	2.57	0.52
1:A:365:LYS:HG2	1:A:419:TRP:CZ2	2.45	0.52
1:B:899:GLU:O	1:B:901:ASN:N	2.42	0.52
1:A:295:GLN:OE1	9:A:1204:HOH:O	2.18	0.52
1:C:373:VAL:HB	9:C:1308:HOH:O	2.09	0.51
1:A:510:GLN:HG2	9:A:1261:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:CYS:HB2	9:A:1248:HOH:O	2.10	0.51
1:D:4:VAL:HG11	1:D:7:LYS:HG3	1.91	0.51
1:D:258:GLY:O	1:D:259:LYS:HE2	2.11	0.51
1:A:29:HIS:HB2	9:B:1269:HOH:O	2.11	0.51
1:A:457:ASN:HB3	1:A:463:GLU:CG	2.41	0.51
1:B:889:ILE:O	1:B:893:GLU:HG2	2.11	0.51
1:C:552:ALA:HB2	5:C:1108:FNR:H7M3	1.93	0.51
1:A:23:GLN:NE2	1:B:96:ASP:OD2	2.42	0.50
1:C:457:ASN:HB3	1:C:463:GLU:CG	2.40	0.50
1:C:1007:ARG:HD3	1:C:1011:TYR:HB2	1.94	0.50
1:A:948:ILE:HD13	1:A:980:PRO:HG2	1.92	0.50
1:A:485:MET:SD	1:B:32:LEU:HD13	2.52	0.50
1:C:780:THR:HG22	1:D:762:TYR:CZ	2.46	0.50
1:C:686:GLN:HG2	1:C:714:VAL:HG12	1.93	0.50
1:B:241:VAL:O	1:B:245:ILE:HG12	2.12	0.49
1:B:413:GLN:HG2	1:B:417:GLY:HA2	1.93	0.49
1:C:323:ALA:O	9:C:1205:HOH:O	2.20	0.49
1:A:394:ARG:HG3	1:A:409:VAL:HG13	1.95	0.49
1:B:722:ARG:NH1	9:B:1219:HOH:O	2.42	0.49
1:A:367:PHE:HZ	1:A:387:PHE:HB2	1.76	0.49
1:A:41:TRP:CE2	1:B:89:LYS:HD2	2.49	0.48
1:B:893:GLU:O	1:B:897:LEU:N	2.44	0.48
1:A:179:GLN:HA	1:A:182:MET:HG2	1.96	0.48
1:B:692:ARG:NH2	9:B:1220:HOH:O	2.44	0.48
1:A:1015:ARG:NE	1:B:582:ILE:HD11	2.29	0.48
6:A:1108:ALA:HB2	1:B:756:ALA:HB2	1.96	0.48
1:C:669:LEU:HD13	1:C:691:VAL:HG22	1.96	0.48
1:C:612:LEU:HD11	1:D:935:PHE:CE2	2.49	0.48
1:A:868:ILE:HB	1:A:871:LEU:HB2	1.95	0.47
1:B:289:LYS:HA	1:B:289:LYS:HD2	1.44	0.47
1:A:167:ASN:ND2	1:A:910:LYS:O	2.47	0.47
1:A:948:ILE:HG12	1:A:1002:ILE:HG12	1.97	0.47
1:A:74:ARG:NH2	9:A:1222:HOH:O	2.41	0.47
1:B:409:VAL:HG12	1:B:426:ILE:CD1	2.45	0.47
1:B:242:ASN:O	1:B:246:GLU:HG3	2.15	0.46
1:A:259:LYS:HD2	1:A:259:LYS:N	2.30	0.46
1:B:642:MET:HE1	1:B:670:SER:HB2	1.96	0.46
1:C:1017:LEU:C	8:C:1101:PRO:N	2.69	0.46
1:D:457:ASN:HB3	1:D:463:GLU:HG3	1.97	0.46
1:D:574:LYS:HE3	5:D:1109:FNR:O4	2.16	0.46
1:A:82:CYS:O	1:A:98:LYS:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:912:PHE:C	1:B:913:ILE:HD13	2.36	0.46
1:A:292:ASP:OD2	1:A:292:ASP:N	2.49	0.45
1:C:844:GLU:OE1	1:C:915:LYS:HE3	2.16	0.45
1:D:691:VAL:HG21	1:D:720:ILE:HG23	1.98	0.45
1:D:868:ILE:O	1:D:872:MET:HG3	2.16	0.45
1:D:900:GLN:CD	1:D:901:ASN:H	2.20	0.45
1:A:424:ASP:OD1	1:A:424:ASP:N	2.46	0.45
1:B:868:ILE:HD13	1:B:893:GLU:HG3	1.98	0.45
1:A:373:VAL:HG12	1:B:47:LYS:HD3	1.97	0.45
1:D:622:CYS:SG	1:D:656:LYS:HG2	2.56	0.45
1:A:669:LEU:HD13	1:A:691:VAL:HG22	1.99	0.45
1:C:191:ALA:O	1:C:279:ALA:HA	2.17	0.45
1:A:441:VAL:HG21	1:A:443:ARG:HH21	1.80	0.45
1:B:381:LYS:HD2	1:B:387:PHE:HE1	1.80	0.45
1:B:934:THR:OG1	1:B:937:GLU:HG3	2.17	0.45
1:C:9:VAL:HG23	1:C:11:ASP:OD2	2.16	0.45
1:C:696:ARG:HG3	1:C:727:GLY:HA2	1.99	0.44
9:A:1220:HOH:O	6:D:1102:ALA:HB1	2.17	0.44
1:B:734:ALA:HA	1:B:735:THR:HA	1.73	0.44
1:D:888:LYS:HE2	1:D:888:LYS:HB2	1.63	0.44
1:D:910:LYS:HD3	1:D:910:LYS:C	2.38	0.44
1:A:642:MET:CE	1:A:670:SER:HB2	2.48	0.44
1:D:734:ALA:HA	1:D:735:THR:HA	1.66	0.44
1:A:574:LYS:NZ	5:A:1107:FNR:H5	2.15	0.44
1:C:779:THR:HG22	1:C:808:SER:HB3	2.00	0.44
1:C:272:LYS:HB2	1:C:272:LYS:HE3	1.91	0.43
1:B:870:GLU:OE1	1:B:870:GLU:N	2.49	0.43
1:A:734:ALA:HA	1:A:735:THR:HA	1.72	0.43
1:D:345:PHE:HE1	1:D:387:PHE:HE1	1.66	0.43
1:B:696:ARG:HH11	1:B:696:ARG:CG	2.31	0.43
1:D:1007[B]:ARG:NH1	1:D:1009:THR:OG1	2.51	0.43
1:C:948:ILE:HG12	1:C:1002:ILE:HG12	2.00	0.43
1:A:179:GLN:HA	1:A:182:MET:CG	2.49	0.43
1:B:381:LYS:HD2	1:B:387:PHE:CE1	2.54	0.43
1:C:783:ARG:HG3	1:C:929:LEU:HD22	2.01	0.43
1:D:82:CYS:O	1:D:98:LYS:HD2	2.19	0.43
1:D:331:ILE:O	1:D:332:ARG:HD3	2.19	0.43
1:A:50:PHE:HD2	1:B:369:ASN:ND2	2.16	0.42
1:A:412:GLU:O	1:A:419:TRP:HA	2.18	0.42
1:C:442:LEU:HD22	1:C:482:ILE:HD11	2.00	0.42
1:C:710:LEU:HD22	1:C:720:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:PRO:O	1:D:315:LYS:HG3	2.19	0.42
1:D:990:THR:O	1:D:990:THR:HG22	2.19	0.42
1:A:867:ARG:HA	1:A:872:MET:HE3	2.01	0.42
1:B:501:TRP:CZ2	1:B:519:PRO:HA	2.55	0.42
1:D:1018:PRO:O	9:D:1207:HOH:O	2.21	0.42
1:A:143:TYR:O	1:B:861:LYS:HE2	2.19	0.42
1:A:455:LYS:HD2	1:A:456:PHE:O	2.19	0.42
1:A:1007:ARG:HD3	1:A:1011:TYR:HB2	2.02	0.42
1:B:990:THR:HG22	1:B:990:THR:O	2.19	0.42
1:C:470:GLN:HG2	9:C:1266:HOH:O	2.20	0.42
1:C:589:ARG:O	1:C:609:ASN:HA	2.19	0.42
1:C:598:PRO:HD2	1:D:77:MET:SD	2.58	0.42
1:A:249:LYS:CE	9:A:1212:HOH:O	2.67	0.42
1:A:922:LYS:NZ	9:A:1246:HOH:O	2.53	0.42
1:D:12:ILE:HA	1:D:15:ILE:HG22	2.02	0.42
1:D:888:LYS:O	1:D:892:GLU:HB2	2.19	0.42
1:A:39:LYS:HA	1:A:39:LYS:HD3	1.82	0.42
1:B:289:LYS:HD3	1:B:441:VAL:CG2	2.47	0.42
1:A:574:LYS:HZ3	5:A:1107:FNR:H5	1.67	0.41
1:B:629:LYS:HD2	1:B:629:LYS:HA	1.90	0.41
1:A:735:THR:O	1:A:793:THR:OG1	2.38	0.41
1:A:593:GLY:HA3	1:A:606:SER:OG	2.20	0.41
1:A:670:SER:OG	9:A:1201:HOH:O	1.93	0.41
1:A:8:ASP:OD1	9:A:1206:HOH:O	2.22	0.41
1:A:381:LYS:HE2	1:A:381:LYS:HB3	1.68	0.41
1:B:442:LEU:HD22	1:B:482:ILE:HD11	2.00	0.41
1:B:501:TRP:CE2	1:B:519:PRO:HA	2.56	0.41
1:C:4:VAL:HG11	1:C:7:LYS:HG3	2.03	0.41
1:C:485:MET:CE	1:D:32:LEU:HB2	2.50	0.41
1:C:775:LEU:O	1:C:779:THR:HG23	2.21	0.41
1:B:452:SER:HA	1:B:453:PRO:HA	1.81	0.41
1:C:455:LYS:HE2	1:C:455:LYS:HA	2.03	0.41
1:C:457:ASN:HB3	1:C:463:GLU:HG2	2.02	0.41
1:C:861:LYS:HG3	1:D:144:ALA:O	2.20	0.41
1:B:875:LYS:O	1:B:875:LYS:CG	2.69	0.41
1:C:700:GLN:HG3	9:C:1712:HOH:O	2.20	0.41
1:C:1014:LYS:HD3	1:D:616:LYS:HE3	2.03	0.41
1:B:395:LYS:HG3	1:B:407:GLN:HB3	2.03	0.40
1:B:972:GLN:O	1:B:980:PRO:HA	2.21	0.40
1:D:452:SER:HA	1:D:453:PRO:HA	1.88	0.40
1:D:705:PRO:HA	1:D:730:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:THR:HG22	1:B:762:TYR:CZ	2.55	0.40
1:A:53:GLU:N	9:A:1248:HOH:O	2.54	0.40
1:D:574:LYS:HG3	1:D:614:SER:HB2	2.03	0.40
1:A:612:LEU:HD11	1:B:935:PHE:CE2	2.56	0.40
1:C:386:GLU:OE2	1:D:368:VAL:HG22	2.22	0.40
1:C:734:ALA:HA	1:C:735:THR:HA	1.77	0.40
1:C:519:PRO:HB3	1:D:28:LEU:HD22	2.03	0.40
1:D:444:ASP:O	1:D:448:LYS:HG3	2.21	0.40
1:D:735:THR:O	1:D:793:THR:OG1	2.39	0.40

All (2) 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)
9:C:1769:HOH:O	9:D:1800:HOH:O[2_555]	1.92	0.28
9:B:1321:HOH:O	9:D:1657:HOH:O[2_646]	2.10	0.10

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	1007/1025 (98%)	971 (96%)	34 (3%)	2 (0%)	47	33
1	B	1006/1025 (98%)	969 (96%)	32 (3%)	5 (0%)	29	15
1	C	1005/1025 (98%)	967 (96%)	34 (3%)	4 (0%)	34	21
1	D	1009/1025 (98%)	972 (96%)	35 (4%)	2 (0%)	47	33
All	All	4027/4100 (98%)	3879 (96%)	135 (3%)	13 (0%)	41	27

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	905	PRO
1	A	1018	PRO
1	B	905	PRO
1	C	414	ASP
1	B	900	GLN
1	C	683	ALA
1	D	417	GLY
1	C	325	HIS
1	C	321	MET
1	D	901	ASN
1	B	904	PHE
1	B	906	PRO
1	B	613	ILE

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	825/853 (97%)	820 (99%)	5 (1%)	86	83
1	B	838/853 (98%)	832 (99%)	6 (1%)	84	80
1	C	830/853 (97%)	823 (99%)	7 (1%)	81	77
1	D	835/853 (98%)	823 (99%)	12 (1%)	67	58
All	All	3328/3412 (98%)	3298 (99%)	30 (1%)	78	74

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

Mol	Chain	Res	Type
1	A	25	HIS
1	A	100	PHE
1	A	292	ASP
1	A	330	SER
1	A	910	LYS
1	B	11	ASP
1	B	100	PHE
1	B	289	LYS
1	B	363	PHE

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Mol	Chain	Res	Type
1	B	364	ARG
1	B	518	LYS
1	C	64	HIS
1	C	100	PHE
1	C	167	ASN
1	C	364	ARG
1	C	402	ARG
1	C	793	THR
1	C	888	LYS
1	D	47	LYS
1	D	100	PHE
1	D	263	GLU
1	D	289	LYS
1	D	300	ASP
1	D	358	ARG
1	D	363	PHE
1	D	364	ARG
1	D	395	LYS
1	D	487	ASN
1	D	1007[A]	ARG
1	D	1007[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	885	GLN
1	C	269	ASN
1	C	407	GLN
1	D	847	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	URA	C	1107	-	8,8,8	5.31	7 (87%)	9,10,10	3.26	5 (55%)
2	SF4	A	1103	1	0,12,12	-	-	-		
4	URA	A	1106	-	8,8,8	5.30	8 (100%)	9,10,10	3.39	6 (66%)
5	FNR	B	1108	-	32,33,33	3.55	15 (46%)	40,50,50	1.44	7 (17%)
7	LEU	B	1101	-	5,7,8	0.49	0	5,8,10	0.22	0
2	SF4	D	1106	1	0,12,12	-	-	-		
2	SF4	B	1105	1	0,12,12	-	-	-		
2	SF4	D	1104	1	0,12,12	-	-	-		
2	SF4	D	1103	1	0,12,12	-	-	-		
5	FNR	A	1107	-	32,33,33	3.53	14 (43%)	40,50,50	1.48	7 (17%)
2	SF4	C	1103	1	0,12,12	-	-	-		
2	SF4	D	1105	1	0,12,12	-	-	-		
3	FAD	C	1106	-	53,58,58	0.47	0	68,89,89	0.48	1 (1%)
6	ALA	D	1102	6	3,4,5	0.63	0	2,4,6	0.85	0
2	SF4	B	1104	1	0,12,12	-	-	-		
6	ALA	A	1108	6	3,4,5	0.62	0	2,4,6	0.84	0
8	PRO	C	1101	7	5,7,8	0.47	0	7,8,10	1.32	0
2	SF4	A	1102	1	0,12,12	-	-	-		
2	SF4	A	1101	1	0,12,12	-	-	-		
2	SF4	A	1104	1	0,12,12	-	-	-		
5	FNR	D	1109	-	32,33,33	3.52	14 (43%)	40,50,50	1.52	6 (15%)
3	FAD	B	1106	-	53,58,58	0.49	0	68,89,89	0.53	1 (1%)
2	SF4	C	1102	1	0,12,12	-	-	-		
2	SF4	C	1104	1	0,12,12	-	-	-		
7	LEU	D	1101	8	5,7,8	0.51	0	5,8,10	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	URA	D	1108	-	8,8,8	5.24	7 (87%)	9,10,10	3.29	5 (55%)
3	FAD	D	1107	-	53,58,58	0.47	0	68,89,89	0.51	1 (1%)
5	FNR	C	1108	-	32,33,33	3.57	14 (43%)	40,50,50	1.51	7 (17%)
3	FAD	A	1105	-	53,58,58	0.53	0	68,89,89	0.52	1 (1%)
2	SF4	B	1103	1	0,12,12	-	-	-		
2	SF4	B	1102	1	0,12,12	-	-	-		
4	URA	B	1107	-	8,8,8	5.36	7 (87%)	9,10,10	3.07	5 (55%)
2	SF4	C	1105	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	URA	C	1107	-	-	-	0/1/1/1
2	SF4	A	1103	1	-	-	0/6/5/5
5	FNR	B	1108	-	-	1/18/18/18	0/3/3/3
4	URA	A	1106	-	-	-	0/1/1/1
7	LEU	B	1101	-	-	2/5/6/8	-
2	SF4	D	1106	1	-	-	0/6/5/5
2	SF4	B	1105	1	-	-	0/6/5/5
2	SF4	D	1104	1	-	-	0/6/5/5
2	SF4	D	1103	1	-	-	0/6/5/5
5	FNR	A	1107	-	-	1/18/18/18	0/3/3/3
2	SF4	C	1103	1	-	-	0/6/5/5
2	SF4	D	1105	1	-	-	0/6/5/5
3	FAD	C	1106	-	-	2/30/50/50	0/6/6/6
6	ALA	D	1102	6	-	0/0/2/4	-
2	SF4	B	1104	1	-	-	0/6/5/5
6	ALA	A	1108	6	-	0/0/2/4	-
8	PRO	C	1101	7	-	0/0/9/11	0/1/1/1
2	SF4	A	1102	1	-	-	0/6/5/5
2	SF4	A	1101	1	-	-	0/6/5/5
2	SF4	A	1104	1	-	-	0/6/5/5
5	FNR	D	1109	-	-	1/18/18/18	0/3/3/3
3	FAD	B	1106	-	-	2/30/50/50	0/6/6/6
2	SF4	C	1102	1	-	-	0/6/5/5
2	SF4	C	1104	1	-	-	0/6/5/5
7	LEU	D	1101	8	-	0/5/6/8	-
4	URA	D	1108	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	D	1107	-	-	2/30/50/50	0/6/6/6
5	FNR	C	1108	-	-	1/18/18/18	0/3/3/3
3	FAD	A	1105	-	-	2/30/50/50	0/6/6/6
2	SF4	B	1103	1	-	-	0/6/5/5
2	SF4	B	1102	1	-	-	0/6/5/5
4	URA	B	1107	-	-	-	0/1/1/1
2	SF4	C	1105	1	-	-	0/6/5/5

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1106	URA	C2-N1	9.35	1.49	1.36
4	B	1107	URA	C2-N1	9.04	1.49	1.36
4	C	1107	URA	C2-N1	8.99	1.48	1.36
4	D	1108	URA	C2-N1	8.86	1.48	1.36
5	C	1108	FNR	O4-C4	8.44	1.39	1.23
5	A	1107	FNR	O4-C4	8.43	1.39	1.23
5	B	1108	FNR	O4-C4	8.23	1.39	1.23
5	C	1108	FNR	C5A-C9A	-8.16	1.31	1.40
5	A	1107	FNR	C5A-C9A	-8.09	1.31	1.40
5	D	1109	FNR	C5A-C9A	-7.87	1.31	1.40
5	D	1109	FNR	O4-C4	7.86	1.38	1.23
5	B	1108	FNR	C5A-C9A	-7.80	1.31	1.40
5	A	1107	FNR	O2-C2	7.67	1.39	1.23
5	D	1109	FNR	O2-C2	7.46	1.39	1.23
5	B	1108	FNR	O2-C2	7.29	1.38	1.23
5	C	1108	FNR	O2-C2	7.03	1.38	1.23
5	B	1108	FNR	C9-C9A	7.00	1.51	1.39
5	A	1107	FNR	C6-C5A	6.95	1.50	1.39
5	D	1109	FNR	C6-C5A	6.81	1.50	1.39
4	B	1107	URA	C6-N1	6.76	1.46	1.36
4	C	1107	URA	C2-N3	6.68	1.48	1.37
5	C	1108	FNR	C6-C5A	6.56	1.49	1.39
4	B	1107	URA	C2-N3	6.55	1.48	1.37
4	C	1107	URA	C6-N1	6.49	1.46	1.36
5	C	1108	FNR	C9-C9A	6.48	1.50	1.39
5	D	1109	FNR	C9-C9A	6.43	1.50	1.39
4	D	1108	URA	C6-N1	6.41	1.45	1.36
4	D	1108	URA	C2-N3	6.37	1.48	1.37
4	A	1106	URA	C6-N1	6.34	1.45	1.36
5	B	1108	FNR	C6-C5A	6.22	1.49	1.39
4	A	1106	URA	C2-N3	6.22	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1107	FNR	C9-C9A	6.19	1.49	1.39
5	B	1108	FNR	CAA-N1	5.97	1.48	1.37
5	D	1109	FNR	CAA-N1	5.69	1.47	1.37
5	C	1108	FNR	CAA-N1	5.33	1.46	1.37
4	B	1107	URA	C6-C5	5.01	1.44	1.34
4	D	1108	URA	C6-C5	4.92	1.44	1.34
4	A	1106	URA	C6-C5	4.82	1.44	1.34
5	A	1107	FNR	CAA-N1	4.77	1.45	1.37
4	C	1107	URA	C6-C5	4.70	1.44	1.34
4	C	1107	URA	C4-N3	4.36	1.46	1.38
5	A	1107	FNR	C2-N1	4.32	1.44	1.37
5	C	1108	FNR	C4A-C4	4.26	1.53	1.42
4	B	1107	URA	C4-N3	4.11	1.45	1.38
4	D	1108	URA	C4-N3	4.10	1.45	1.38
5	C	1108	FNR	C2-N1	4.05	1.44	1.37
5	B	1108	FNR	C2-N1	3.93	1.44	1.37
4	A	1106	URA	C4-N3	3.89	1.45	1.38
5	D	1109	FNR	C4A-C4	3.85	1.52	1.42
5	B	1108	FNR	C4A-C4	3.81	1.52	1.42
5	A	1107	FNR	C4A-C4	3.79	1.52	1.42
5	B	1108	FNR	C9A-N10	3.50	1.47	1.41
5	B	1108	FNR	C4A-N5	3.45	1.43	1.35
5	D	1109	FNR	C9A-N10	3.39	1.47	1.41
5	D	1109	FNR	C2-N1	3.38	1.43	1.37
5	A	1107	FNR	C9A-N10	3.34	1.47	1.41
5	C	1108	FNR	C5A-N5	3.32	1.45	1.39
5	D	1109	FNR	C4A-N5	3.20	1.42	1.35
5	C	1108	FNR	C9A-N10	3.19	1.46	1.41
5	B	1108	FNR	C5A-N5	3.17	1.45	1.39
4	A	1106	URA	C5-C4	3.09	1.50	1.43
4	D	1108	URA	C5-C4	3.07	1.50	1.43
5	C	1108	FNR	C4A-N5	3.05	1.42	1.35
4	B	1107	URA	C5-C4	3.00	1.50	1.43
5	D	1109	FNR	C5A-N5	2.92	1.44	1.39
5	D	1109	FNR	CAA-N10	2.91	1.43	1.38
4	C	1107	URA	C5-C4	2.89	1.50	1.43
5	A	1107	FNR	C4A-N5	2.88	1.42	1.35
5	A	1107	FNR	C5A-N5	2.81	1.44	1.39
5	C	1108	FNR	CAA-N10	2.76	1.43	1.38
5	B	1108	FNR	CAA-N10	2.62	1.43	1.38
5	A	1107	FNR	C2-N3	2.57	1.41	1.37
4	A	1106	URA	O4-C4	-2.57	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1107	URA	O4-C4	-2.53	1.19	1.24
4	B	1107	URA	O4-C4	-2.48	1.19	1.24
4	D	1108	URA	O4-C4	-2.38	1.19	1.24
5	C	1108	FNR	C2-N3	2.37	1.41	1.37
5	A	1107	FNR	CAA-N10	2.36	1.42	1.38
5	B	1108	FNR	P-O3P	-2.17	1.46	1.54
5	D	1109	FNR	P-O3P	-2.16	1.46	1.54
5	D	1109	FNR	C2-N3	2.14	1.41	1.37
5	B	1108	FNR	P-O1P	-2.12	1.46	1.54
4	A	1106	URA	O2-C2	-2.04	1.19	1.23
5	A	1107	FNR	P-O3P	-2.02	1.47	1.54
5	B	1108	FNR	C2-N3	2.01	1.41	1.37
5	C	1108	FNR	P-O3P	-2.01	1.47	1.54

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1106	URA	C6-N1-C2	-5.89	118.79	122.40
4	D	1108	URA	C4-N3-C2	-5.80	119.95	125.70
4	C	1107	URA	C4-N3-C2	-5.76	119.98	125.70
4	A	1106	URA	C4-N3-C2	-5.52	120.23	125.70
5	D	1109	FNR	C4-N3-C2	-5.32	118.67	126.34
4	B	1107	URA	C6-N1-C2	-5.11	119.26	122.40
4	B	1107	URA	C4-N3-C2	-5.10	120.65	125.70
4	D	1108	URA	C6-N1-C2	-4.98	119.34	122.40
4	C	1107	URA	C6-N1-C2	-4.83	119.43	122.40
5	C	1108	FNR	C4-N3-C2	-4.83	119.38	126.34
5	B	1108	FNR	C4-N3-C2	-4.80	119.43	126.34
5	A	1107	FNR	C4-N3-C2	-4.68	119.59	126.34
4	D	1108	URA	N1-C2-N3	4.37	120.08	115.13
4	A	1106	URA	N1-C2-N3	4.21	119.90	115.13
4	C	1107	URA	N1-C2-N3	3.89	119.54	115.13
4	B	1107	URA	N1-C2-N3	3.75	119.38	115.13
5	C	1108	FNR	N3-C2-N1	3.72	121.78	115.80
5	A	1107	FNR	O4-C4-C4A	-3.49	119.25	127.24
5	B	1108	FNR	O4-C4-C4A	-3.27	119.75	127.24
5	D	1109	FNR	O4-C4-C4A	-3.21	119.88	127.24
4	A	1106	URA	C5-C4-N3	3.18	119.60	114.84
4	C	1107	URA	C5-C4-N3	3.17	119.58	114.84
5	D	1109	FNR	N3-C2-N1	3.12	120.81	115.80
5	B	1108	FNR	N3-C2-N1	3.07	120.74	115.80
4	B	1107	URA	C5-C4-N3	3.03	119.37	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1108	URA	C5-C4-N3	2.97	119.29	114.84
4	C	1107	URA	O4-C4-C5	-2.95	119.98	125.16
5	A	1107	FNR	N3-C2-N1	2.94	120.52	115.80
5	C	1108	FNR	O4-C4-C4A	-2.93	120.53	127.24
5	D	1109	FNR	C4A-C4-N3	2.75	120.51	112.31
5	B	1108	FNR	O3P-P-O5'	2.69	113.89	106.73
5	B	1108	FNR	C4A-C4-N3	2.67	120.26	112.31
5	D	1109	FNR	O3P-P-O5'	2.60	113.64	106.73
5	C	1108	FNR	O3P-P-O5'	2.59	113.62	106.73
5	D	1109	FNR	O5'-P-O2P	2.57	113.68	106.47
5	C	1108	FNR	O1P-P-O5'	2.49	113.35	106.73
4	B	1107	URA	O4-C4-C5	-2.44	120.86	125.16
4	D	1108	URA	O4-C4-C5	-2.43	120.89	125.16
5	A	1107	FNR	C4A-C4-N3	2.41	119.49	112.31
5	A	1107	FNR	O3P-P-O5'	2.40	113.12	106.73
5	A	1107	FNR	C9-C9A-N10	-2.37	118.63	121.84
5	A	1107	FNR	O5'-P-O2P	2.31	112.95	106.47
3	A	1105	FAD	C5A-C6A-N6A	2.31	123.86	120.35
3	D	1107	FAD	C5A-C6A-N6A	2.31	123.86	120.35
3	C	1106	FAD	C5A-C6A-N6A	2.30	123.85	120.35
5	C	1108	FNR	C4A-C4-N3	2.26	119.04	112.31
4	A	1106	URA	O4-C4-C5	-2.26	121.19	125.16
3	B	1106	FAD	C5A-C6A-N6A	2.24	123.76	120.35
4	A	1106	URA	O2-C2-N3	-2.14	117.77	121.82
5	B	1108	FNR	O1P-P-O5'	2.13	112.41	106.73
5	C	1108	FNR	O5'-P-O2P	2.13	112.44	106.47
5	B	1108	FNR	O5'-P-O2P	2.05	112.24	106.47

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1105	FAD	PA-O3P-P-O5'
3	B	1106	FAD	PA-O3P-P-O5'
3	C	1106	FAD	PA-O3P-P-O5'
5	A	1107	FNR	C4'-C5'-O5'-P
5	D	1109	FNR	C4'-C5'-O5'-P
3	D	1107	FAD	PA-O3P-P-O5'
7	B	1101	LEU	C-CA-CB-CG
7	B	1101	LEU	N-CA-CB-CG
5	B	1108	FNR	C4'-C5'-O5'-P
5	C	1108	FNR	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
3	A	1105	FAD	O4B-C4B-C5B-O5B
3	B	1106	FAD	O4B-C4B-C5B-O5B
3	C	1106	FAD	O4B-C4B-C5B-O5B
3	D	1107	FAD	O4B-C4B-C5B-O5B

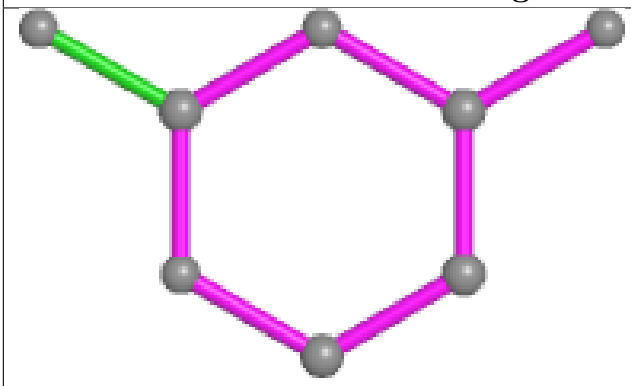
There are no ring outliers.

11 monomers are involved in 15 short contacts:

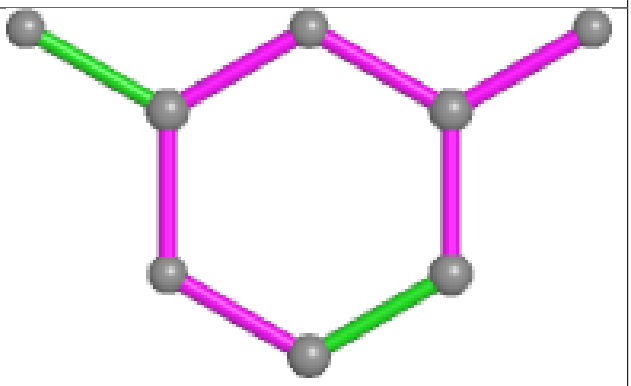
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1108	FNR	2	0
5	A	1107	FNR	3	0
3	C	1106	FAD	1	0
6	D	1102	ALA	1	0
6	A	1108	ALA	2	0
8	C	1101	PRO	1	0
5	D	1109	FNR	1	0
3	B	1106	FAD	1	0
3	D	1107	FAD	1	0
5	C	1108	FNR	1	0
3	A	1105	FAD	1	0

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.

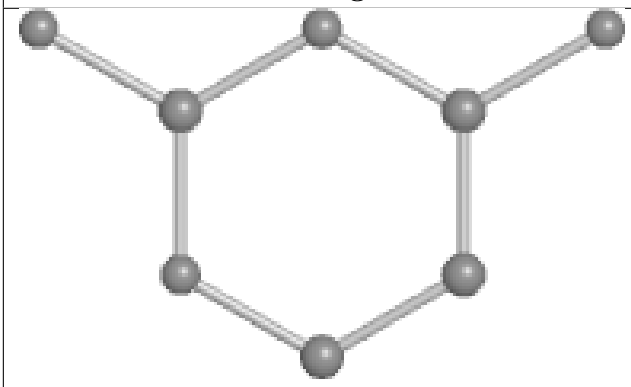
Ligand URA C 1107



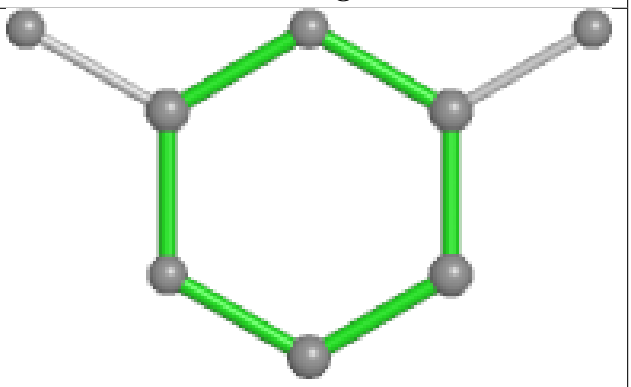
Bond lengths



Bond angles

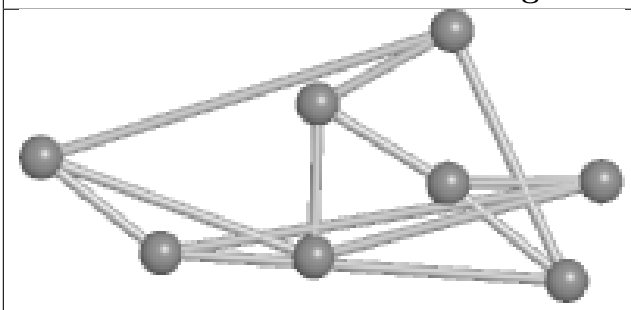


Torsions

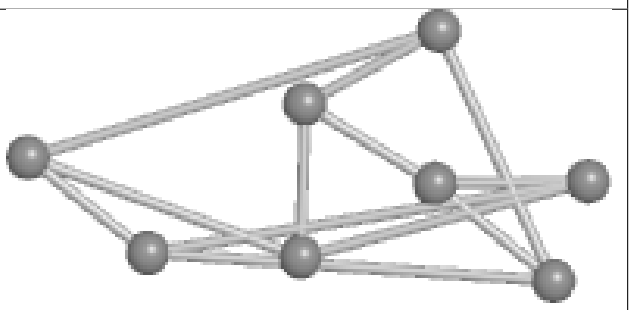


Rings

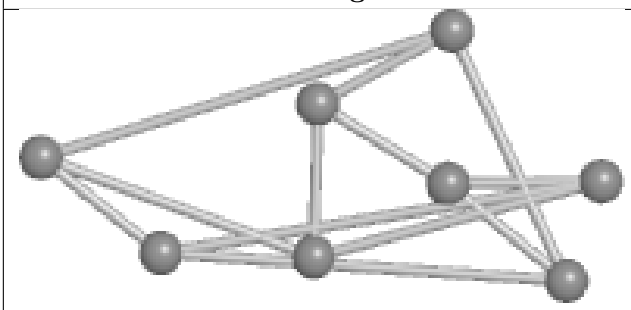
Ligand SF4 A 1103



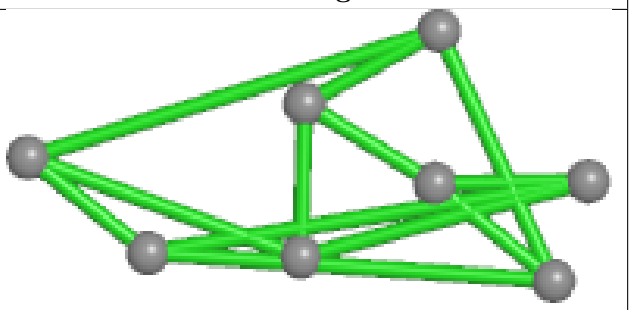
Bond lengths



Bond angles

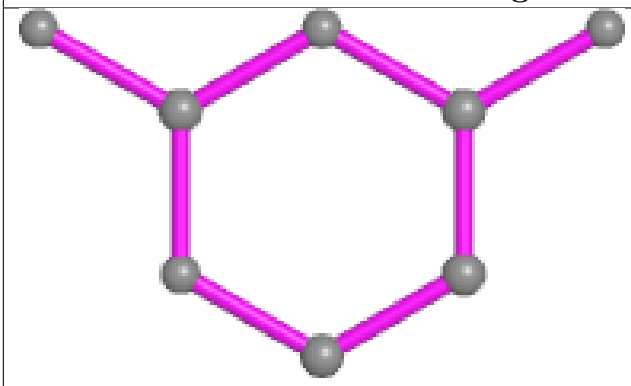


Torsions

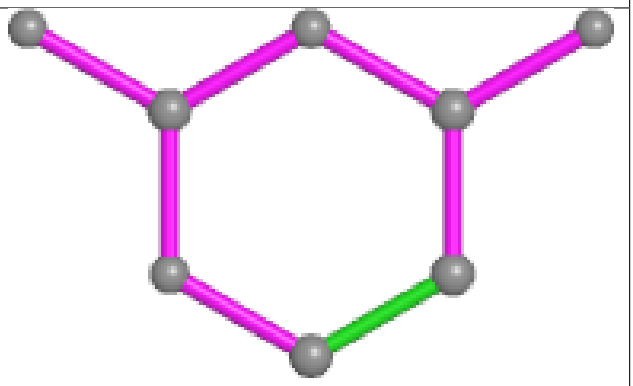


Rings

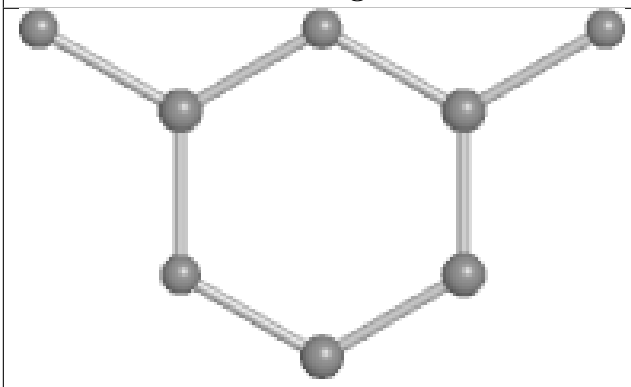
Ligand URA A 1106



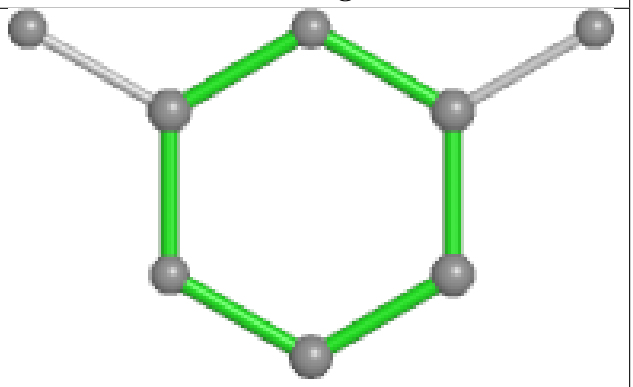
Bond lengths



Bond angles

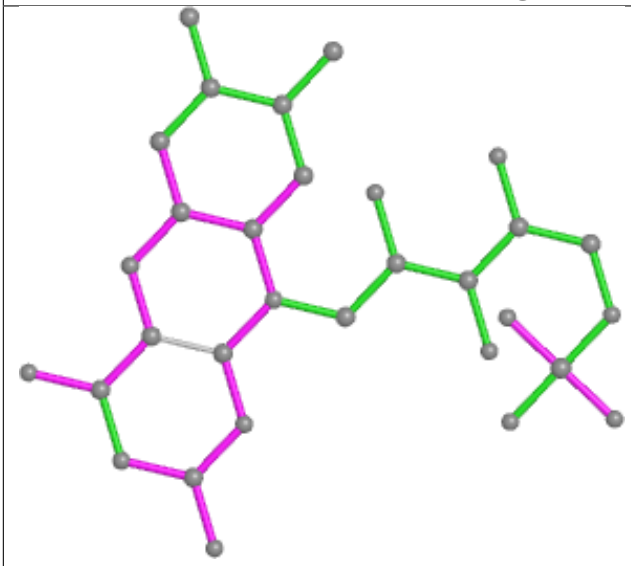


Torsions

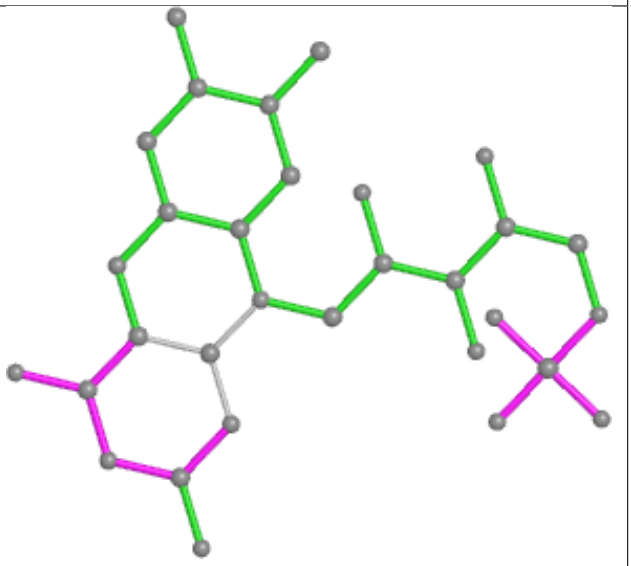


Rings

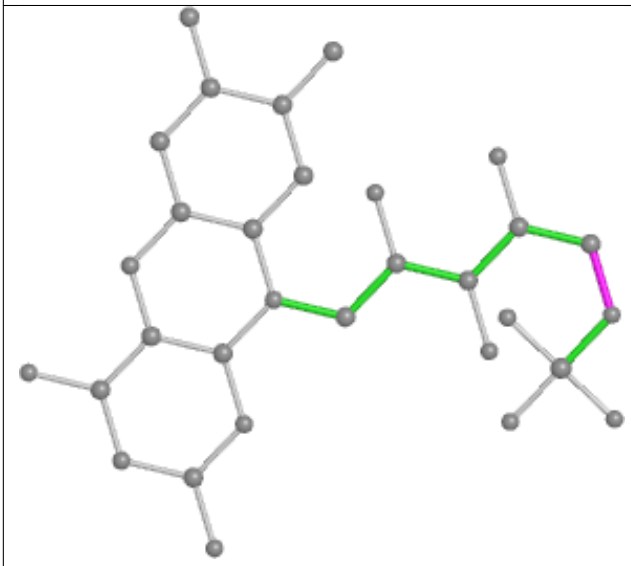
Ligand FNR B 1108



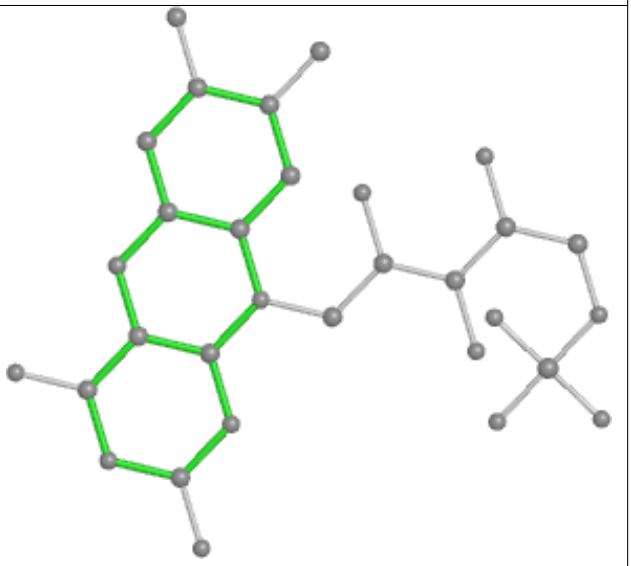
Bond lengths



Bond angles

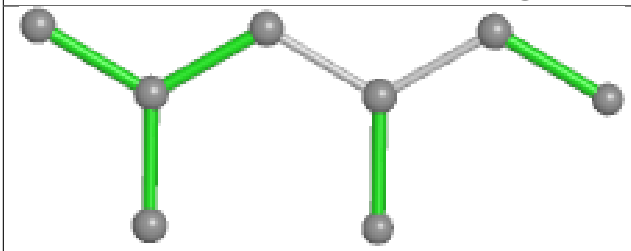


Torsions



Rings

Ligand LEU B 1101



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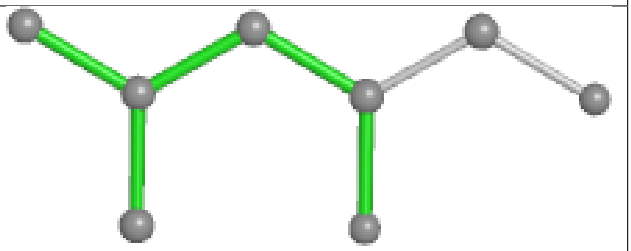
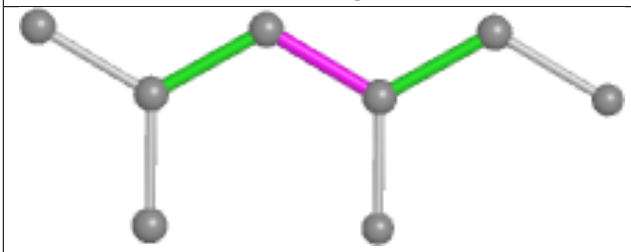


Bond angles



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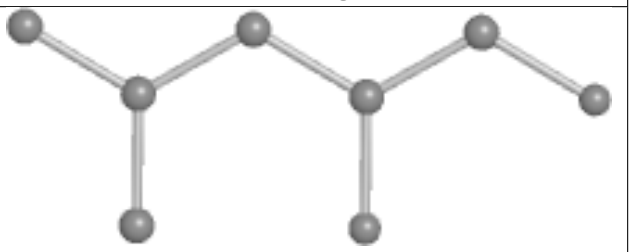
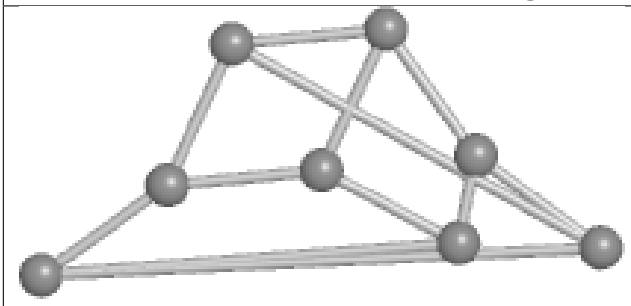


Rings

Ligand SF4 D 1106



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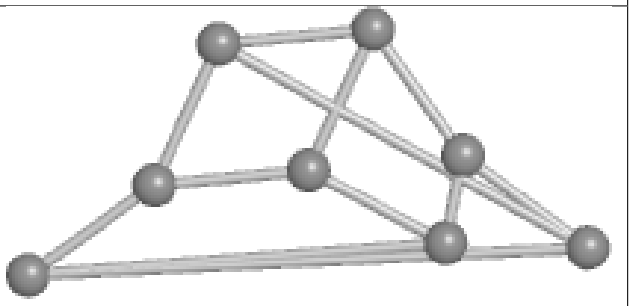
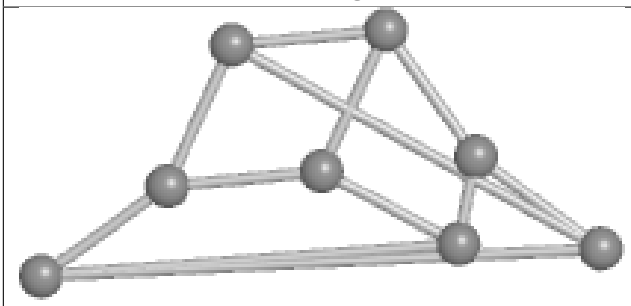
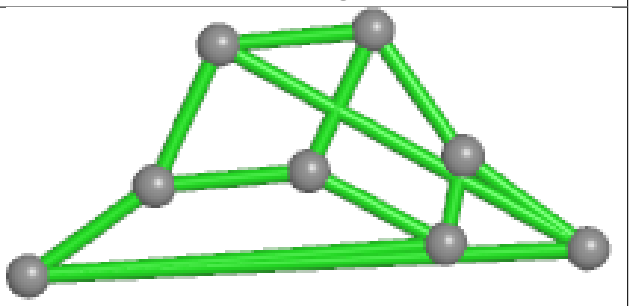


Bond angles

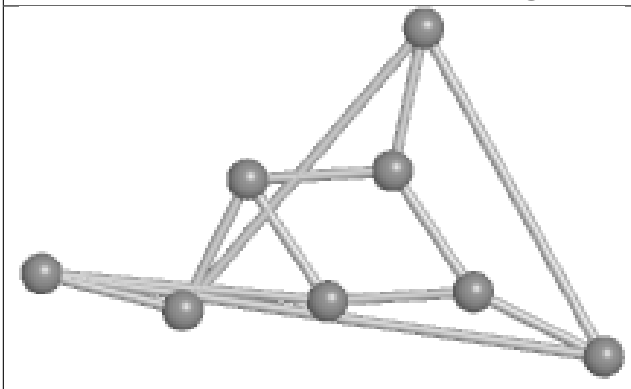


Torsions



Rings

Ligand SF4 B 1105



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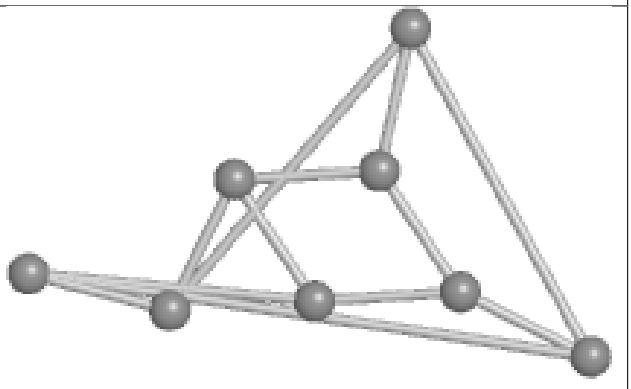
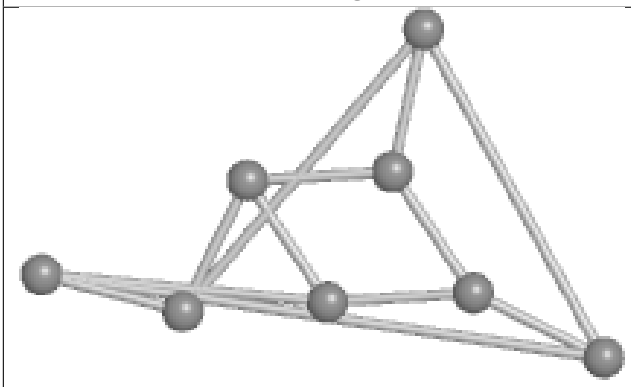


Bond angles



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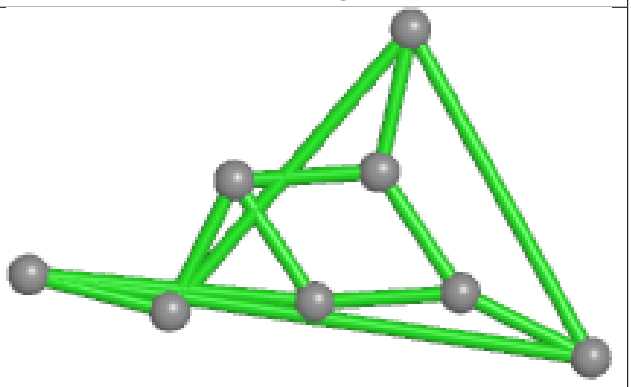
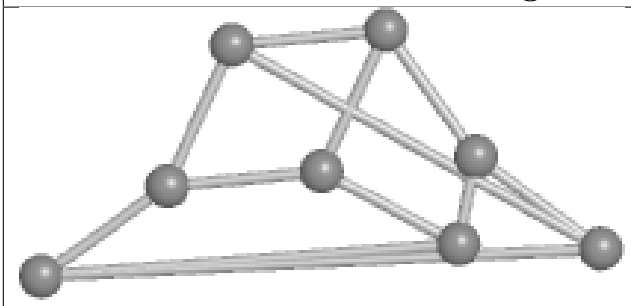


Rings

Ligand SF4 D 1104



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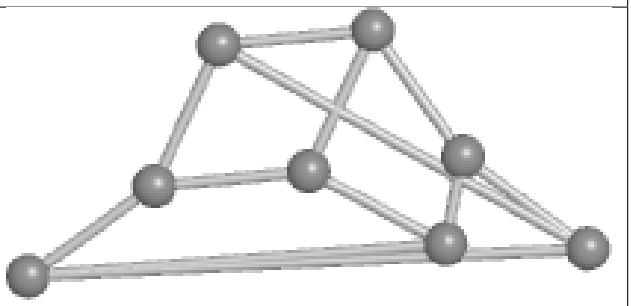
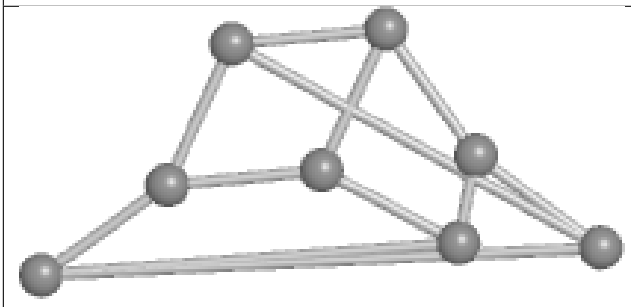


Bond angles



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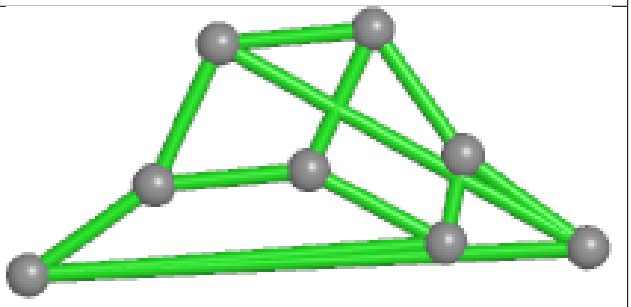
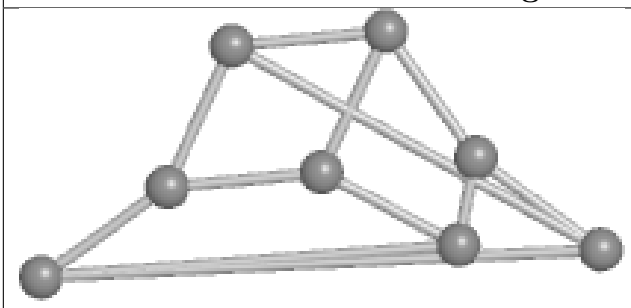


Rings

Ligand SF4 D 1103



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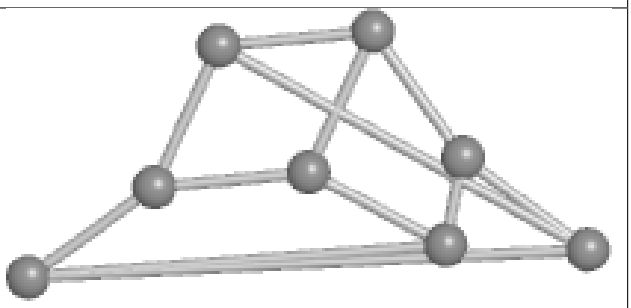
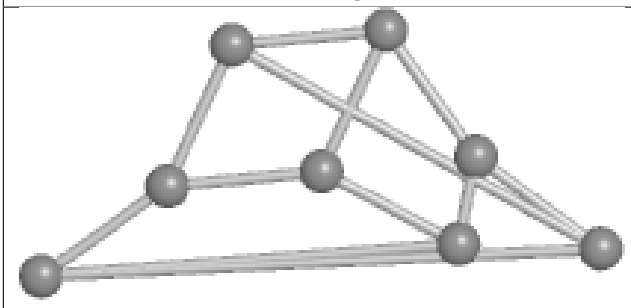


Bond angles



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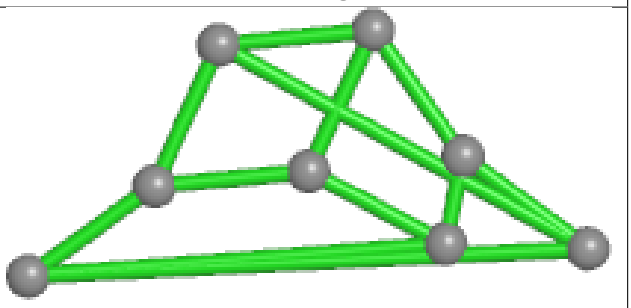
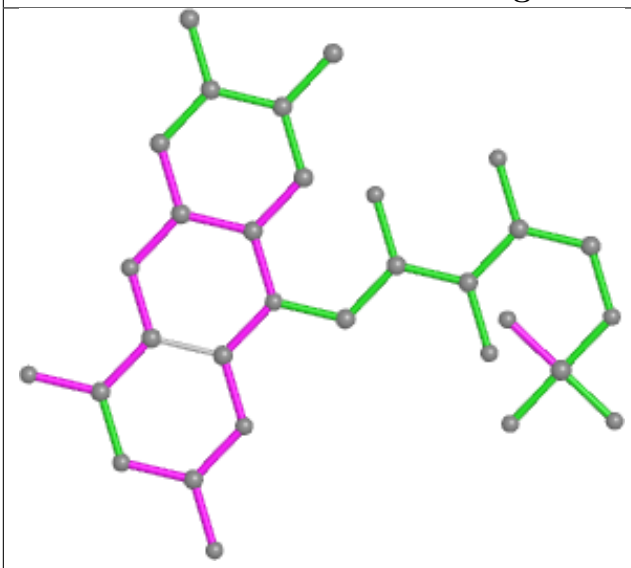


Rings

Ligand FNR A 1107



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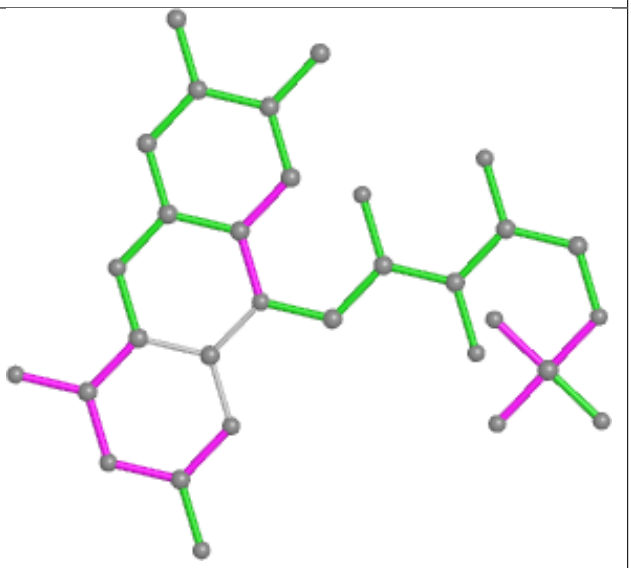
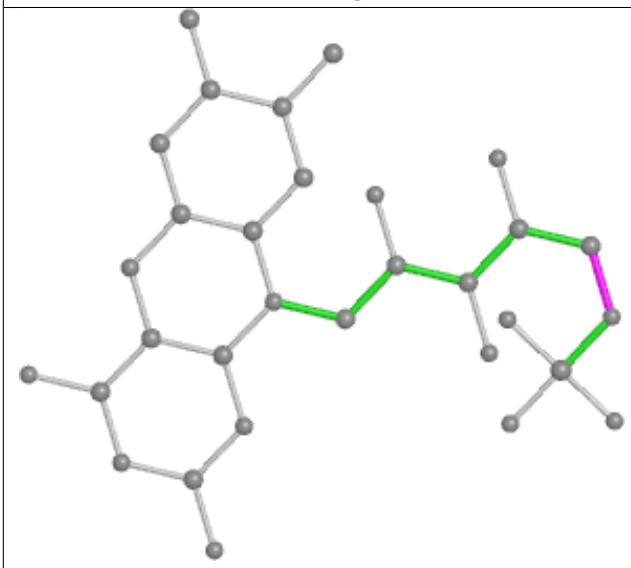
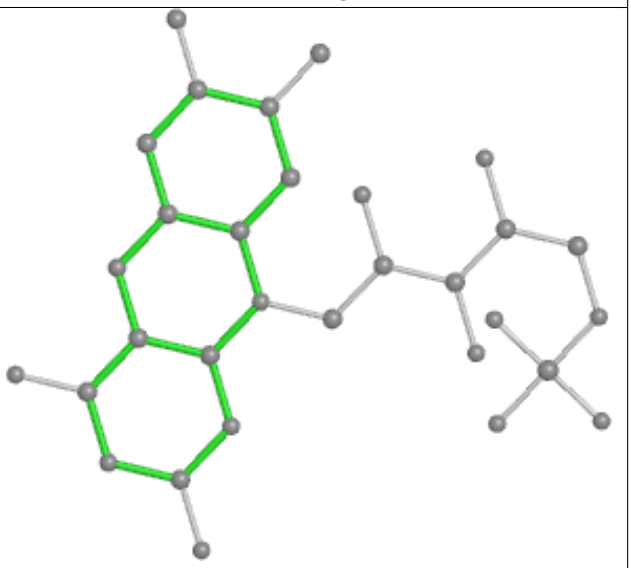


Bond angles

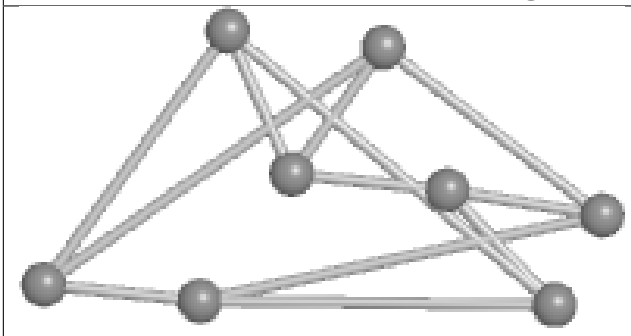


Torsions



Rings

Ligand SF4 C 1103



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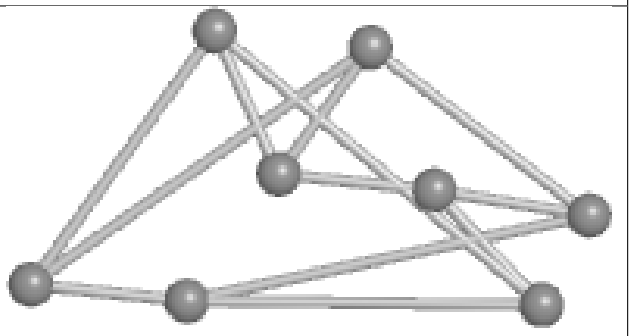
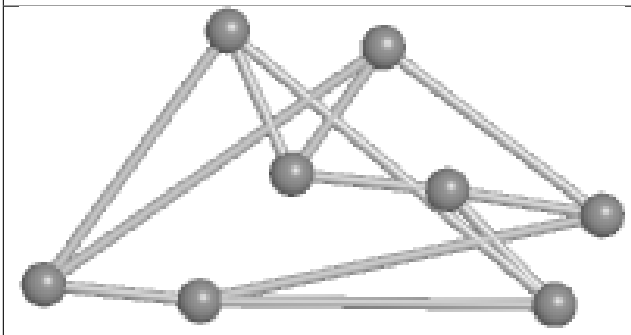


Bond angles



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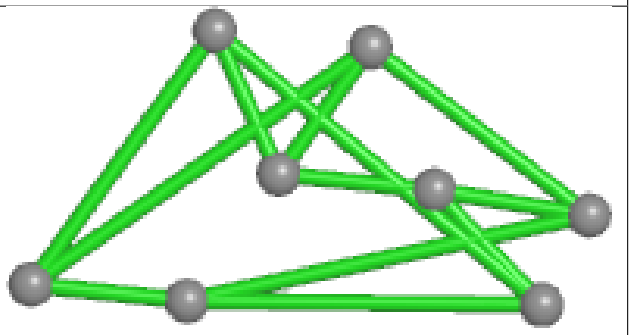
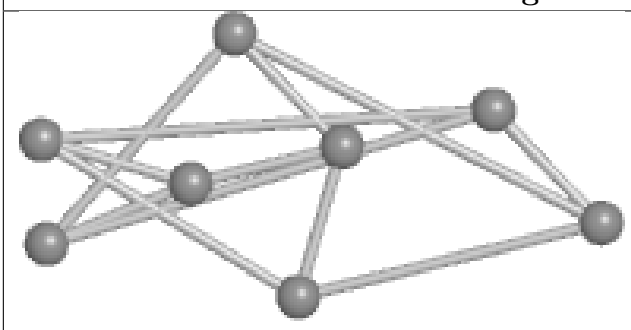


Rings

Ligand SF4 D 1105



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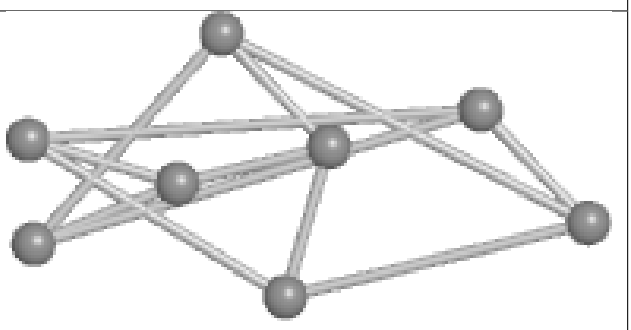
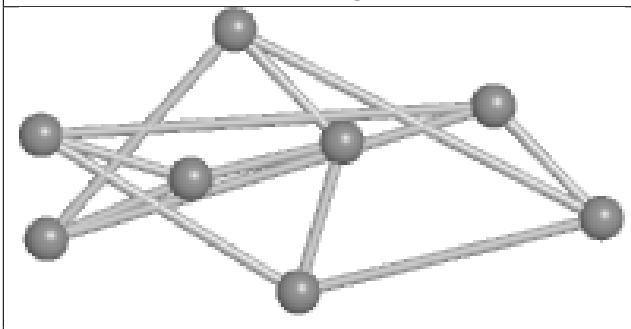


Bond angles



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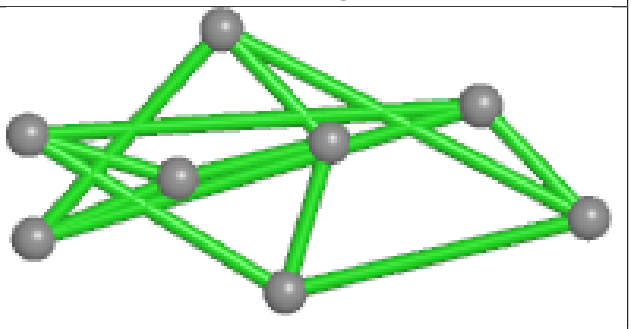
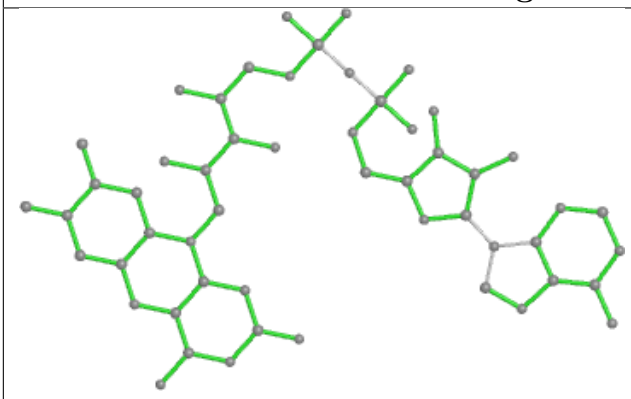


Rings

Ligand FAD C 1106



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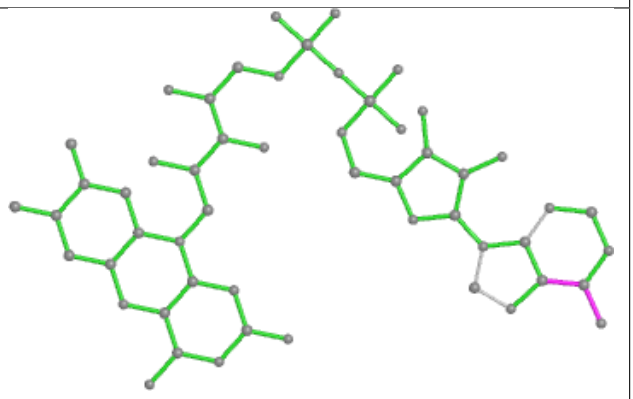
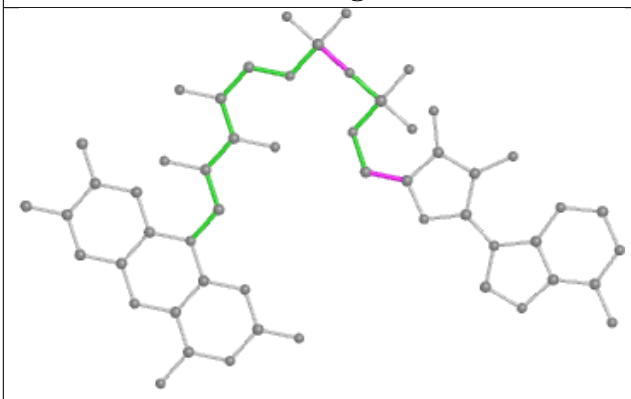
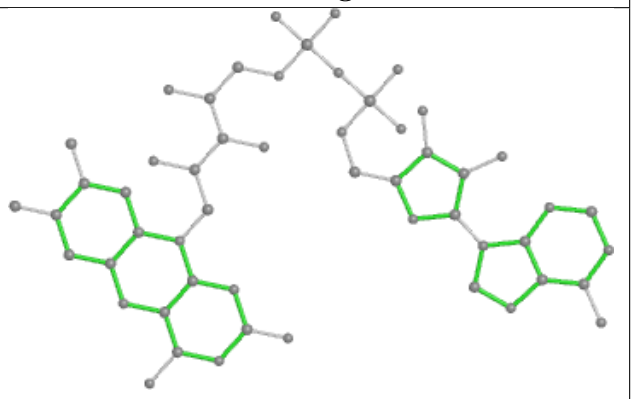


Bond angles

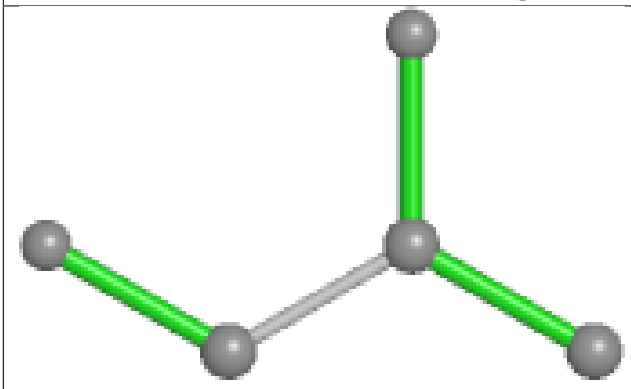


Torsions



Rings

Ligand ALA D 1102



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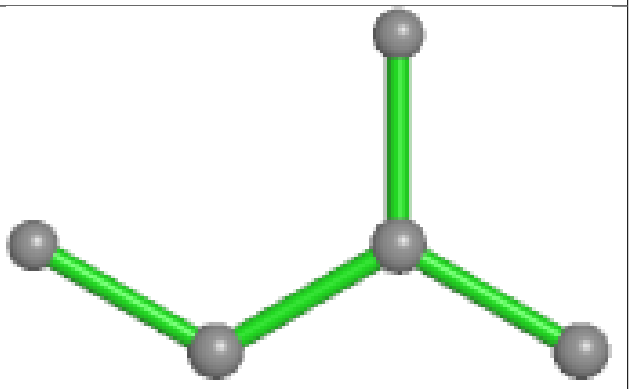
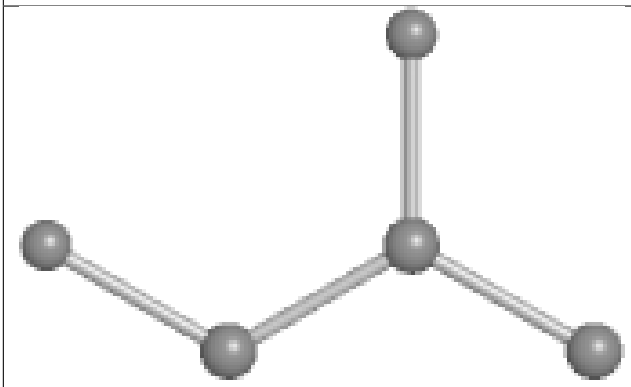


Bond angles



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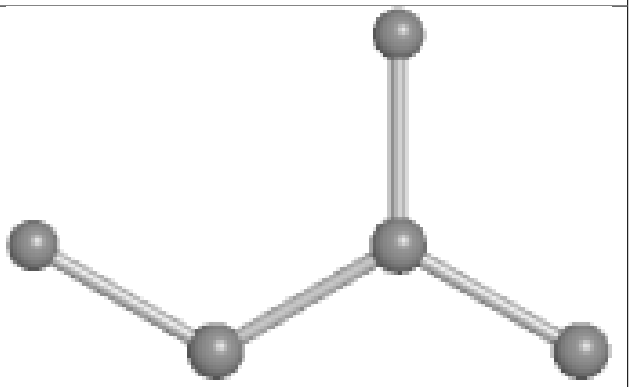
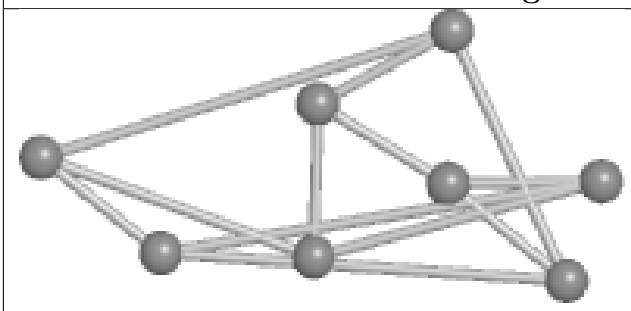


Rings

Ligand SF4 B 1104



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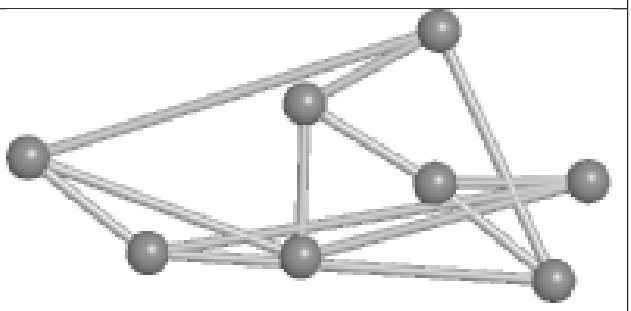
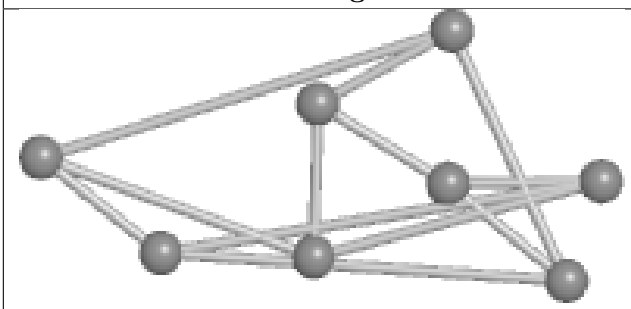
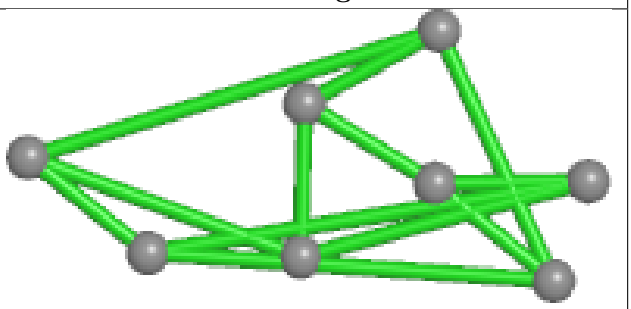


Bond angles

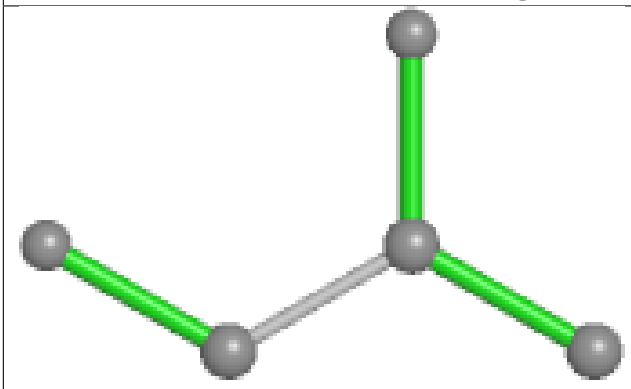


Torsions



Rings

Ligand ALA A 1108



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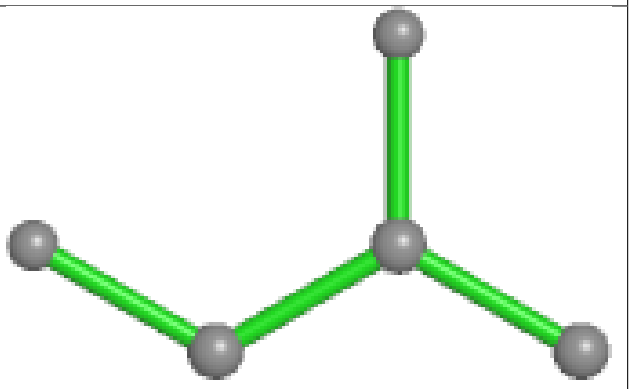
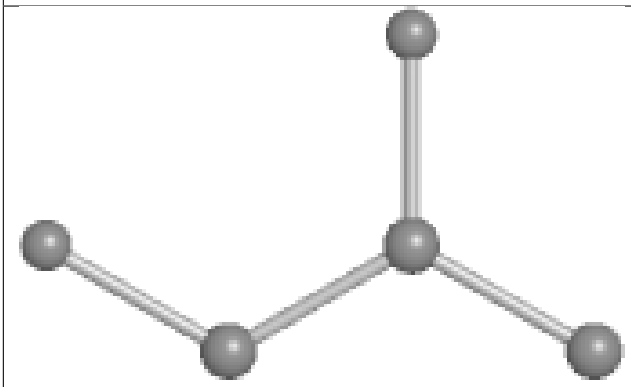


Bond angles



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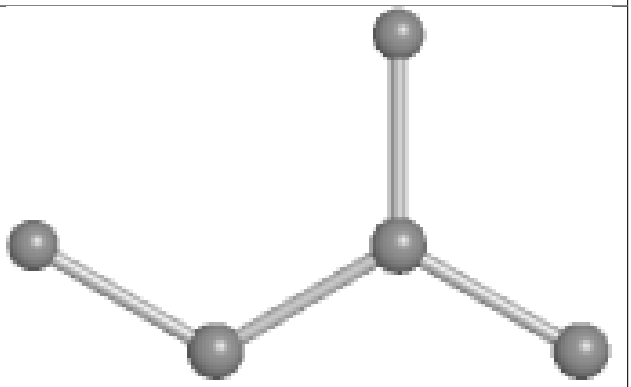
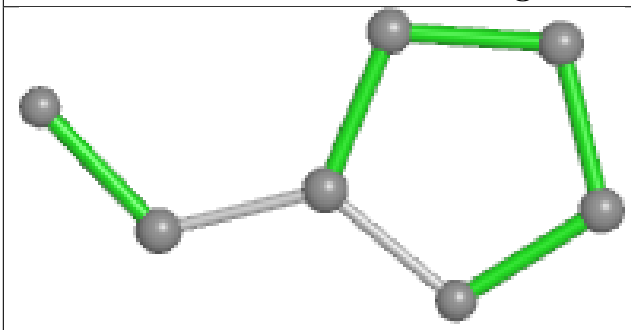


Rings

Ligand PRO C 1101



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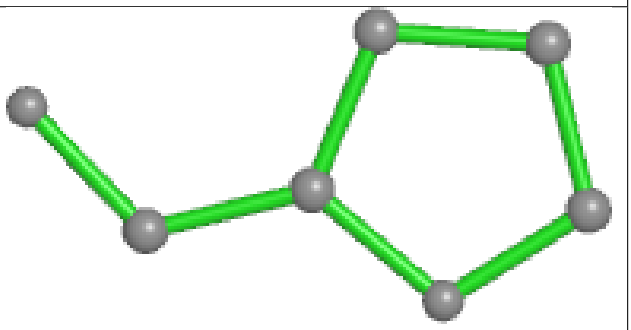
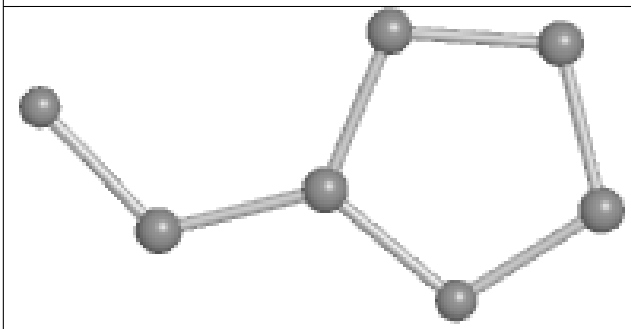
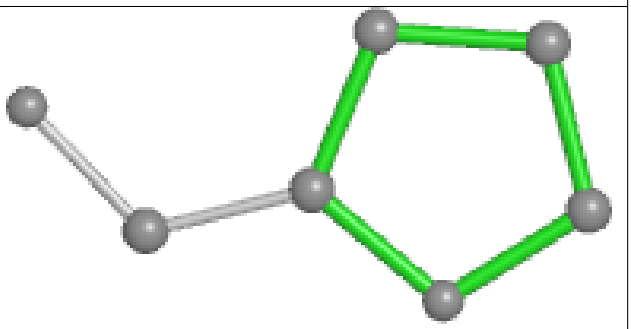


Bond angles

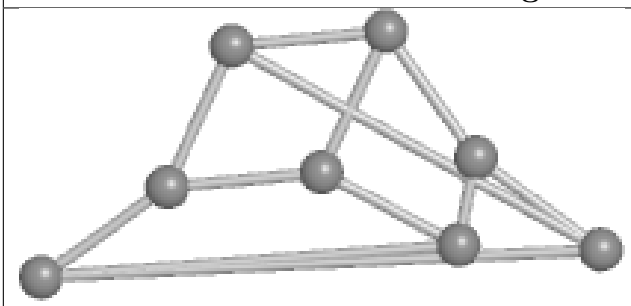


Torsions

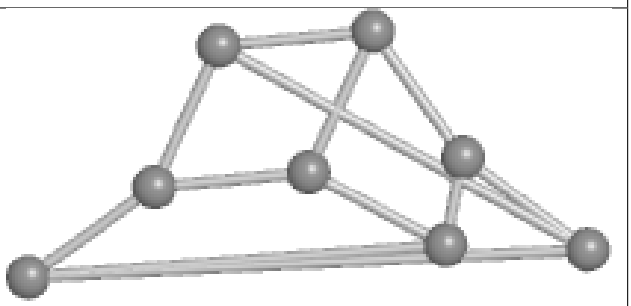


Rings

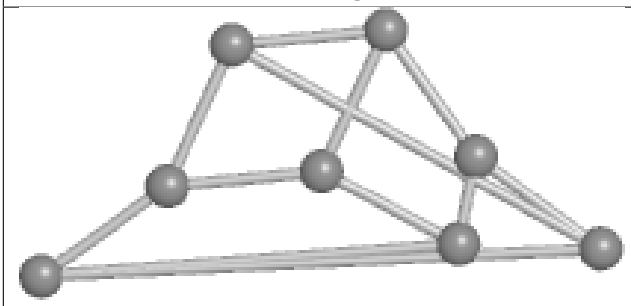
Ligand SF4 A 1102



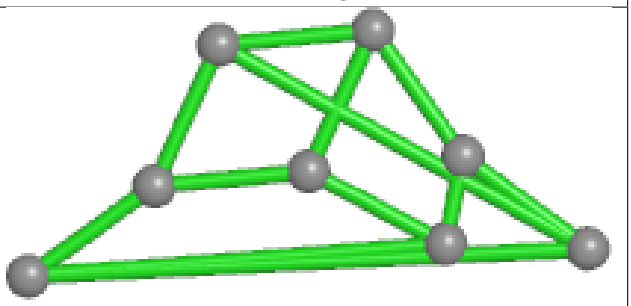
Bond lengths



Bond angles

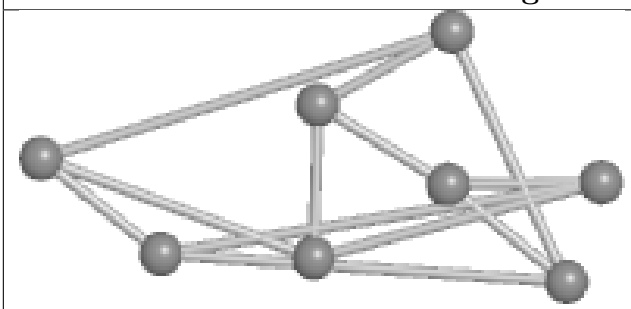


Torsions



Rings

Ligand SF4 A 1101



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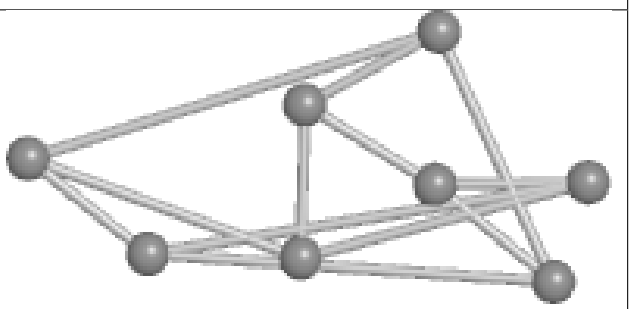
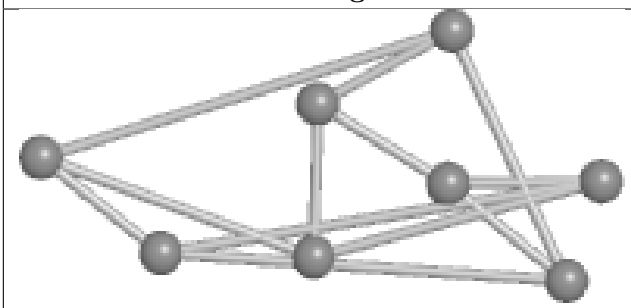


Bond angles



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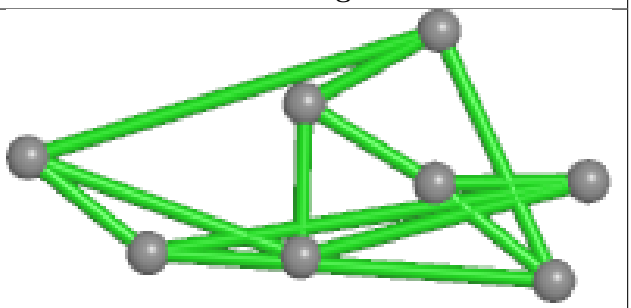
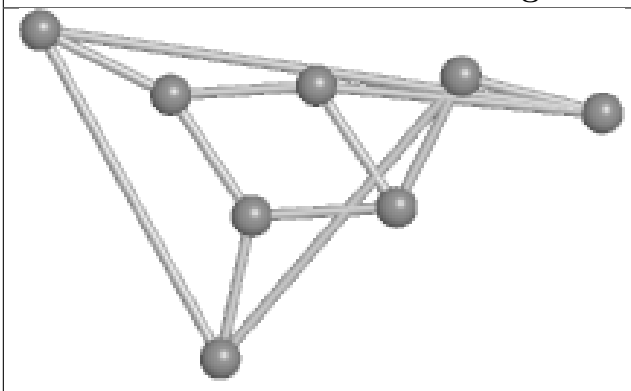


Rings

Ligand SF4 A 1104



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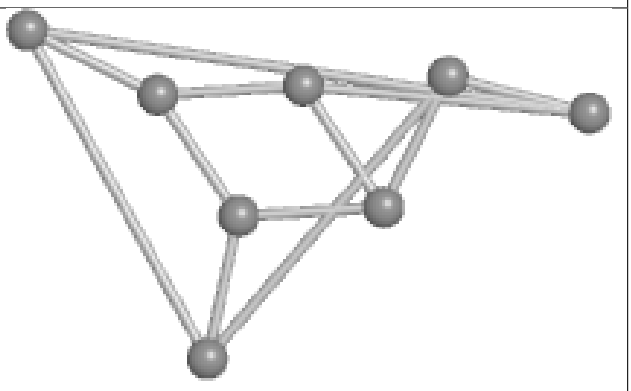
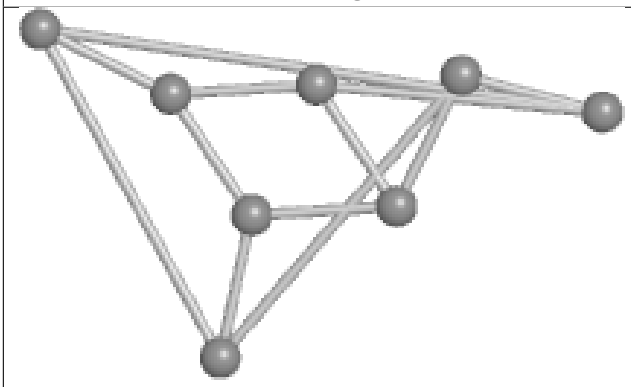


Bond angles



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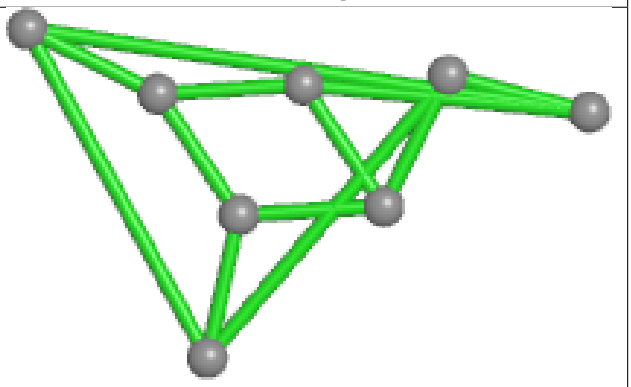
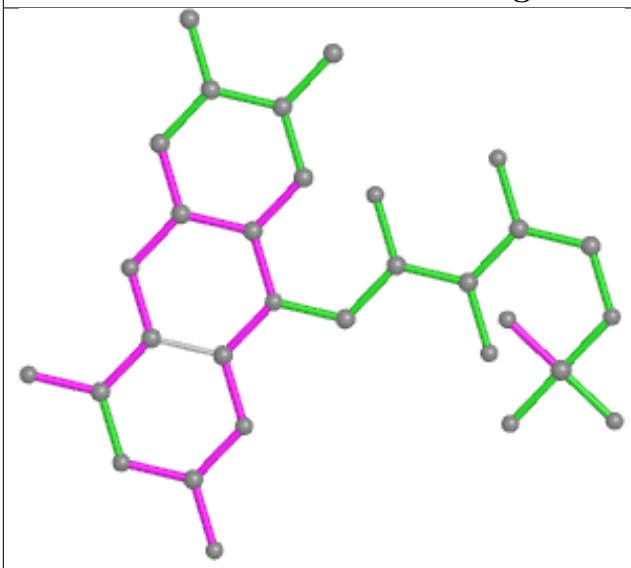


Rings

Ligand FNR D 1109



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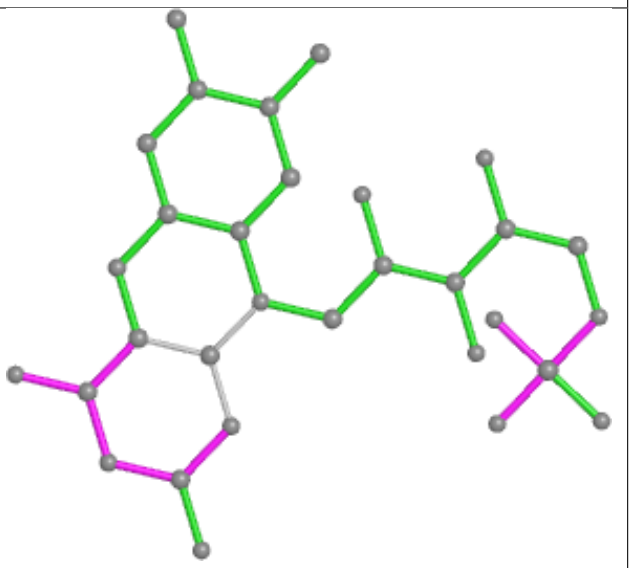

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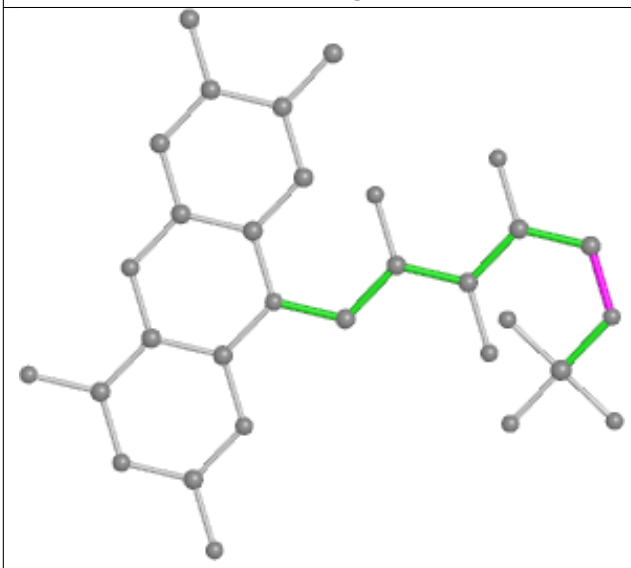

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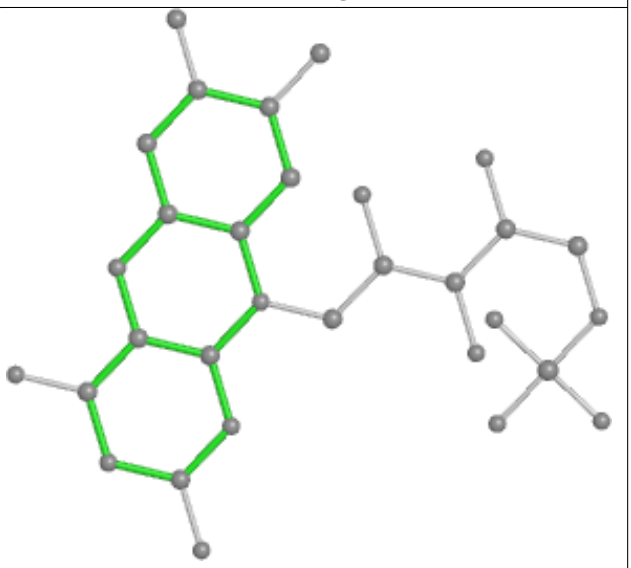
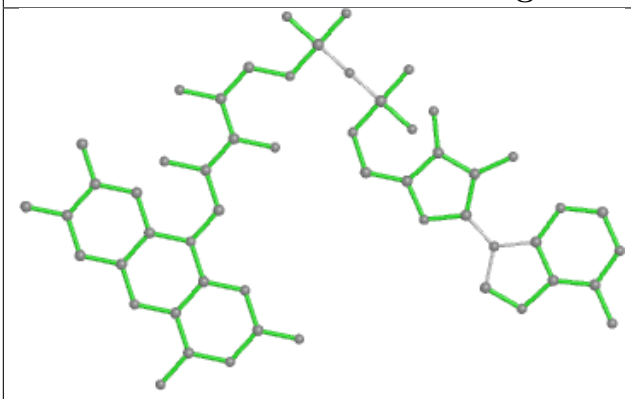


Rings

Ligand FAD B 1106



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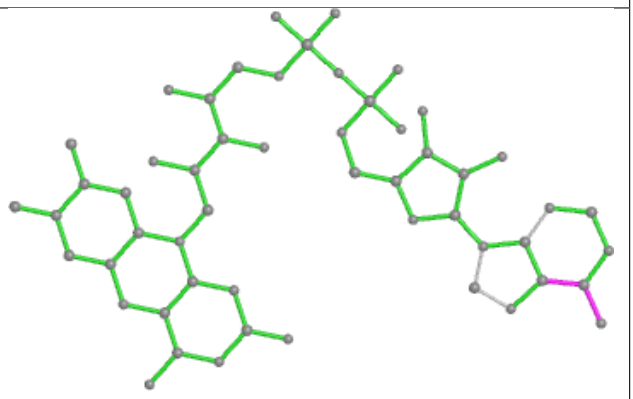
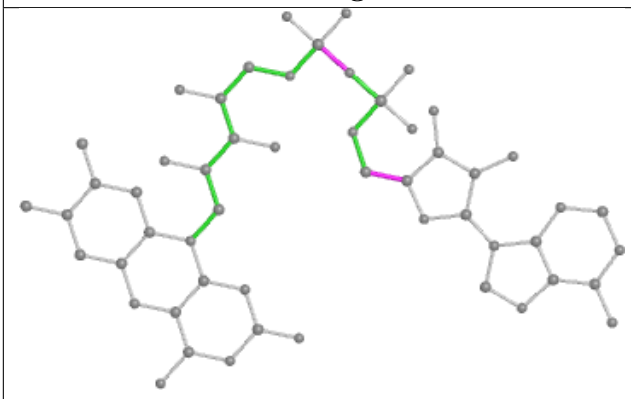


Bond angles



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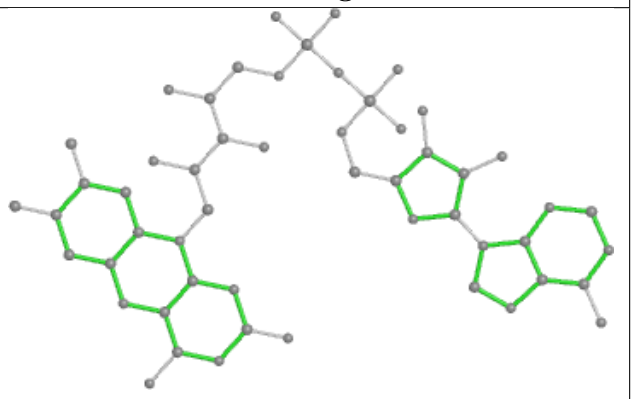
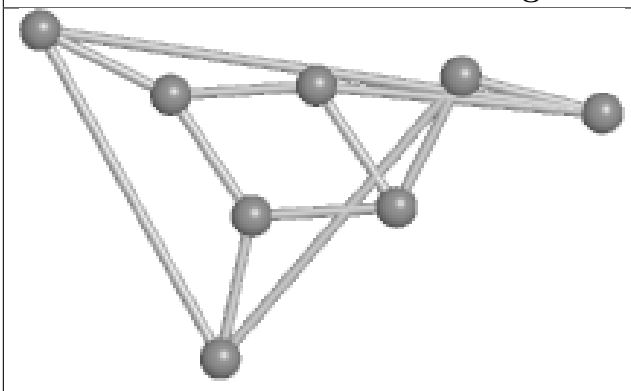


Rings

Ligand SF4 C 1102



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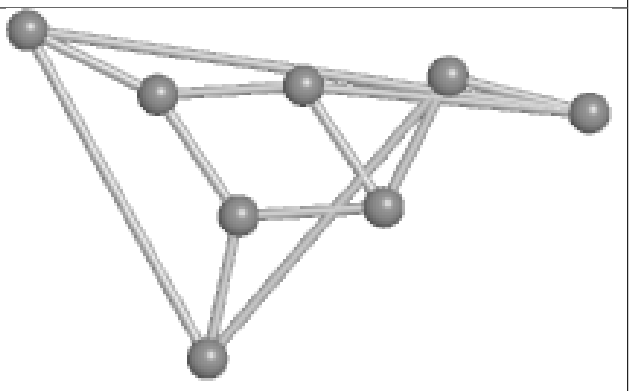
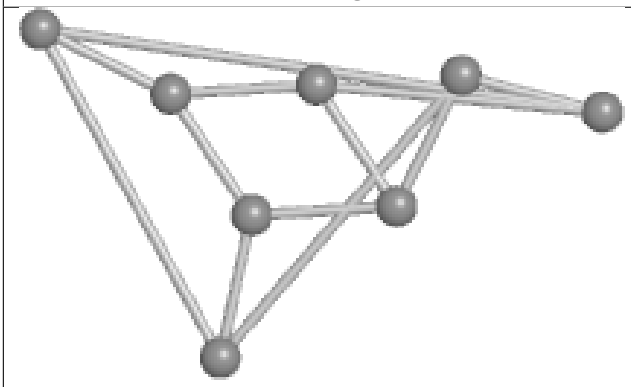


Bond angles



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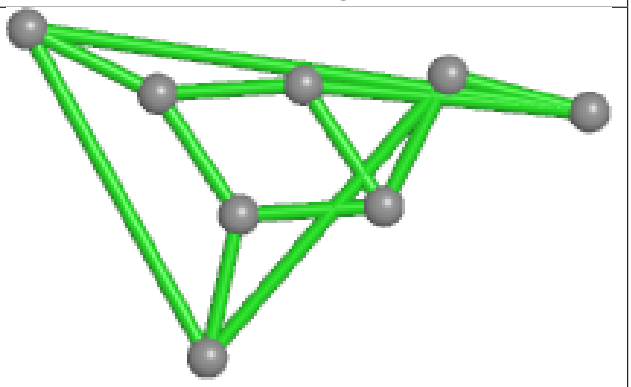
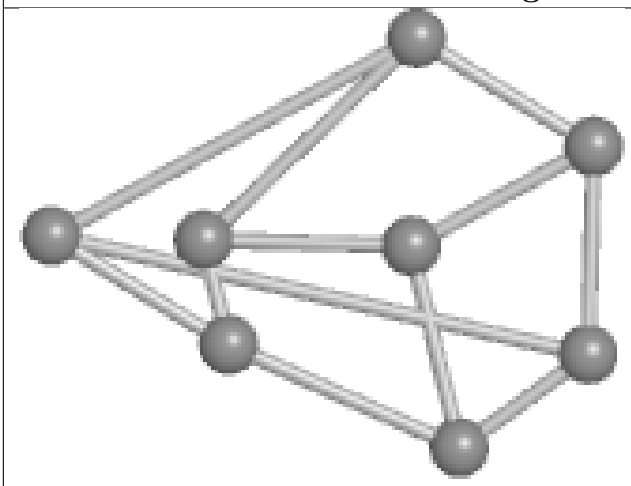


Rings

Ligand SF4 C 1104



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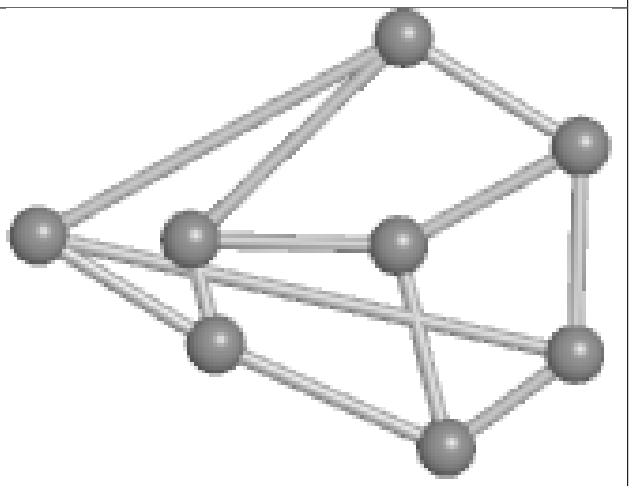

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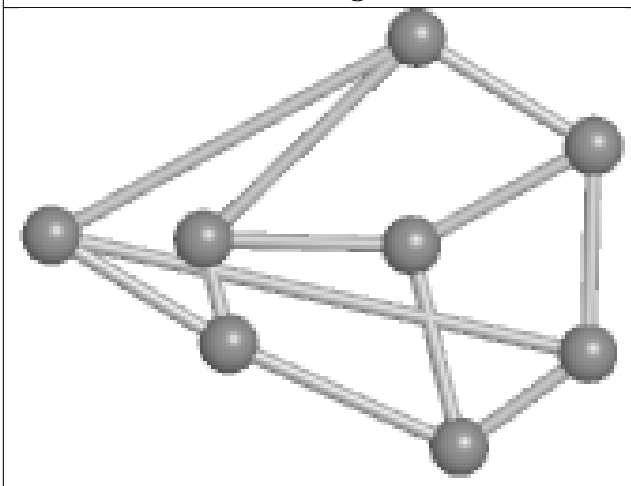

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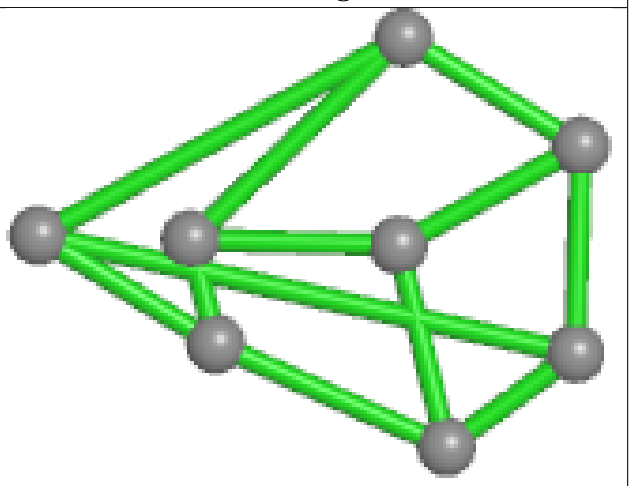
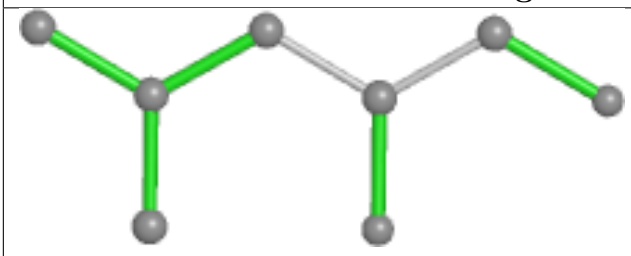


Rings

Ligand LEU D 1101



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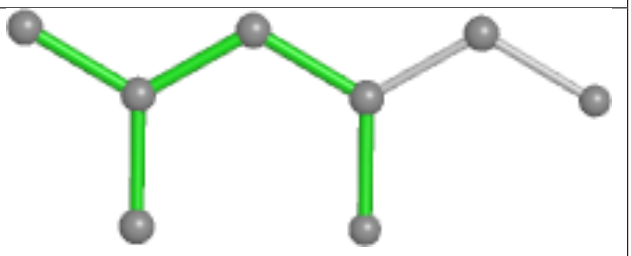
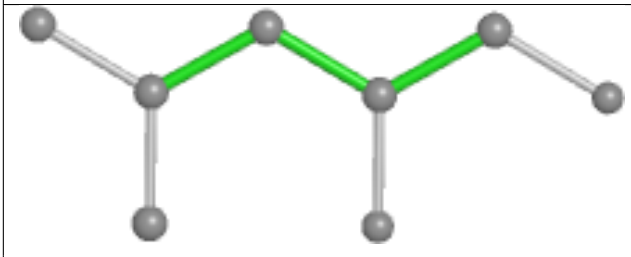


Bond angles



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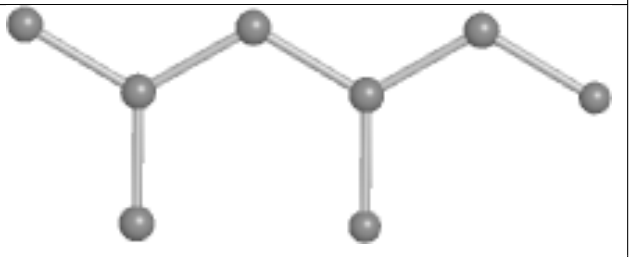
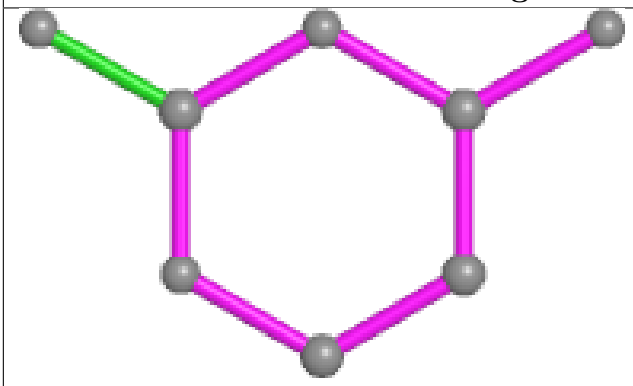


Rings

Ligand URA D 1108



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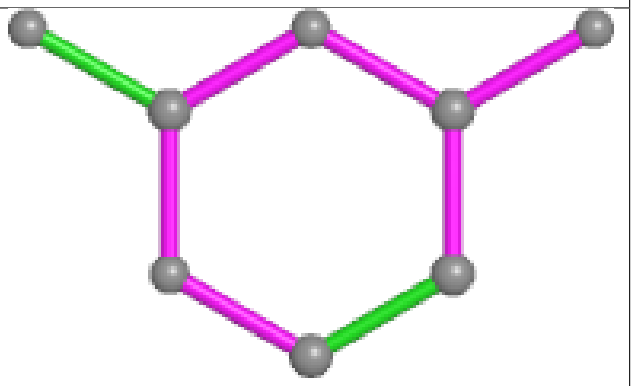
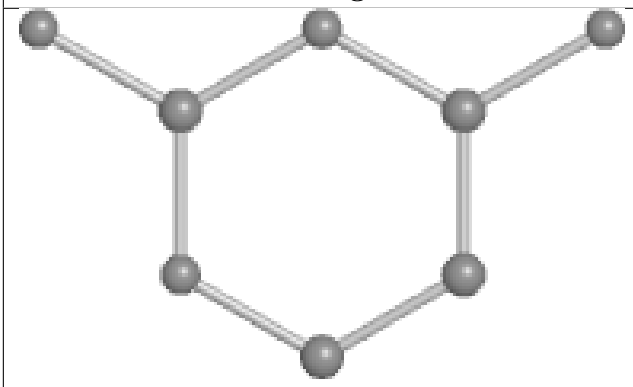


Bond angles



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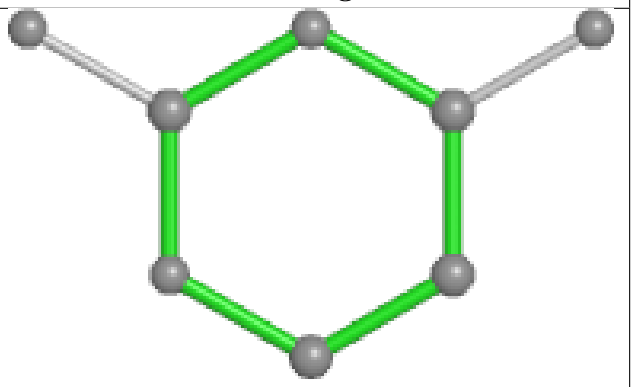
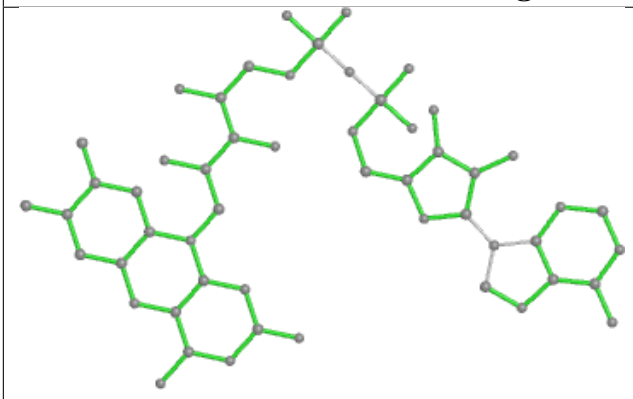


Rings

Ligand FAD D 1107



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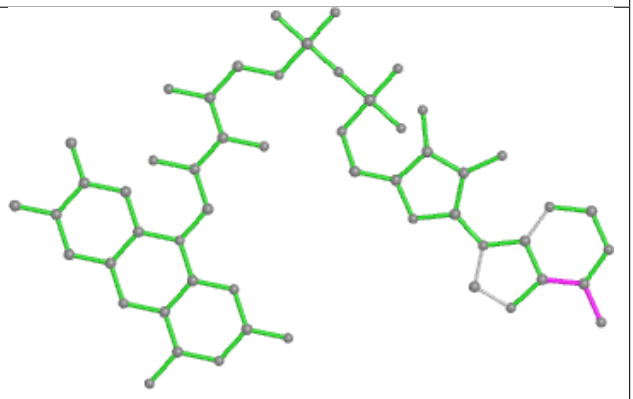
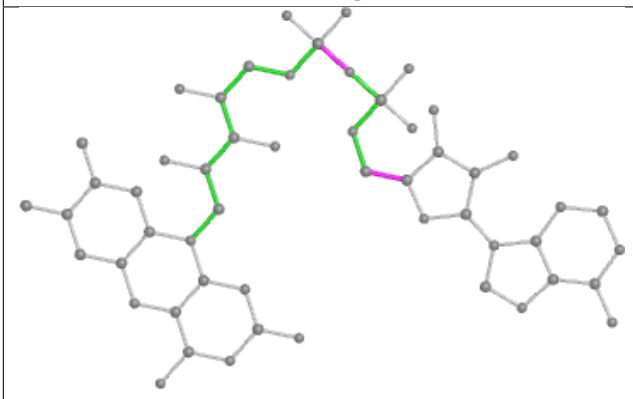
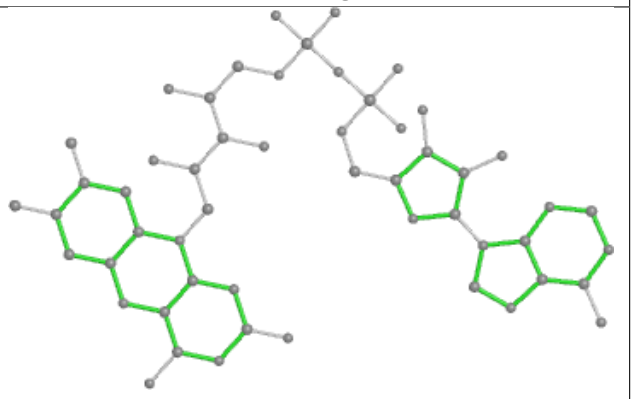


Bond angles

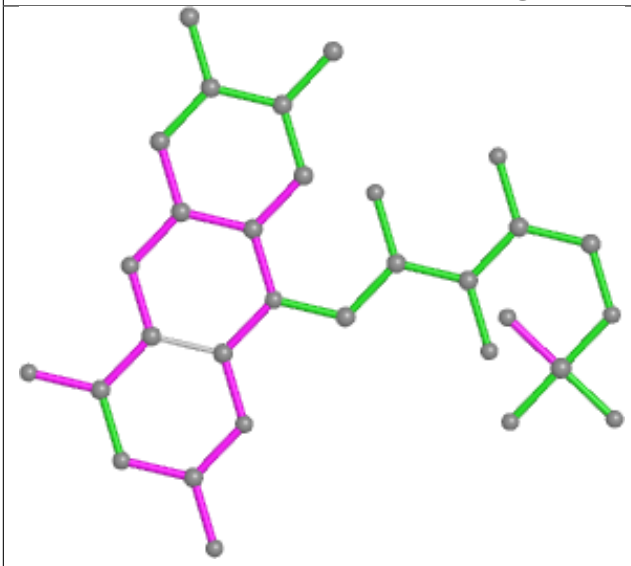


Torsions



Rings

Ligand FNR C 1108



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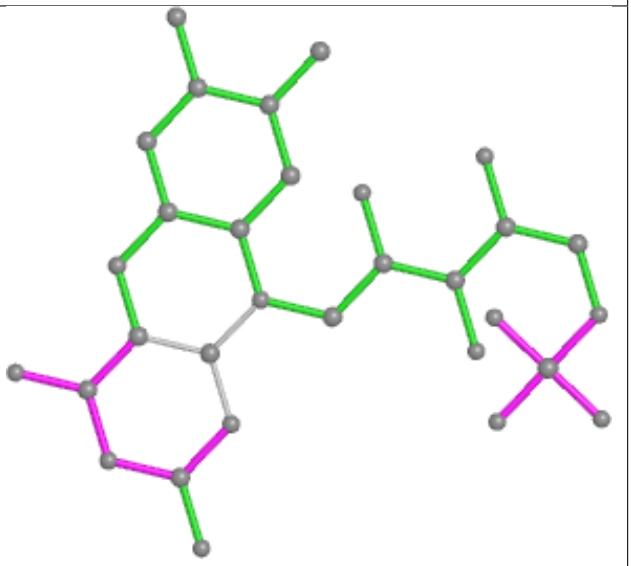
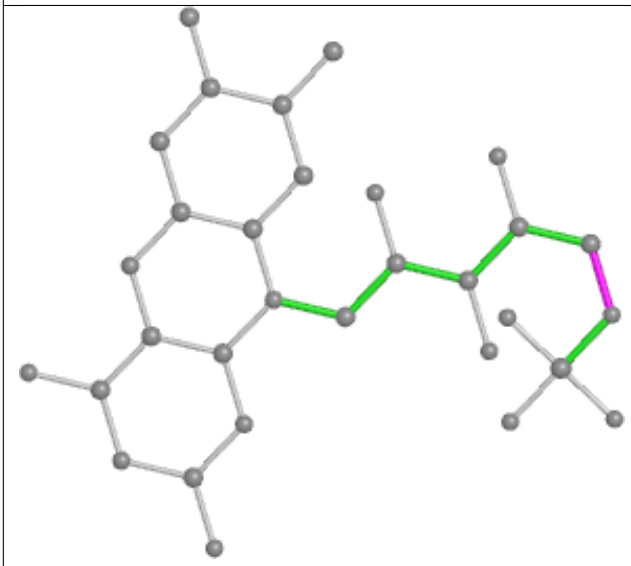


Bond angles



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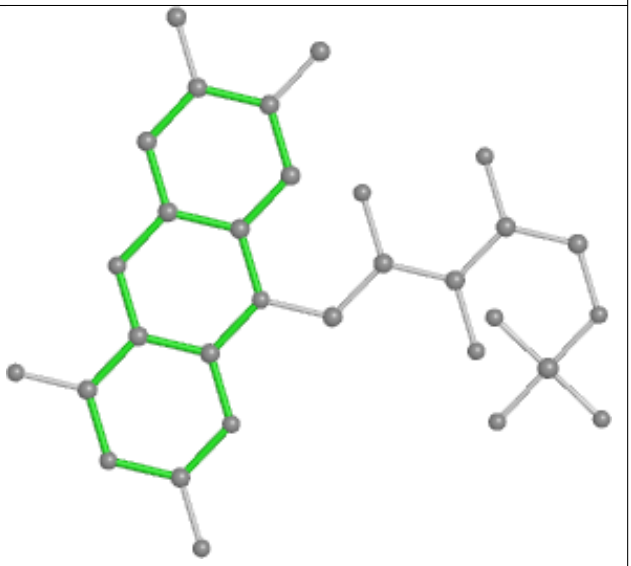
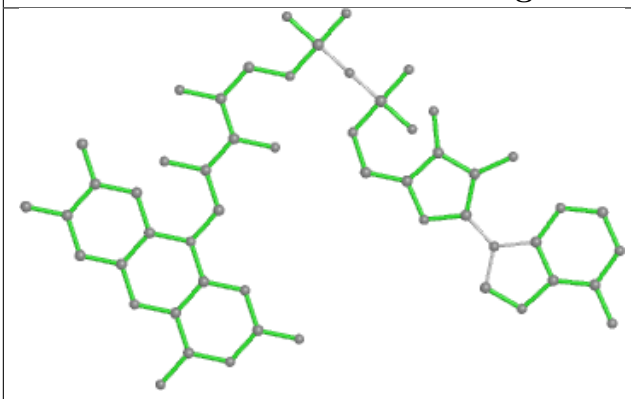


Rings

Ligand FAD A 1105



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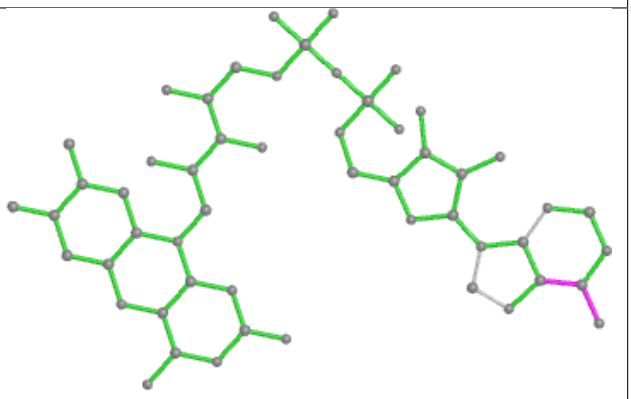
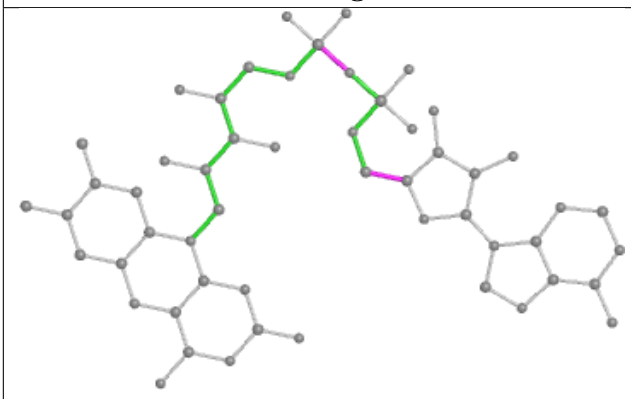
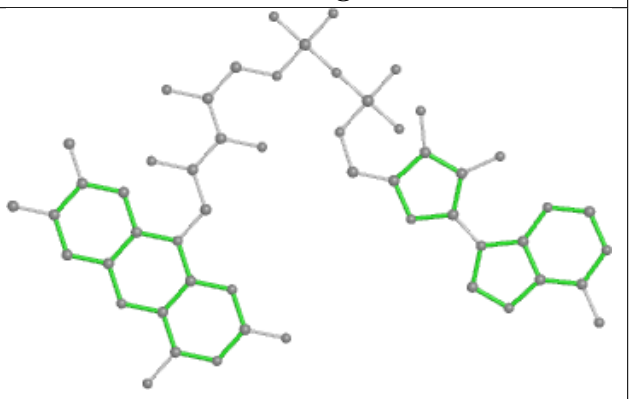


Bond angles

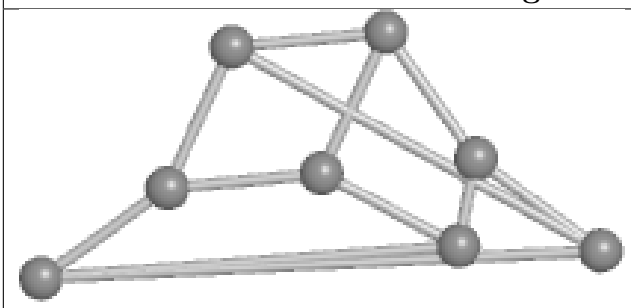


Torsions



Rings

Ligand SF4 B 1103



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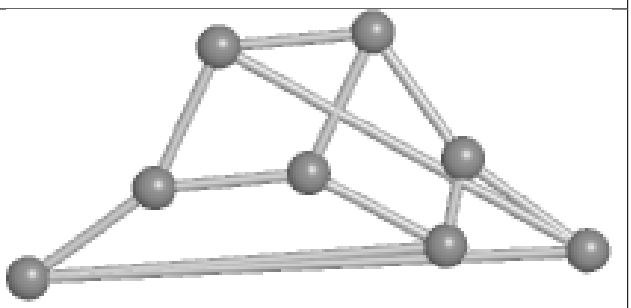
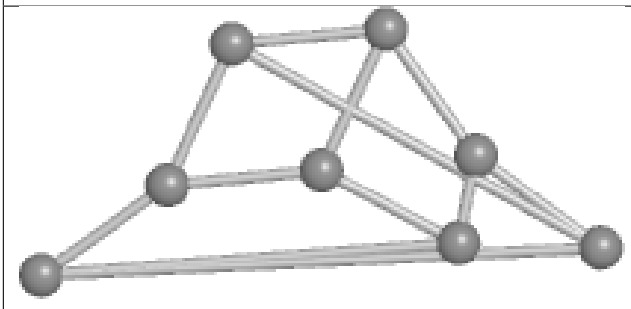
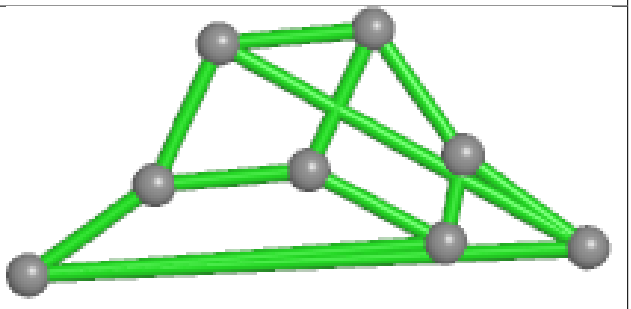


Bond angles

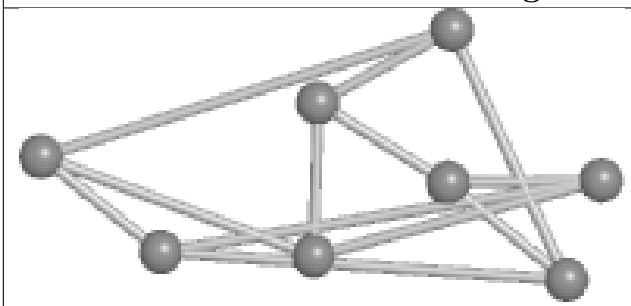


Torsions

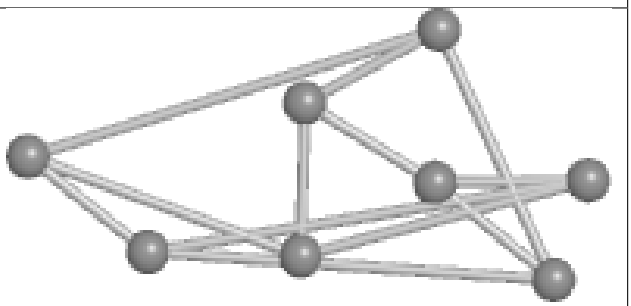


Rings

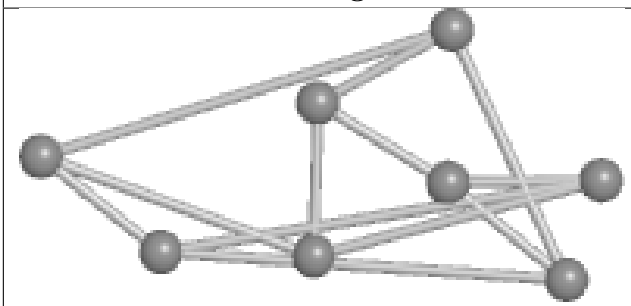
Ligand SF4 B 1102



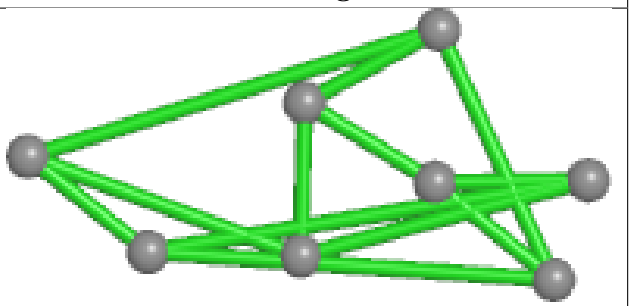
Bond lengths



Bond angles

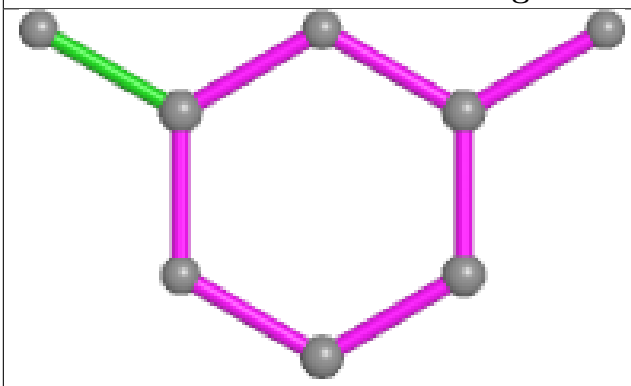


Torsions

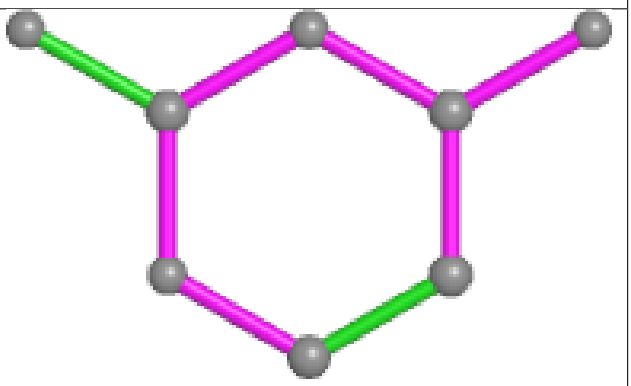


Rings

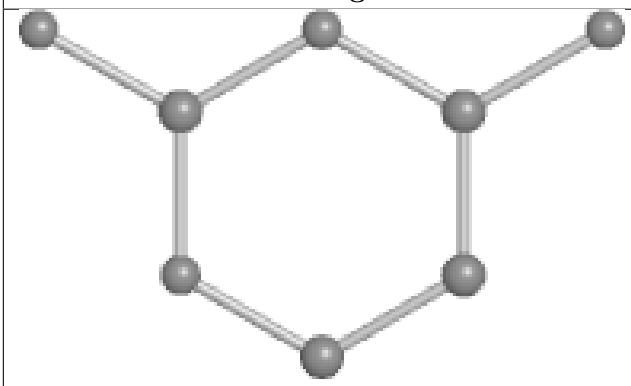
Ligand URA B 1107



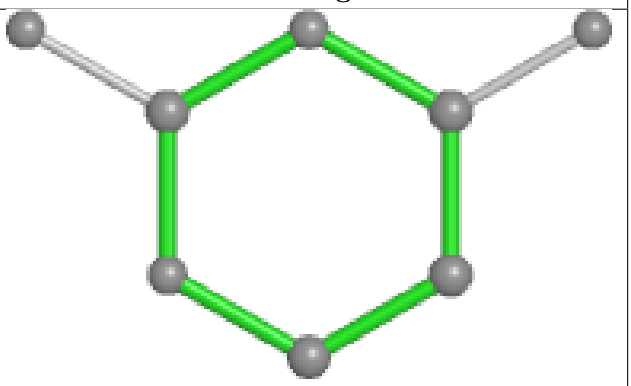
Bond lengths



Bond angles

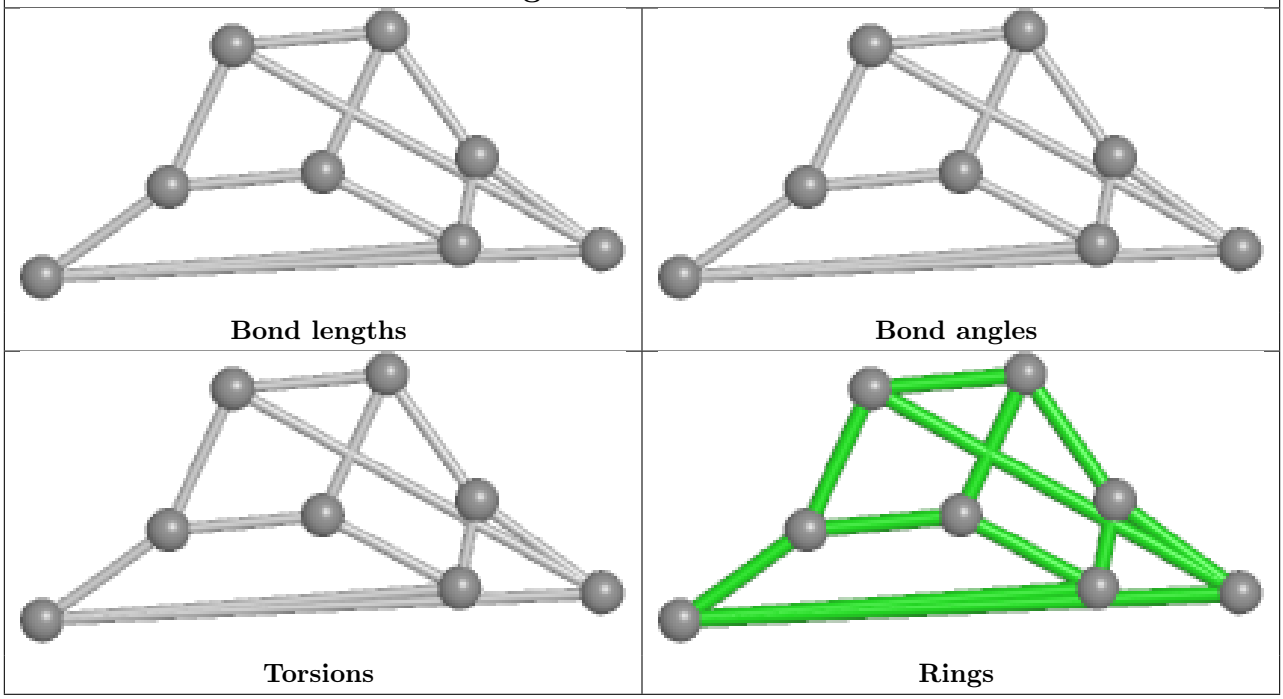


Torsions



Rings

Ligand SF4 C 1105



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	1007/1025 (98%)	-0.05	48 (4%)	30	25	19, 29, 61, 107	0
1	B	1006/1025 (98%)	0.03	56 (5%)	24	19	19, 30, 64, 117	0
1	C	1007/1025 (98%)	-0.08	49 (4%)	29	24	19, 28, 62, 107	0
1	D	1008/1025 (98%)	-0.06	42 (4%)	36	30	19, 29, 61, 111	0
All	All	4028/4100 (98%)	-0.04	195 (4%)	30	25	19, 29, 63, 117	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	897	LEU	15.8
1	A	907	LEU	15.7
1	B	907	LEU	14.9
1	B	900	GLN	10.4
1	D	52	CYS	9.1
1	D	901	ASN	8.9
1	B	871	LEU	8.9
1	A	868	ILE	8.9
1	B	867	ARG	8.8
1	B	870	GLU	8.5
1	B	901	ASN	8.3
1	D	51	HIS	8.2
1	C	415	GLU	8.2
1	B	899	GLU	8.1
1	B	902	ALA	8.0
1	D	902	ALA	8.0
1	A	50	PHE	7.9
1	B	868	ILE	7.5
1	A	52	CYS	7.5
1	B	869	ALA	7.4
1	B	52	CYS	7.1

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Mol	Chain	Res	Type	RSRZ
1	A	1018	PRO	6.7
1	A	908	GLU	6.7
1	A	900	GLN	6.6
1	D	415	GLU	6.5
1	B	324	CYS	6.4
1	A	867	ARG	6.4
1	C	324	CYS	6.3
1	D	869	ALA	6.3
1	C	901	ASN	6.3
1	D	871	LEU	6.2
1	B	415	GLU	6.1
1	B	908	GLU	6.0
1	D	416	THR	6.0
1	D	900	GLN	6.0
1	B	51	HIS	6.0
1	A	864	PRO	5.8
1	B	874	LYS	5.8
1	C	907	LEU	5.7
1	B	872	MET	5.7
1	D	897	LEU	5.6
1	B	865	VAL	5.6
1	A	51	HIS	5.6
1	C	417	GLY	5.4
1	C	52	CYS	5.4
1	B	866	PRO	5.3
1	B	50	PHE	5.2
1	A	417	GLY	5.2
1	A	414	ASP	5.2
1	A	902	ALA	5.2
1	B	898	LYS	5.2
1	A	324	CYS	5.1
1	D	907	LEU	5.1
1	B	896	ARG	5.1
1	D	868	ILE	5.1
1	B	856	THR	5.1
1	C	414	ASP	5.1
1	A	870	GLU	4.9
1	C	872	MET	4.9
1	B	414	ASP	4.8
1	C	320	GLY	4.8
1	C	51	HIS	4.8
1	D	899	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	415	GLU	4.7
1	B	873	GLY	4.7
1	D	870	GLU	4.6
1	C	867	ARG	4.6
1	C	418	LYS	4.6
1	B	53	GLU	4.5
1	A	899	GLU	4.5
1	B	1010	PRO	4.5
1	A	866	PRO	4.4
1	C	322	CYS	4.4
1	A	873	GLY	4.4
1	B	892	GLU	4.3
1	A	897	LEU	4.3
1	D	418	LYS	4.3
1	B	417	GLY	4.3
1	C	870	GLU	4.2
1	D	867	ARG	4.2
1	B	895	MET	4.2
1	D	459	TRP	4.2
1	B	891	ALA	4.2
1	D	873	GLY	4.2
1	C	416	THR	4.2
1	C	1010	PRO	4.1
1	C	908	GLU	4.1
1	A	871	LEU	4.0
1	D	414	ASP	4.0
1	C	866	PRO	4.0
1	B	459	TRP	4.0
1	C	413	GLN	3.9
1	A	416	THR	3.8
1	B	420	ASN	3.8
1	D	866	PRO	3.8
1	C	874	LYS	3.7
1	D	50	PHE	3.7
1	A	326	SER	3.7
1	C	419	TRP	3.6
1	D	419	TRP	3.6
1	D	856	THR	3.6
1	D	53	GLU	3.5
1	A	869	ALA	3.5
1	A	413	GLN	3.5
1	D	909	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	901	ASN	3.4
1	D	908	GLU	3.4
1	C	868	ILE	3.4
1	C	903	ALA	3.4
1	A	332	ARG	3.4
1	D	874	LYS	3.3
1	C	902	ALA	3.3
1	C	904	PHE	3.3
1	D	420	ASN	3.3
1	C	325	HIS	3.3
1	C	906	PRO	3.2
1	C	319	ALA	3.2
1	D	417	GLY	3.2
1	C	900	GLN	3.2
1	C	869	ALA	3.2
1	C	332	ARG	3.2
1	C	330	SER	3.1
1	C	682	LEU	3.1
1	B	325	HIS	3.0
1	B	1008	THR	3.0
1	A	53	GLU	3.0
1	B	419	TRP	3.0
1	C	50	PHE	3.0
1	B	330	SER	3.0
1	A	893	GLU	3.0
1	C	865	VAL	3.0
1	B	367	PHE	3.0
1	B	180	GLU	3.0
1	A	895	MET	3.0
1	C	323	ALA	3.0
1	C	905	PRO	3.0
1	B	416	THR	2.9
1	A	872	MET	2.9
1	A	865	VAL	2.9
1	A	875	LYS	2.9
1	B	893	GLU	2.8
1	B	672	PRO	2.8
1	D	48	ASN	2.8
1	C	899	GLU	2.8
1	D	892	GLU	2.8
1	B	582	ILE	2.7
1	D	895	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	897	LEU	2.7
1	B	332	ARG	2.7
1	C	873	GLY	2.7
1	A	419	TRP	2.7
1	A	891	ALA	2.7
1	A	874	LYS	2.6
1	B	1018	PRO	2.6
1	B	418	LYS	2.6
1	C	1012	GLU	2.6
1	C	327	PRO	2.6
1	C	871	LEU	2.6
1	B	48	ASN	2.6
1	A	1019	LEU	2.6
1	B	371	ARG	2.5
1	A	896	ARG	2.5
1	D	865	VAL	2.4
1	D	857	GLU	2.4
1	B	673	HIS	2.4
1	B	323	ALA	2.4
1	D	458	ARG	2.4
1	B	413	GLN	2.4
1	A	320	GLY	2.3
1	A	367	PHE	2.3
1	D	913	ILE	2.3
1	A	327	PRO	2.3
1	B	857	GLU	2.3
1	B	890	ILE	2.3
1	D	872	MET	2.2
1	D	332	ARG	2.2
1	B	1011	TYR	2.2
1	A	76	ALA	2.2
1	D	675	MET	2.2
1	D	180	GLU	2.2
1	A	857	GLU	2.1
1	A	1009	THR	2.1
1	B	875	LYS	2.1
1	C	420	ASN	2.1
1	C	180	GLU	2.1
1	C	326	SER	2.1
1	C	331	ILE	2.1
1	D	49	CYS	2.1
1	A	1012	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	179	GLN	2.1
1	D	891	ALA	2.1
1	A	1010	PRO	2.1
1	A	898	LYS	2.1
1	A	180	GLU	2.0
1	C	673	HIS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	LEU	B	1101	8/9	0.70	0.35	47,61,70,72	0
6	ALA	A	1108	5/6	0.72	0.31	58,65,68,69	0
6	ALA	D	1102	5/6	0.79	0.22	54,62,66,71	0
8	PRO	C	1101	7/8	0.79	0.28	52,59,62,64	0
7	LEU	D	1101	8/9	0.87	0.26	48,53,65,74	0
4	URA	B	1107	8/8	0.94	0.09	29,32,35,35	0
4	URA	A	1106	8/8	0.94	0.08	27,30,33,35	0
4	URA	D	1108	8/8	0.95	0.08	27,28,33,35	0
4	URA	C	1107	8/8	0.95	0.11	28,31,33,34	0
5	FNR	A	1107	31/31	0.97	0.11	18,21,25,28	0
5	FNR	D	1109	31/31	0.98	0.10	17,21,26,28	0
3	FAD	B	1106	53/53	0.98	0.07	22,28,33,34	0
3	FAD	C	1106	53/53	0.98	0.09	22,26,34,38	0
3	FAD	D	1107	53/53	0.98	0.07	23,27,31,32	0
3	FAD	A	1105	53/53	0.98	0.07	20,24,28,29	0
5	FNR	C	1108	31/31	0.98	0.09	18,21,25,28	0
2	SF4	D	1104	8/8	0.99	0.08	20,21,22,22	0

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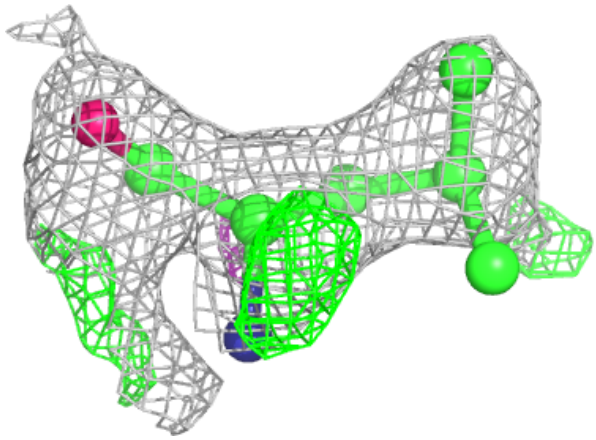
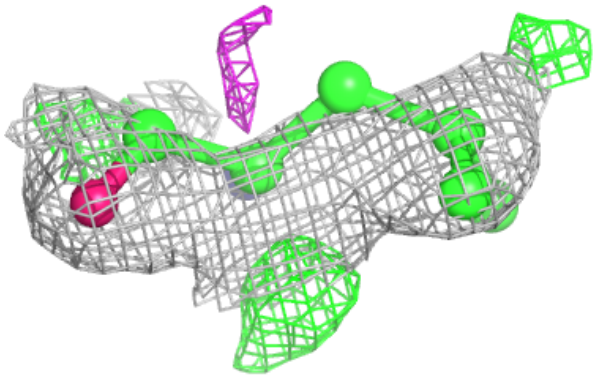
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SF4	D	1105	8/8	0.99	0.09	20,20,21,21	0
2	SF4	D	1106	8/8	0.99	0.07	20,20,22,22	0
2	SF4	B	1103	8/8	0.99	0.08	19,21,22,22	0
2	SF4	C	1105	8/8	0.99	0.09	20,22,23,23	0
2	SF4	D	1103	8/8	0.99	0.07	21,22,23,24	0
5	FNR	B	1108	31/31	0.99	0.09	19,22,27,29	0
2	SF4	A	1104	8/8	1.00	0.06	22,22,23,24	0
2	SF4	B	1102	8/8	1.00	0.09	20,21,22,23	0
2	SF4	A	1101	8/8	1.00	0.08	20,21,22,23	0
2	SF4	B	1104	8/8	1.00	0.07	21,22,24,24	0
2	SF4	B	1105	8/8	1.00	0.07	20,21,21,22	0
2	SF4	C	1102	8/8	1.00	0.07	19,20,21,21	0
2	SF4	C	1103	8/8	1.00	0.06	19,21,21,21	0
2	SF4	C	1104	8/8	1.00	0.08	19,21,21,21	0
2	SF4	A	1102	8/8	1.00	0.10	20,21,21,23	0
2	SF4	A	1103	8/8	1.00	0.07	18,21,22,23	0

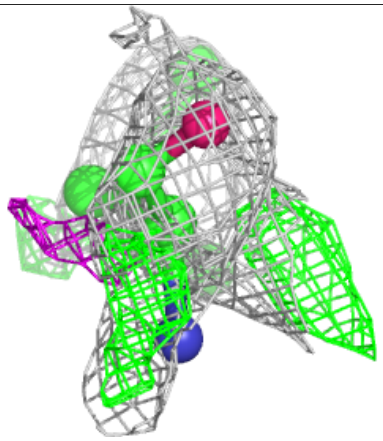
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LEU 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)

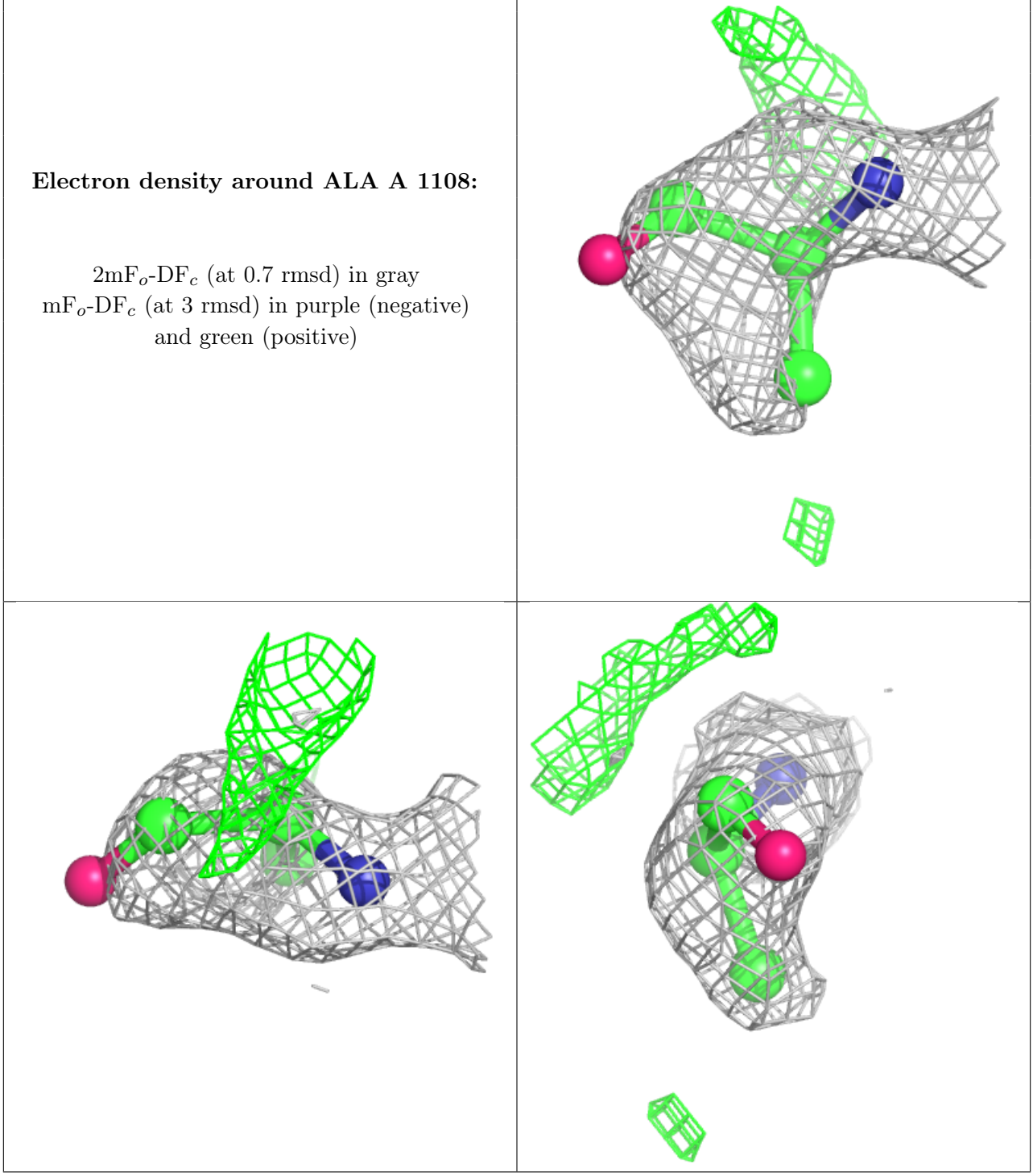






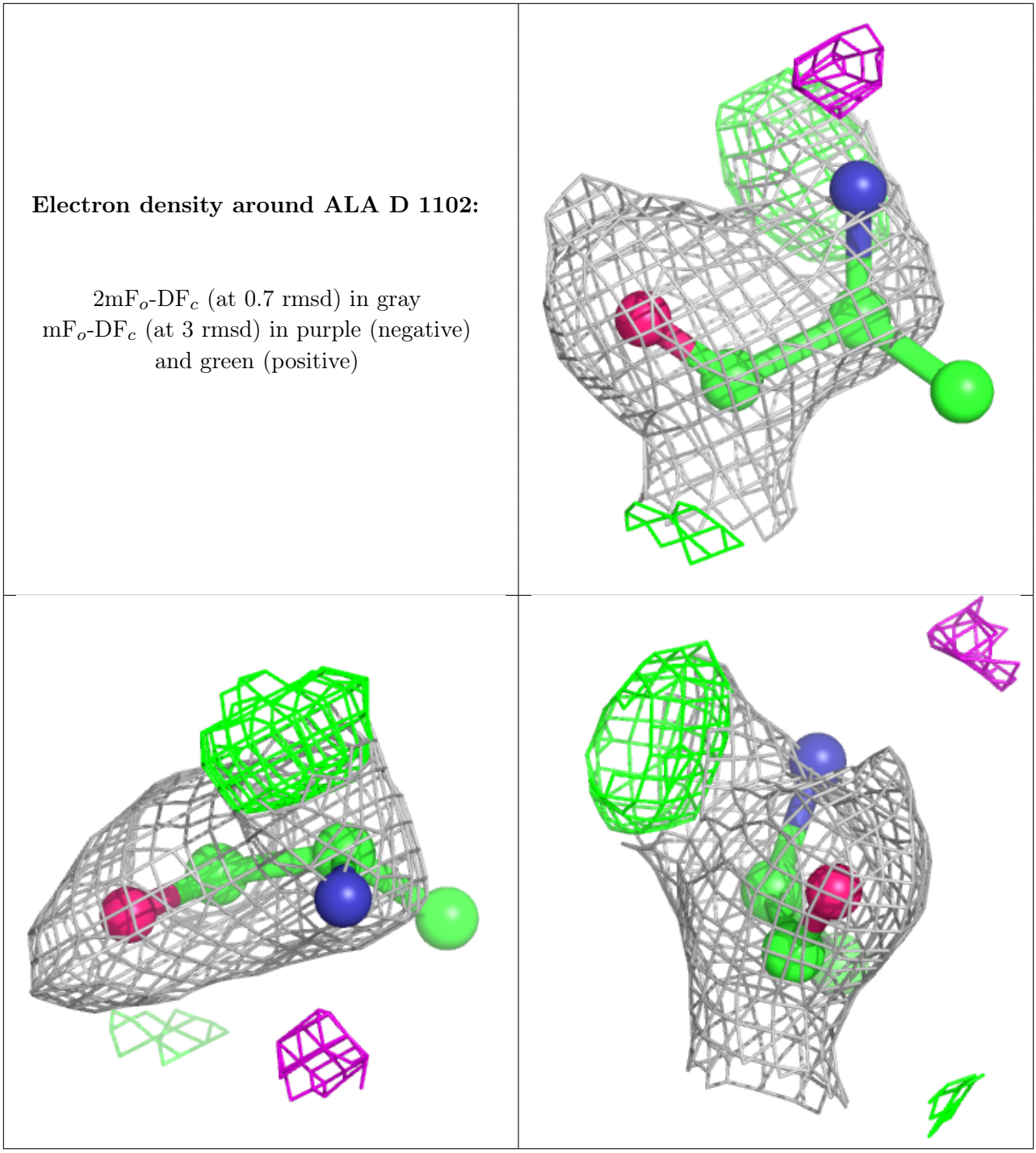
Electron density around ALA A 1108:

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



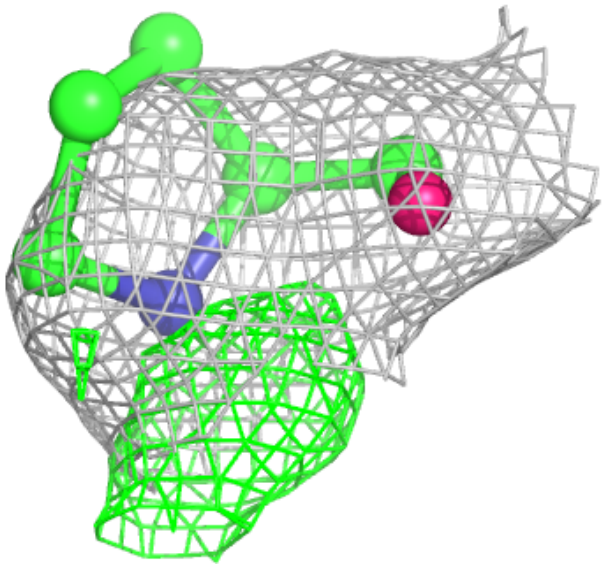
Electron density around ALA D 1102:

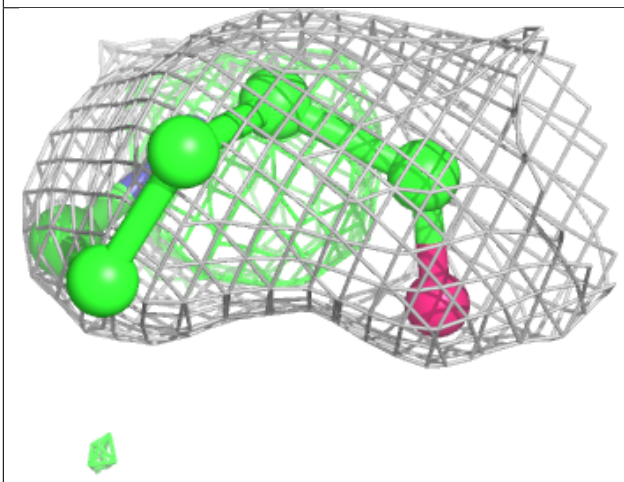
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

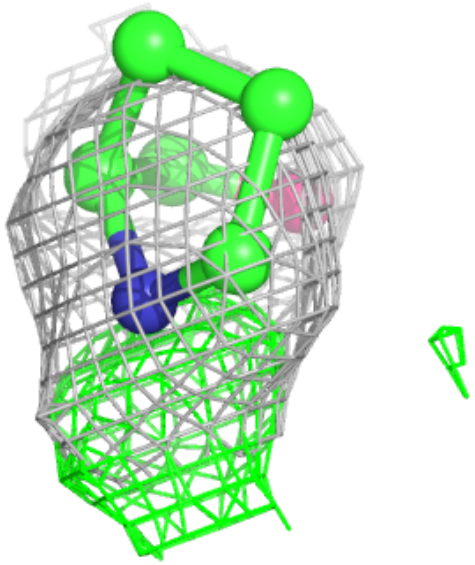


Electron density around PRO C 1101:

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

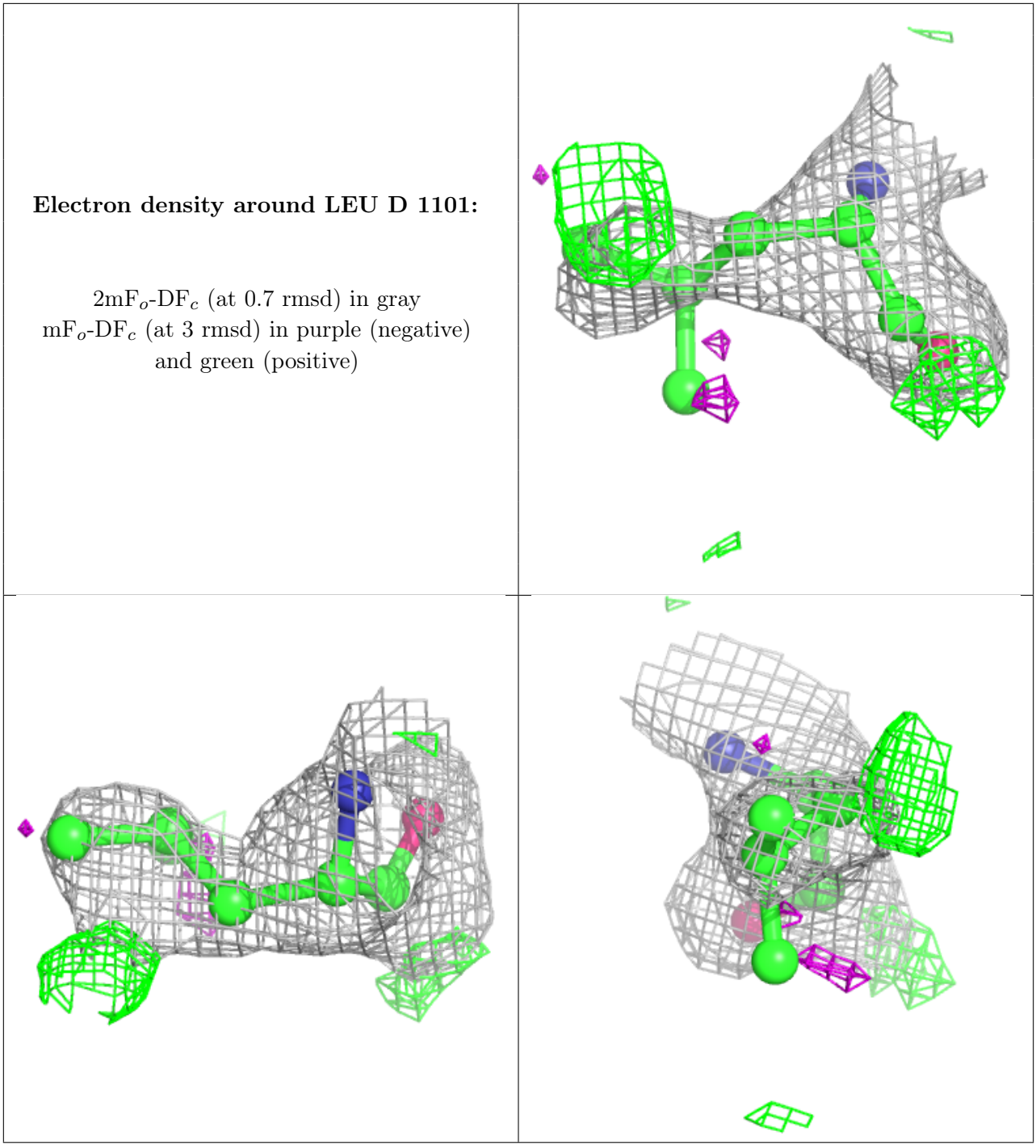






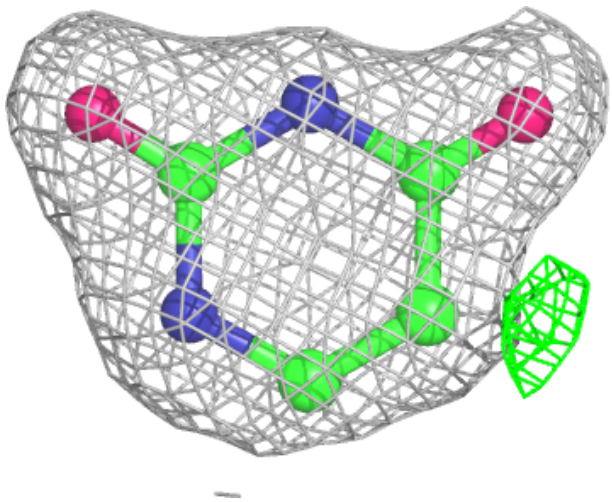
Electron density around LEU D 1101:

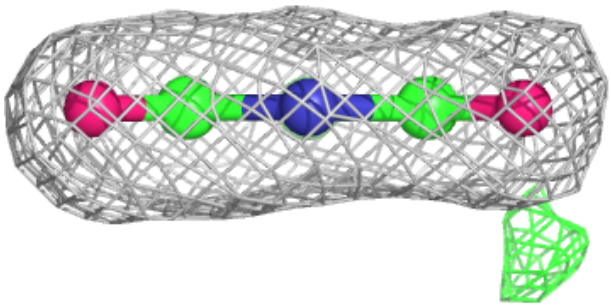
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

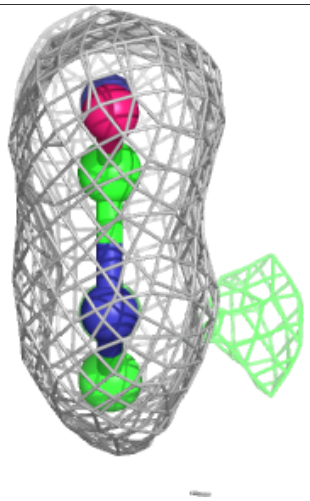


Electron density around URA B 1107:

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

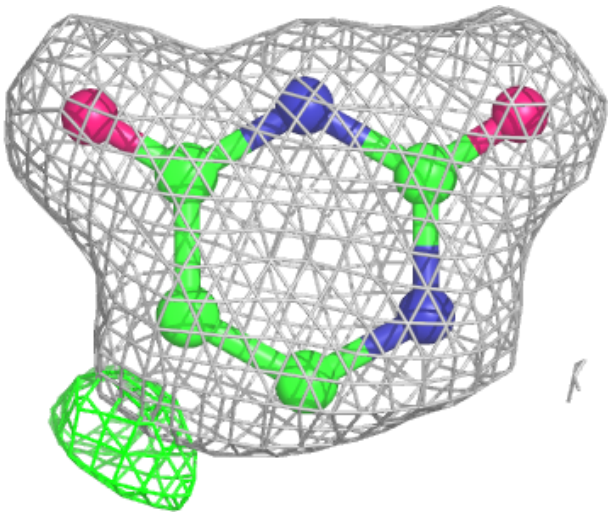


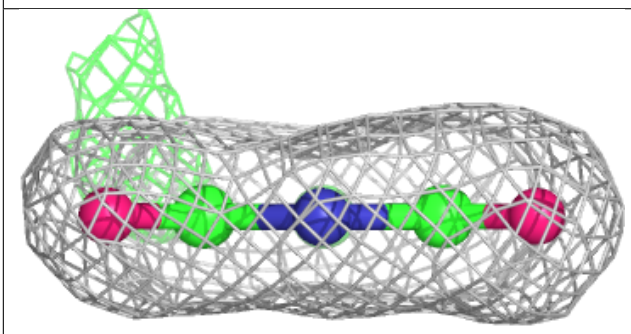


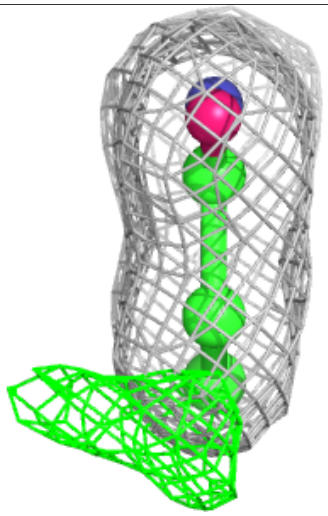


Electron density around URA A 1106:

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

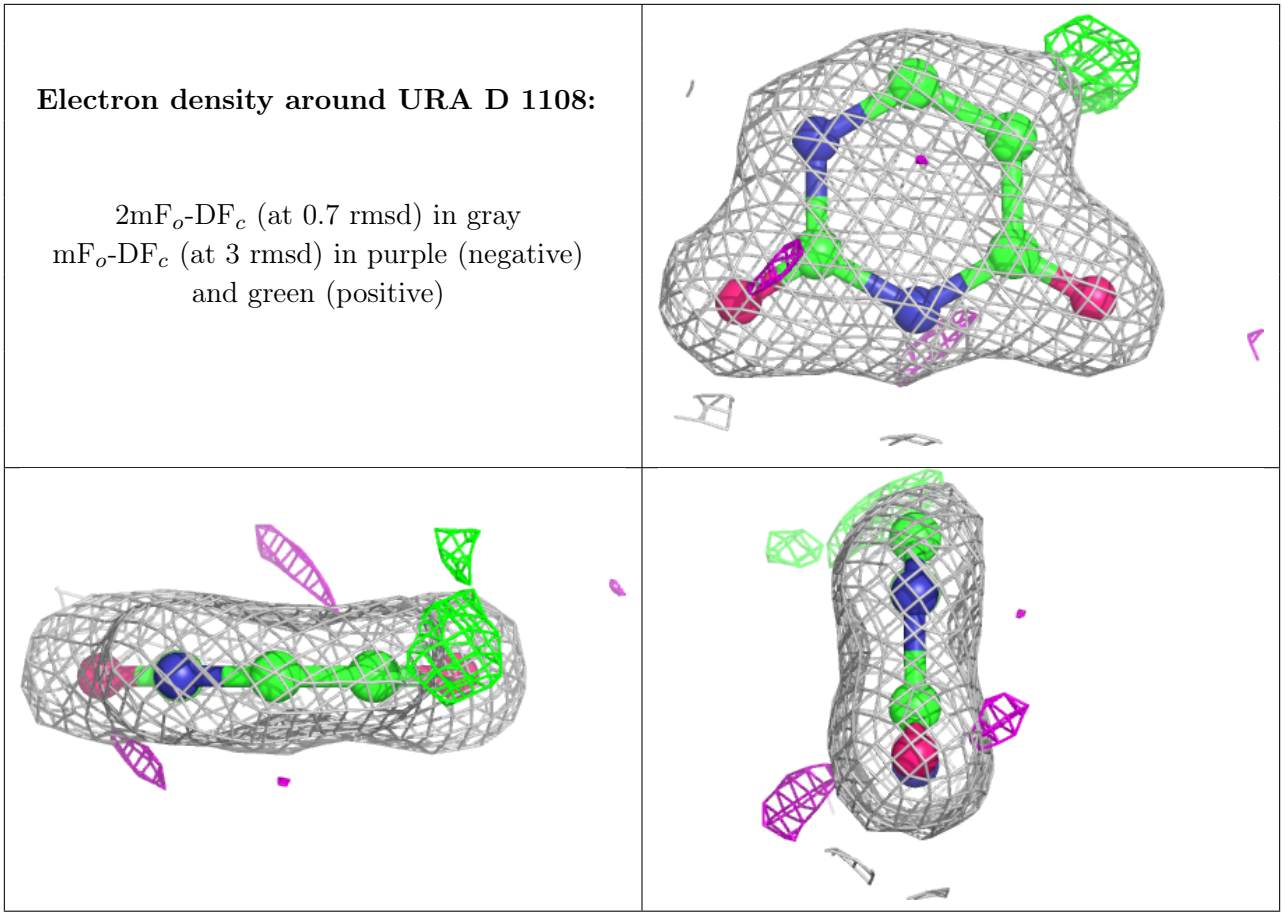






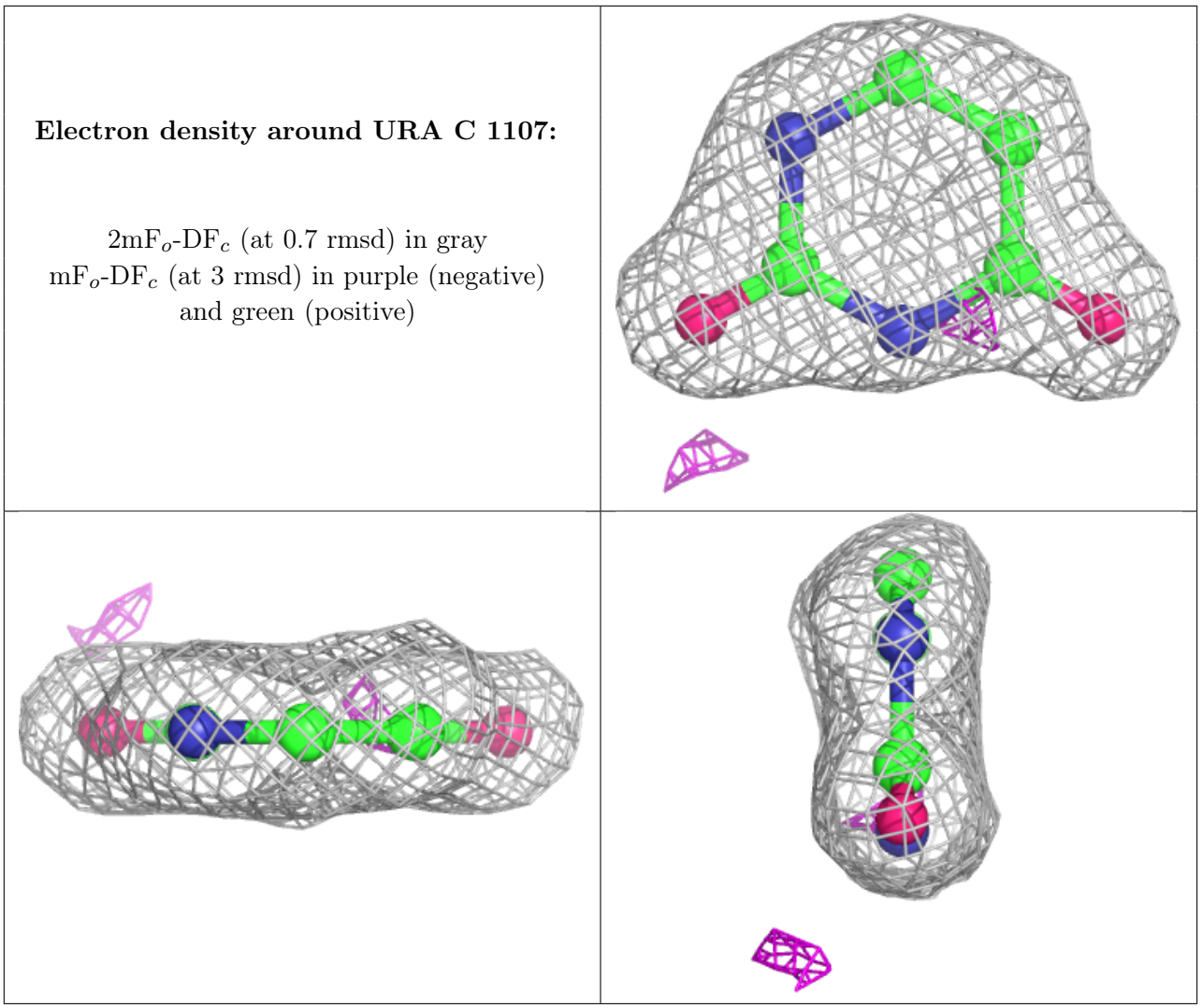
Electron density around URA D 1108:

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



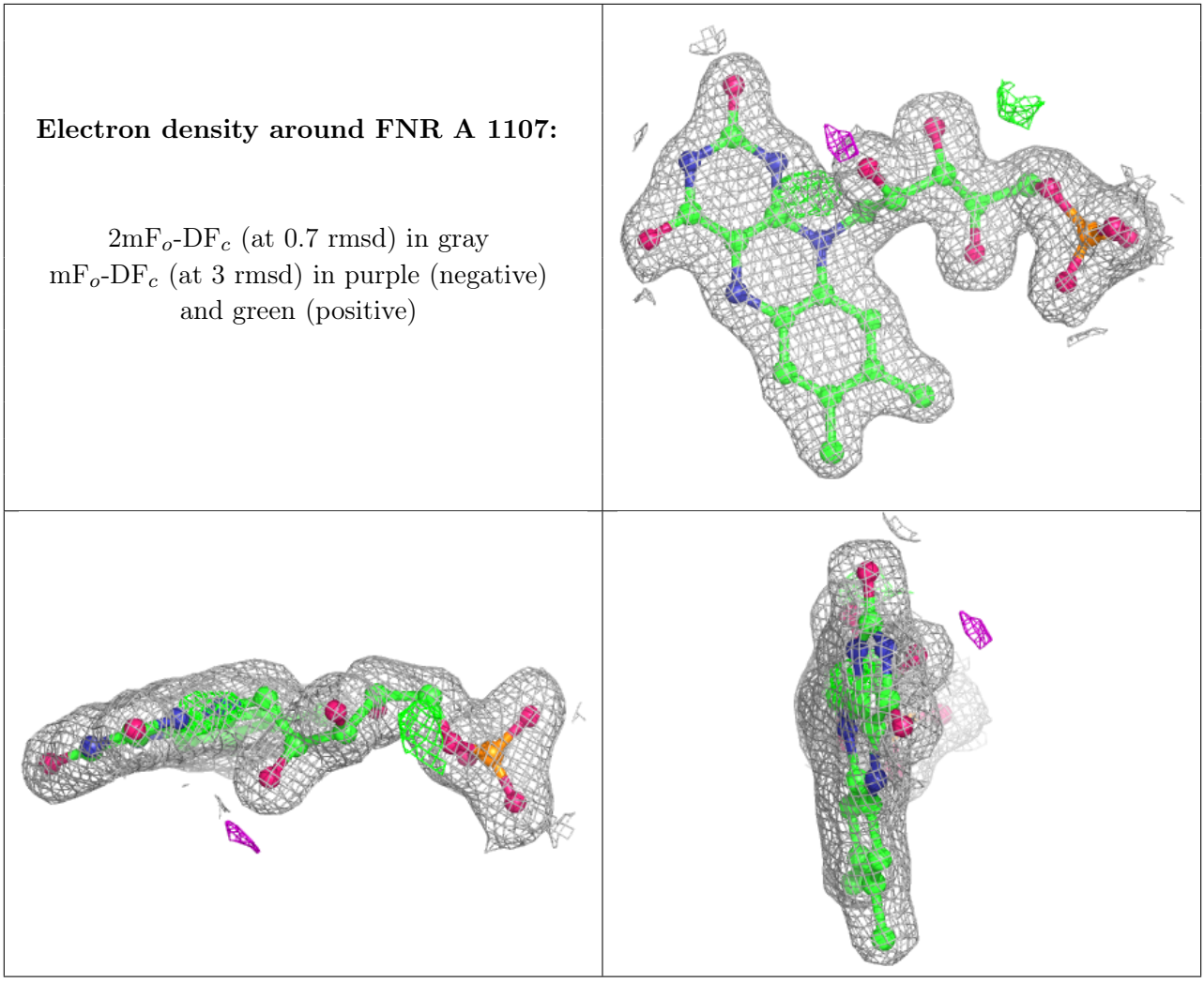
Electron density around URA C 1107:

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



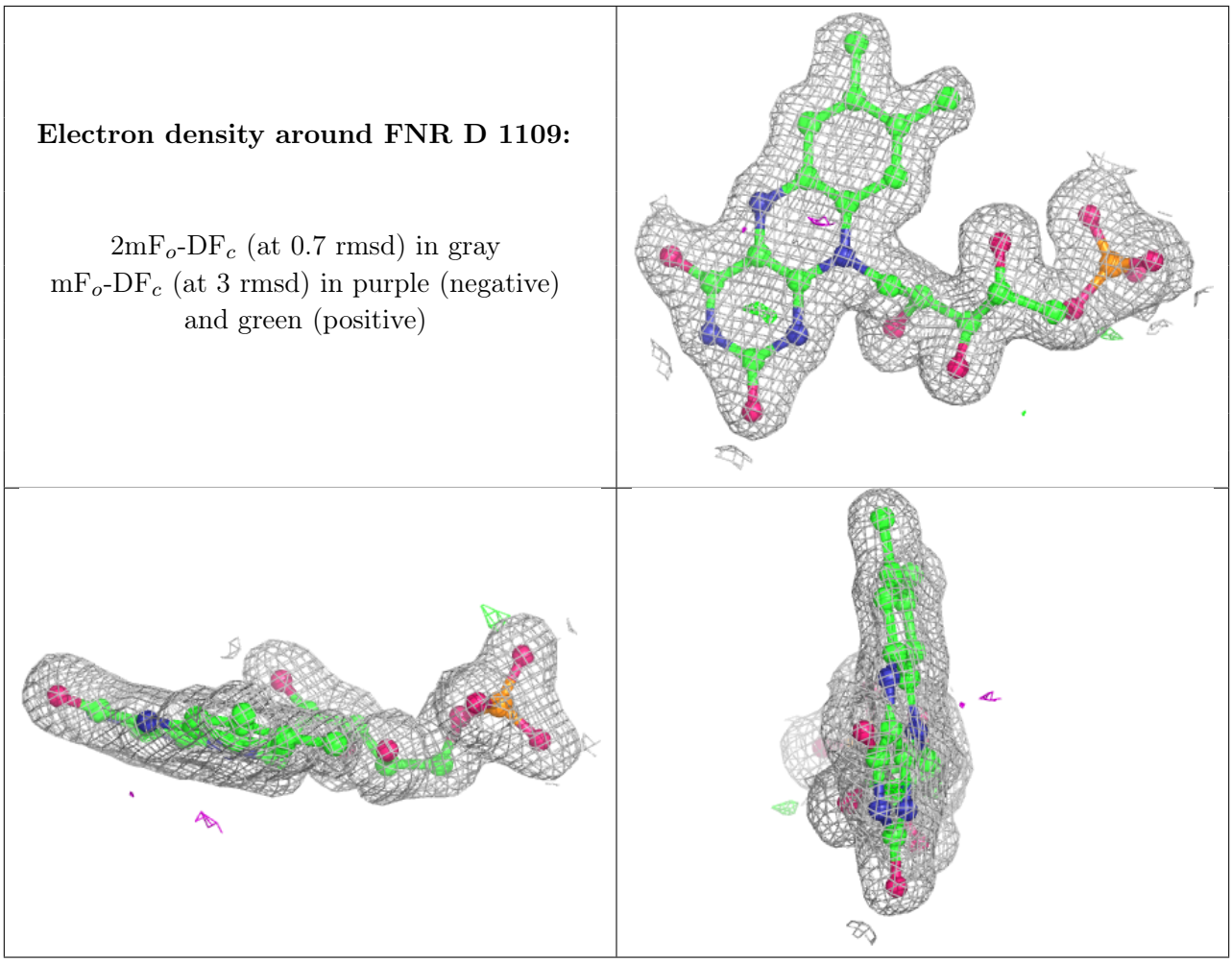
Electron density around FNR A 1107:

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



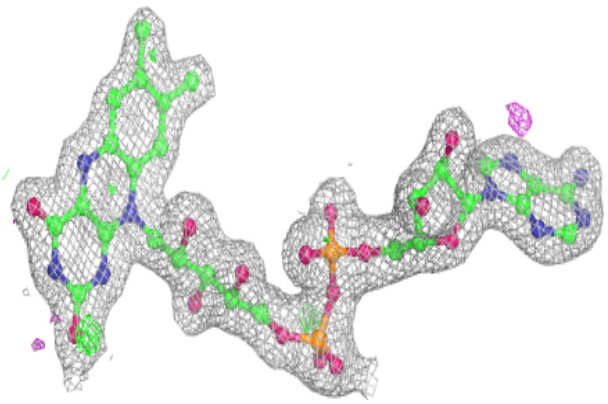
Electron density around FNR D 1109:

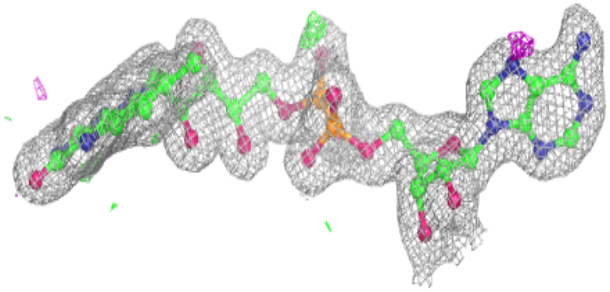
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

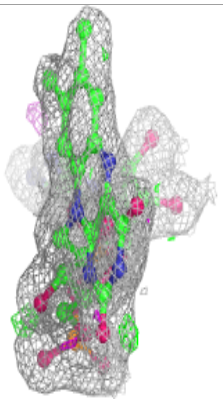


Electron density around FAD B 1106:

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

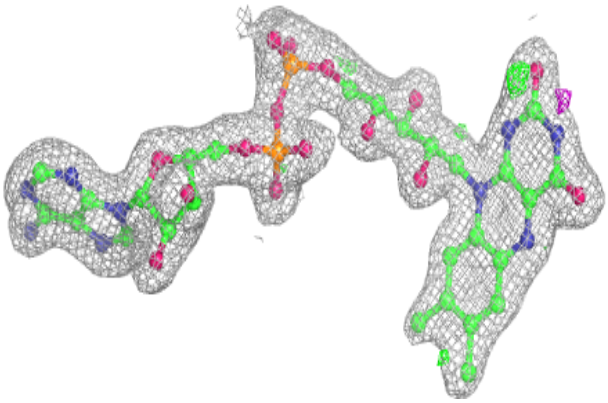


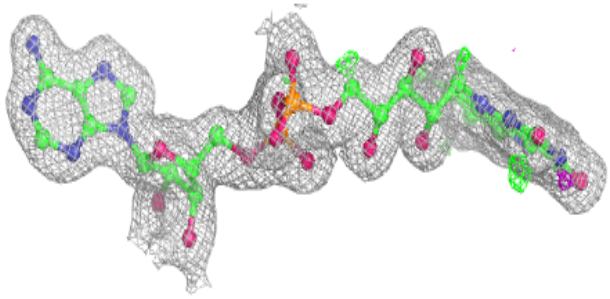


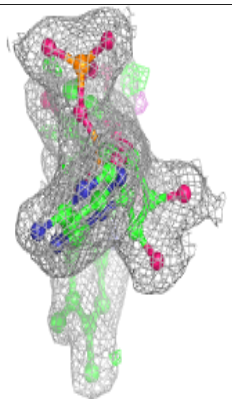


Electron density around FAD C 1106:

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

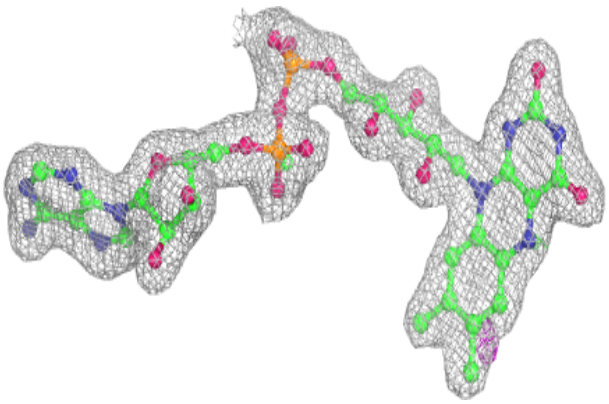


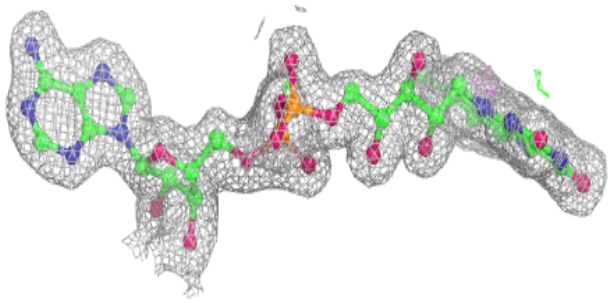


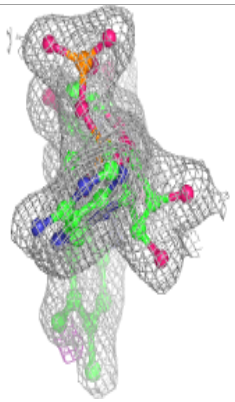


Electron density around FAD D 1107:

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

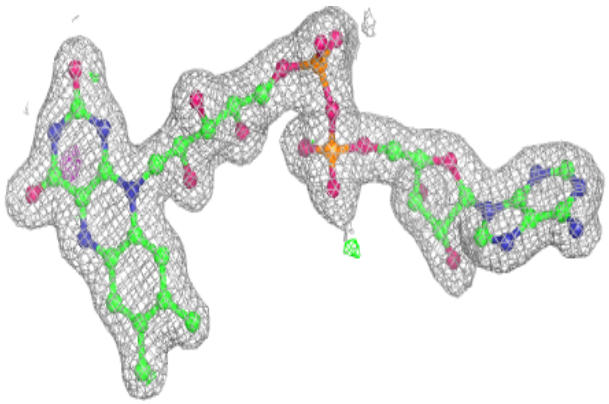


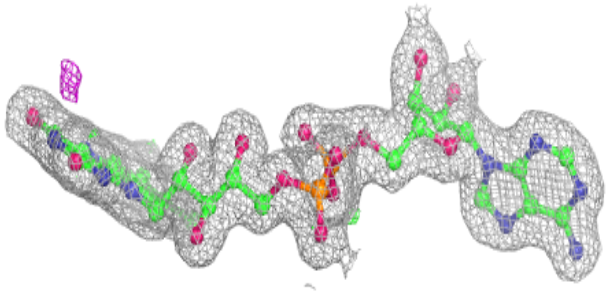


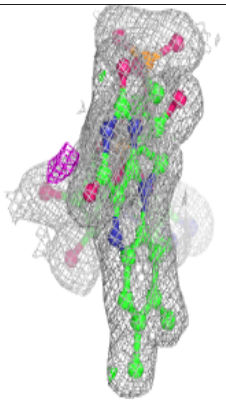


Electron density around FAD A 1105:

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

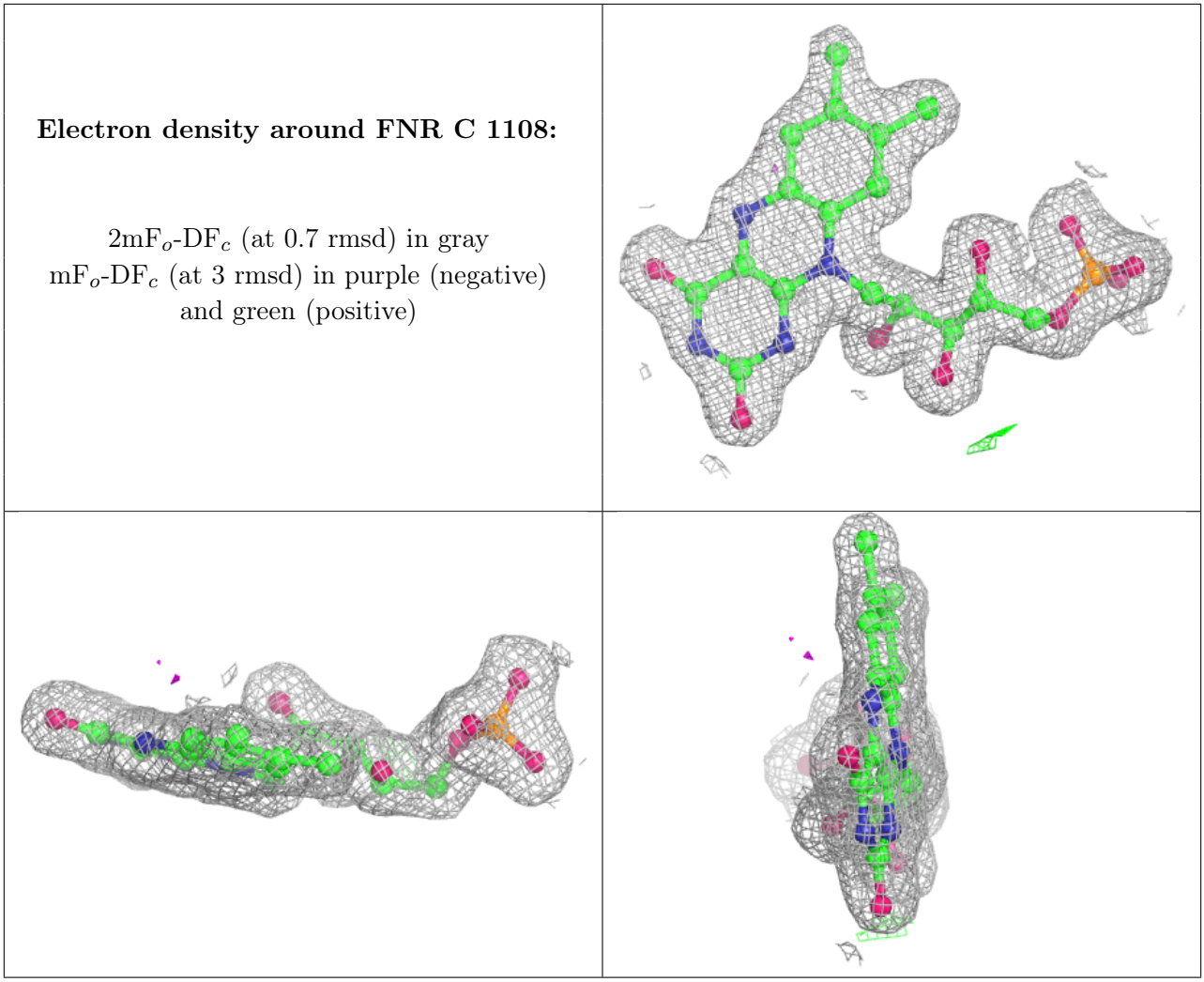






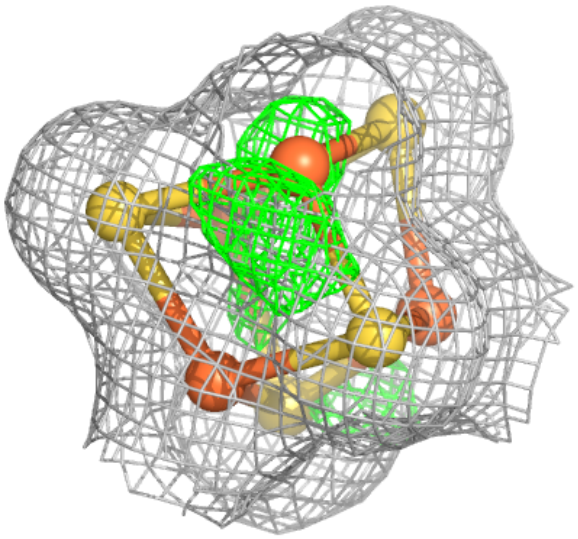
Electron density around FNR C 1108:

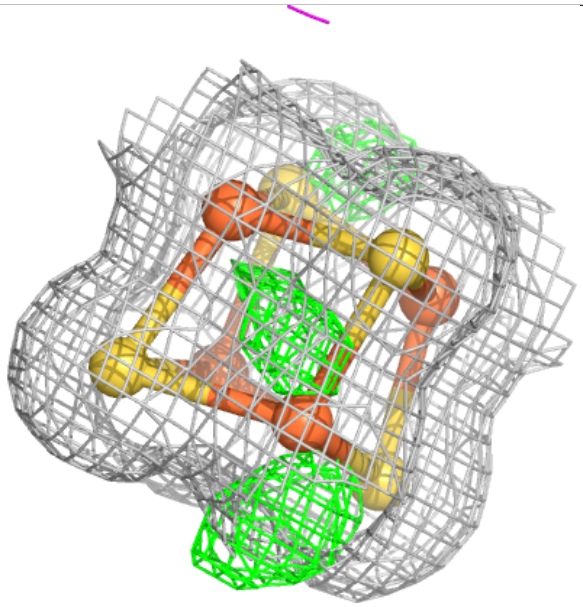
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

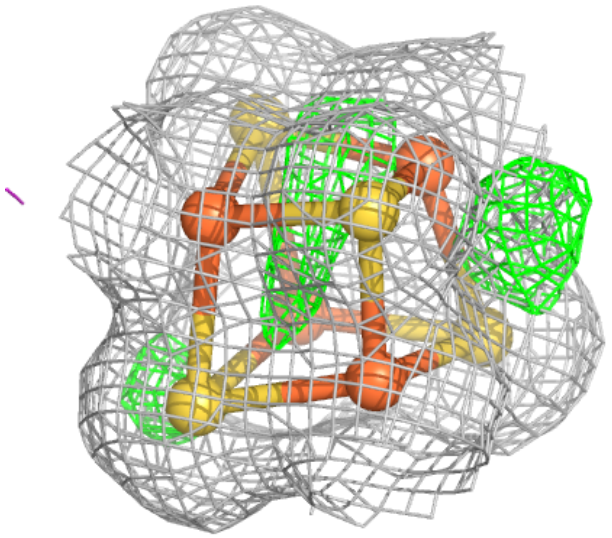


Electron density around SF4 D 1104:

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

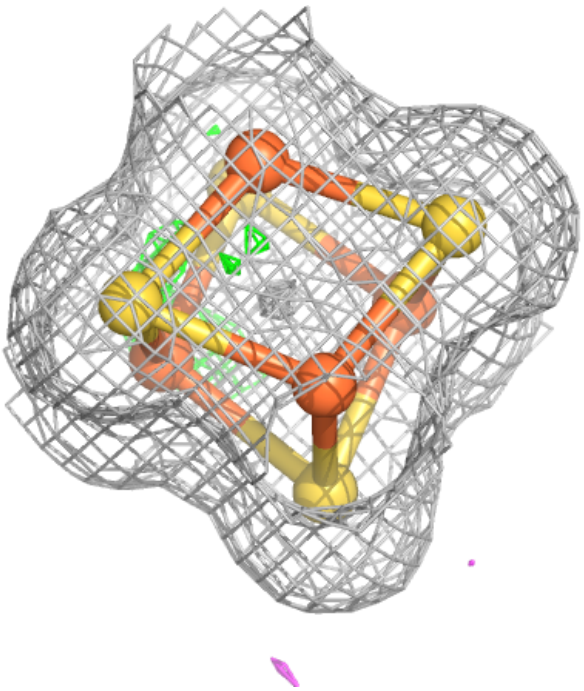


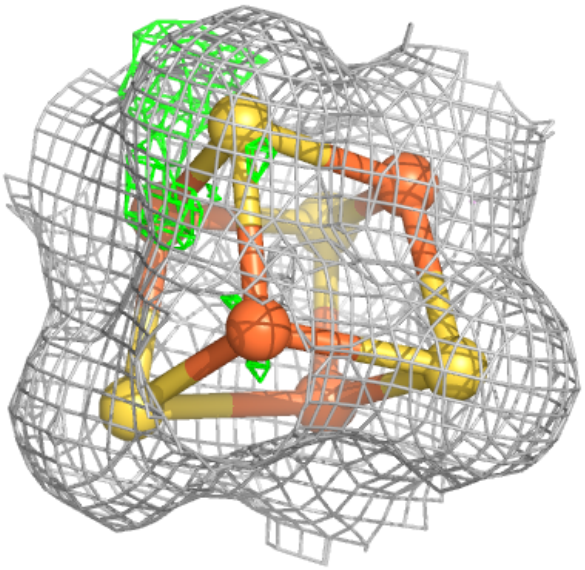


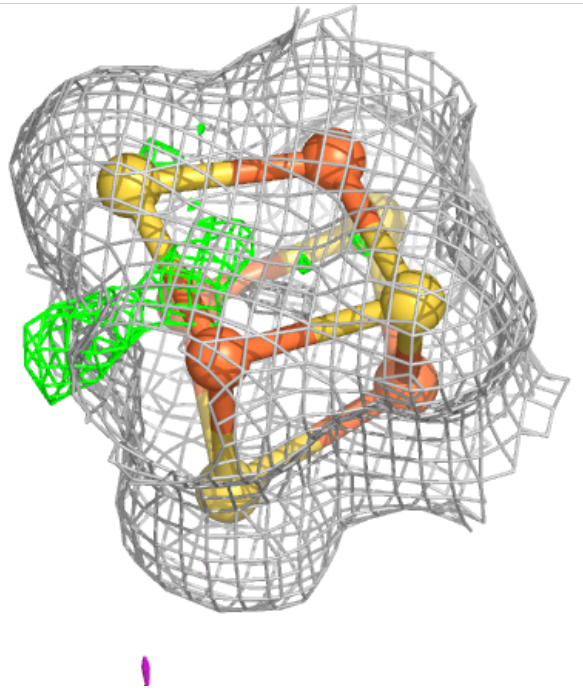


Electron density around SF4 D 1105:

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

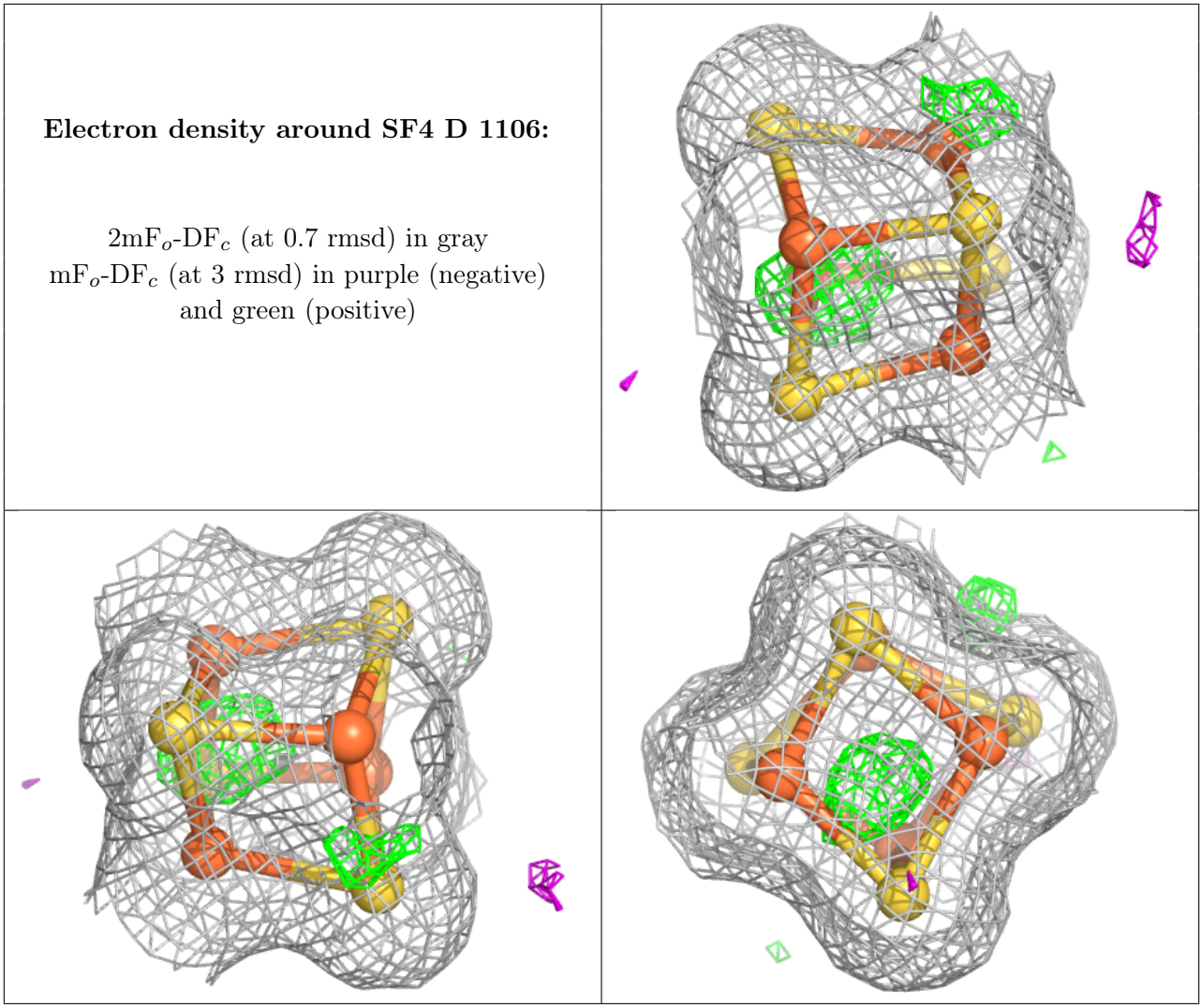






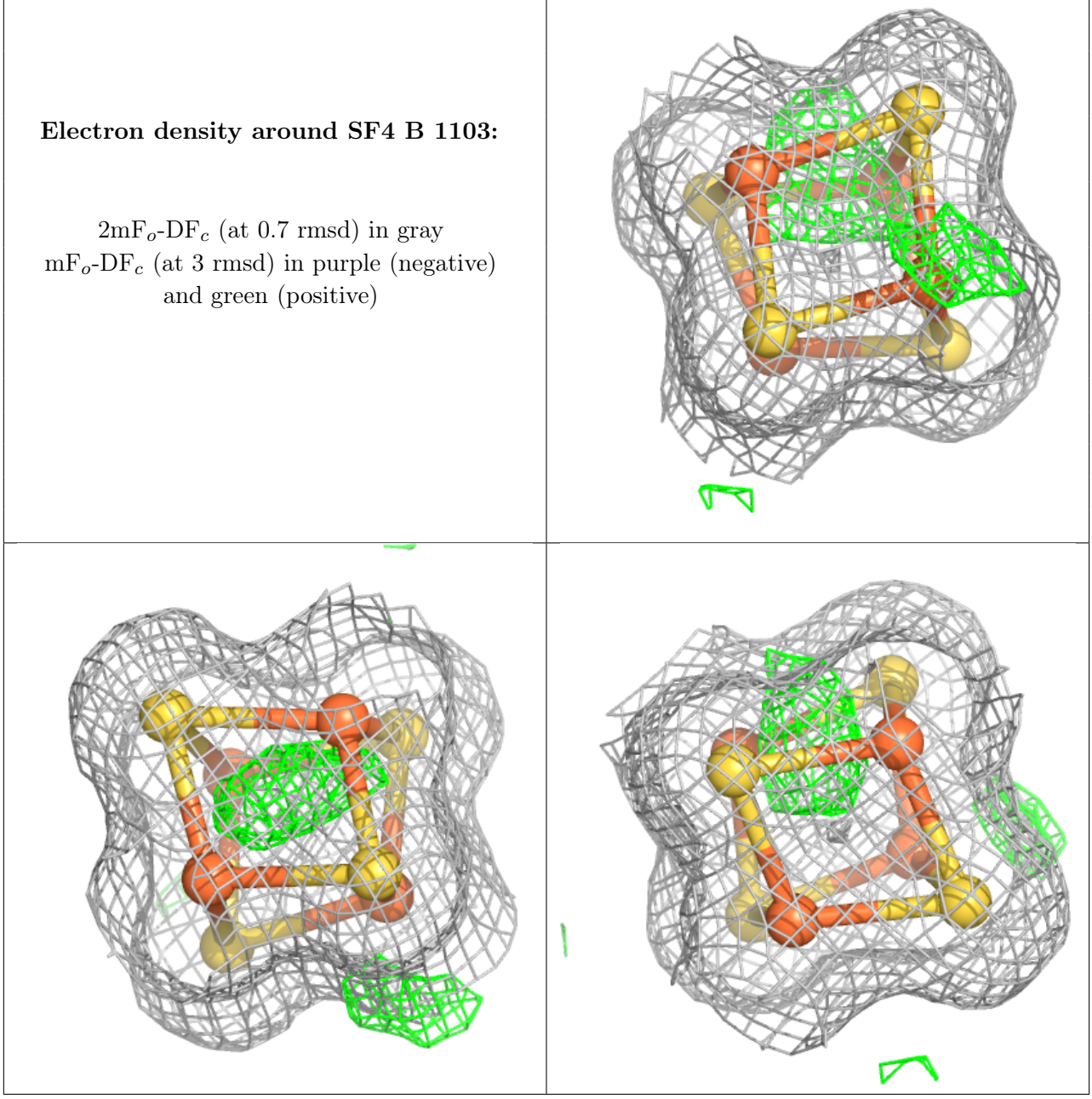
Electron density around SF4 D 1106:

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



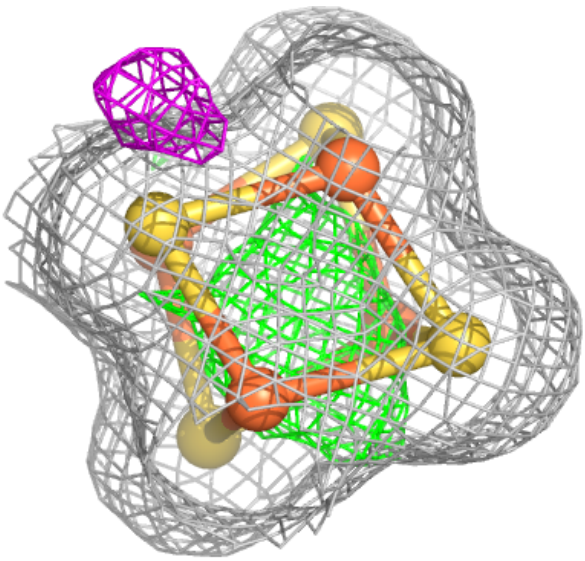
Electron density around SF4 B 1103:

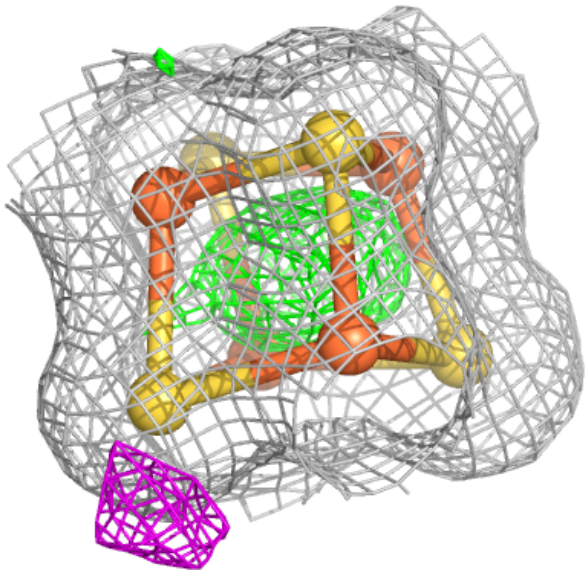
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

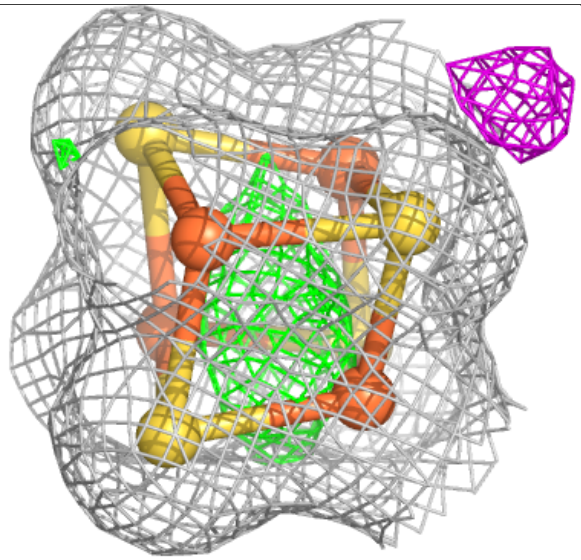


Electron density around SF4 C 1105:

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

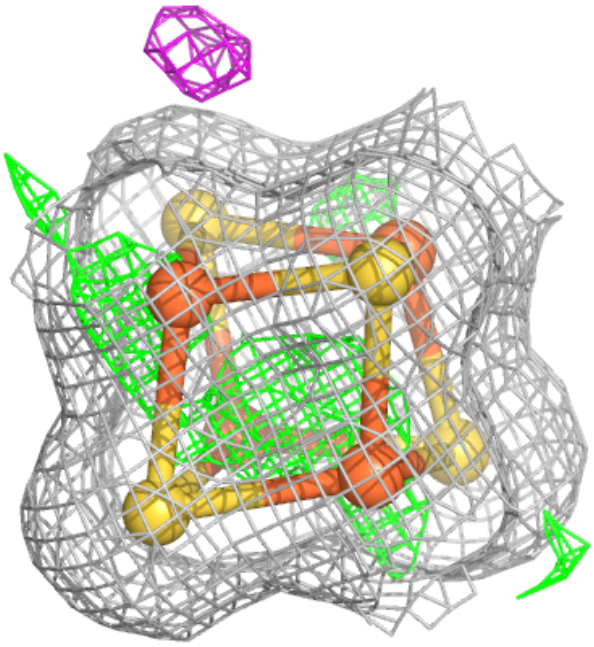


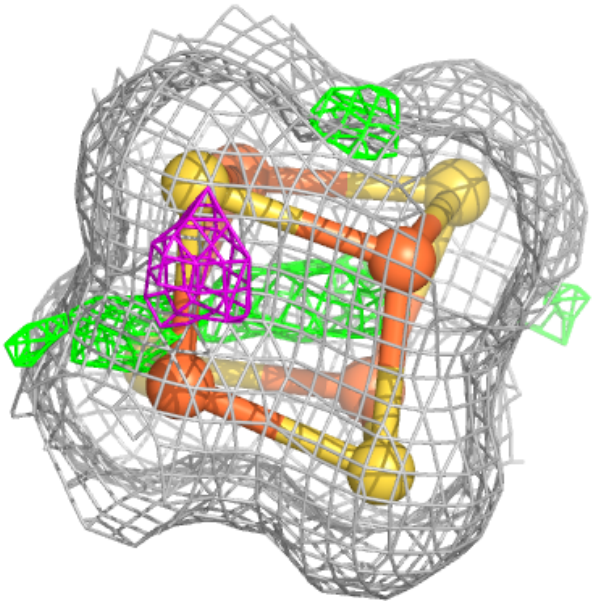


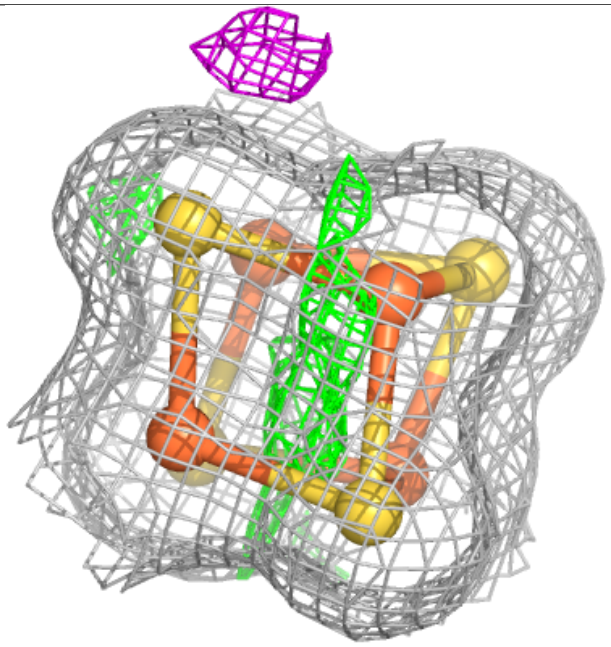


Electron density around SF4 D 1103:

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

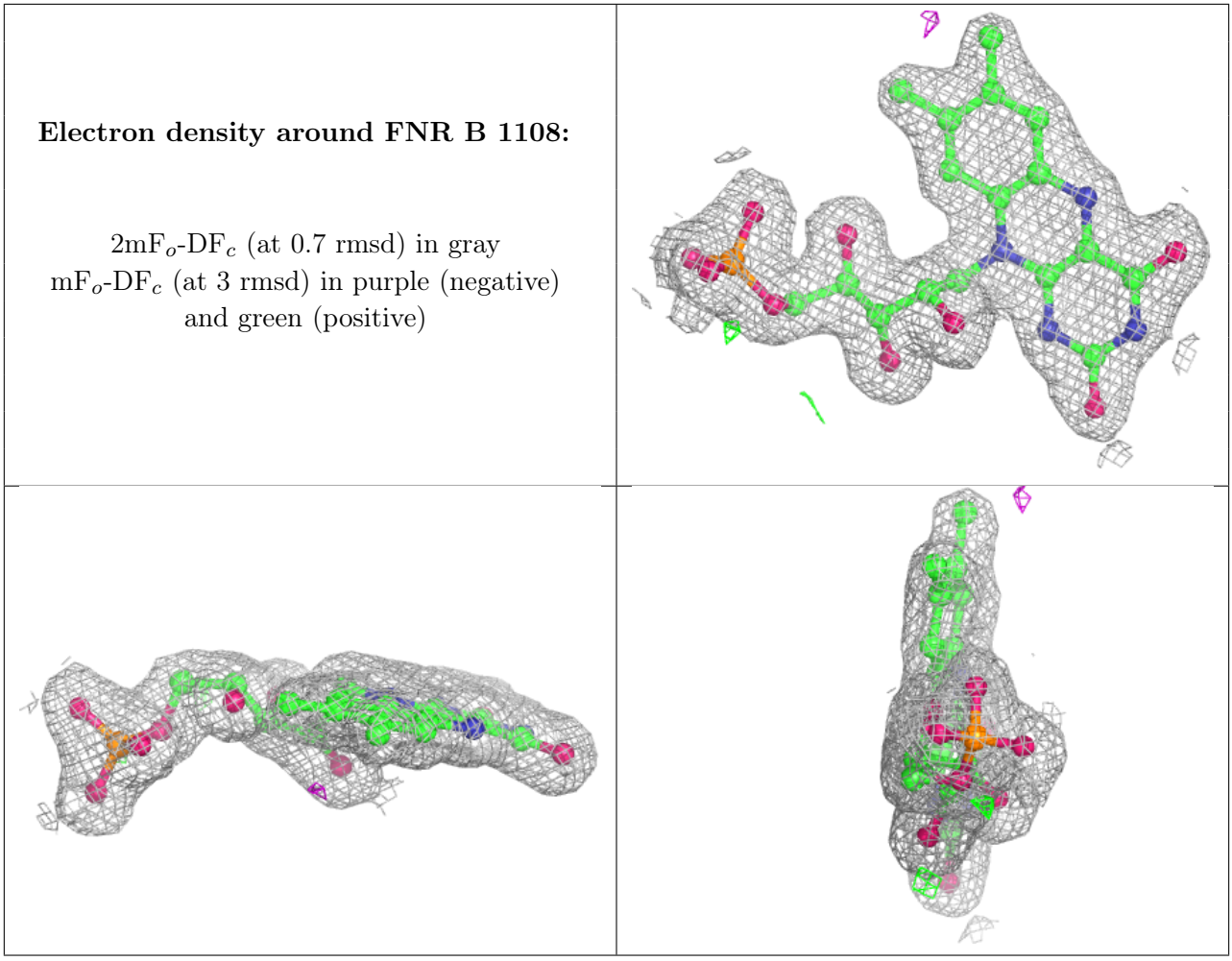






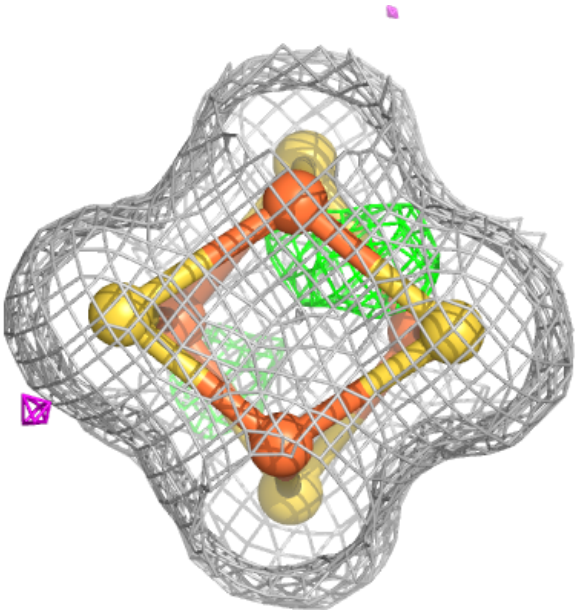
Electron density around FNR B 1108:

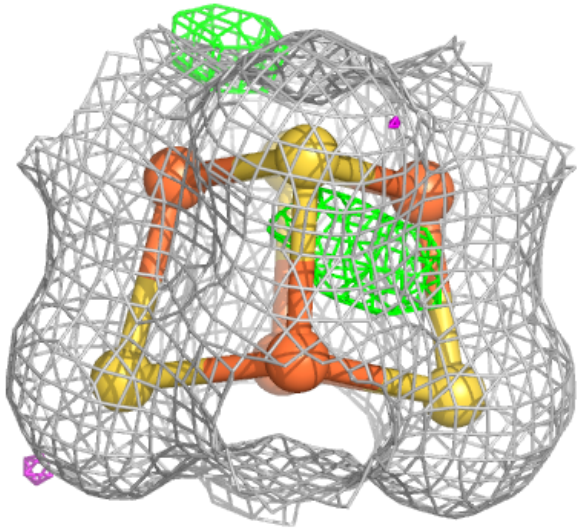
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

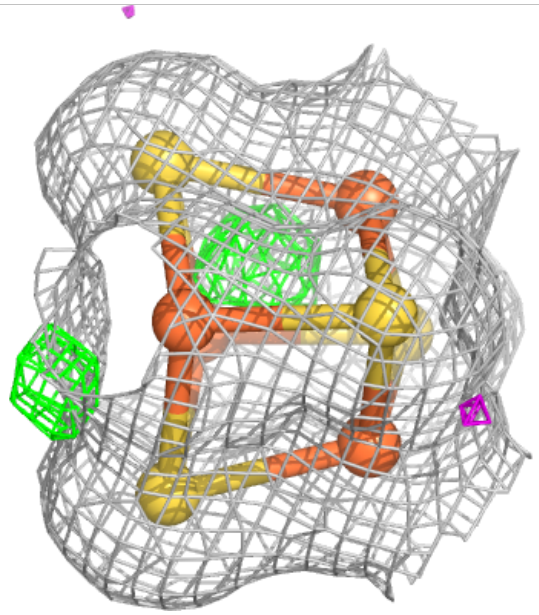


Electron density around SF4 A 1104:

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

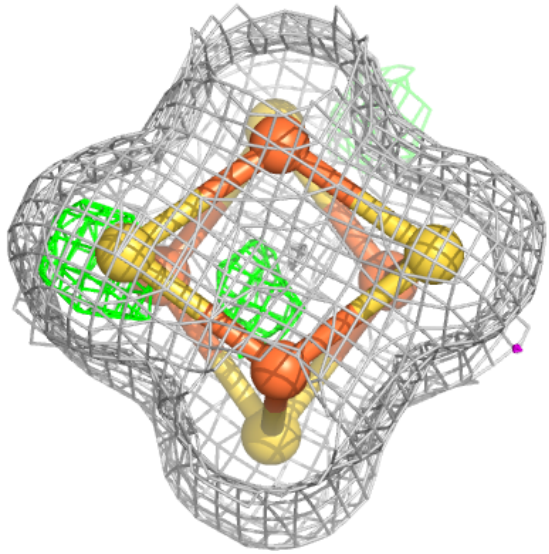


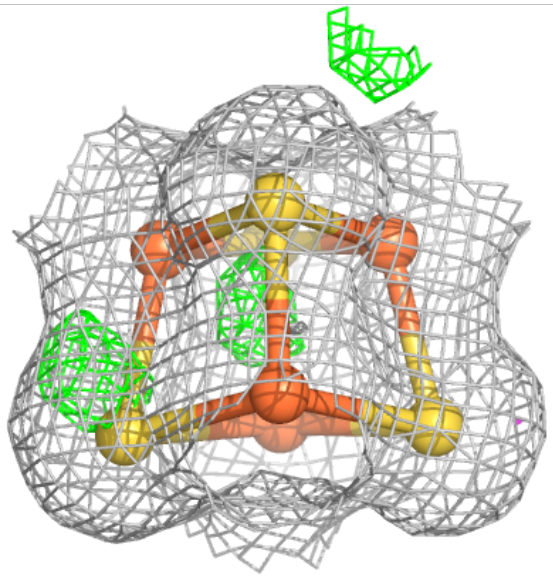


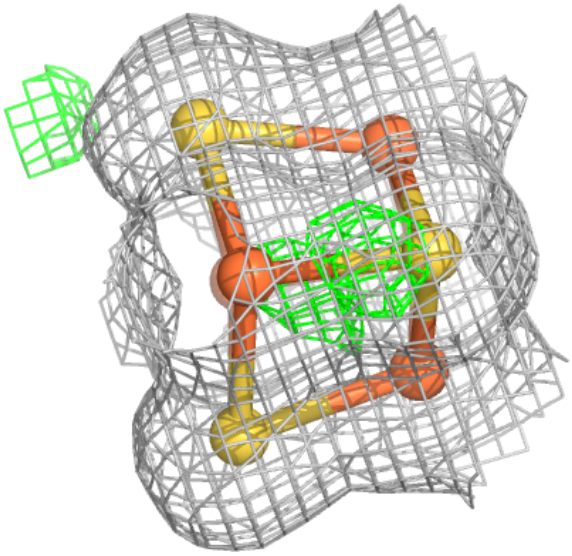


Electron density around SF4 B 1102:

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

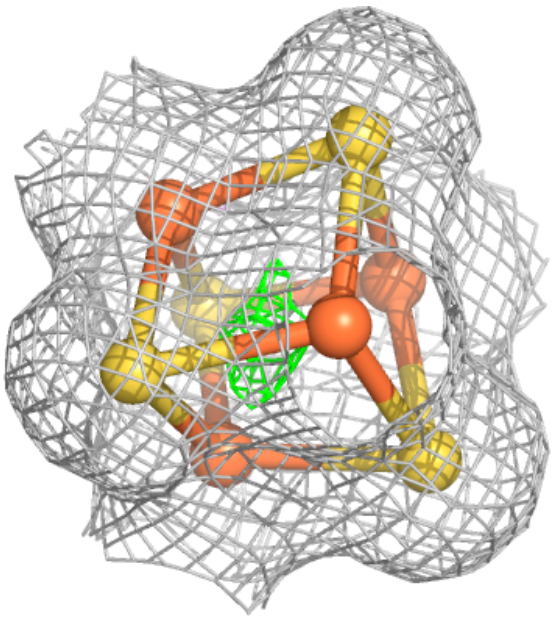


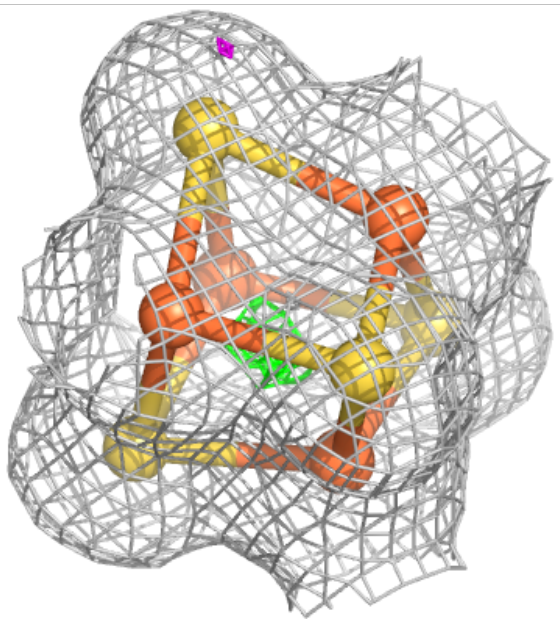


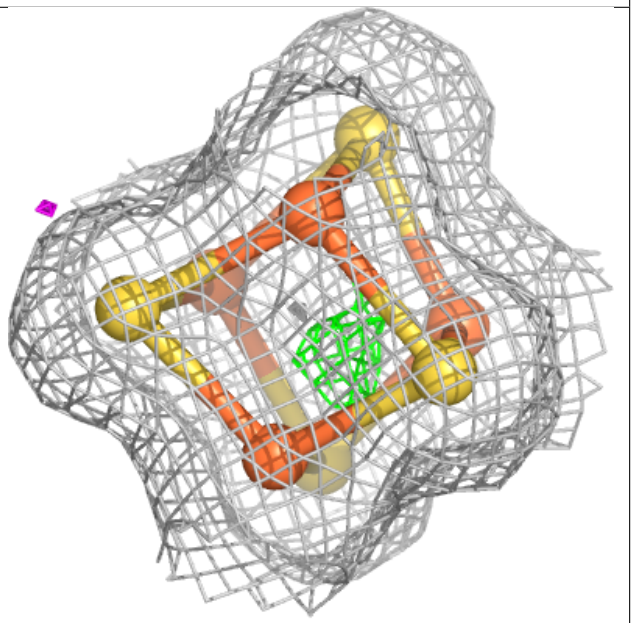


Electron density around SF4 A 1101:

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

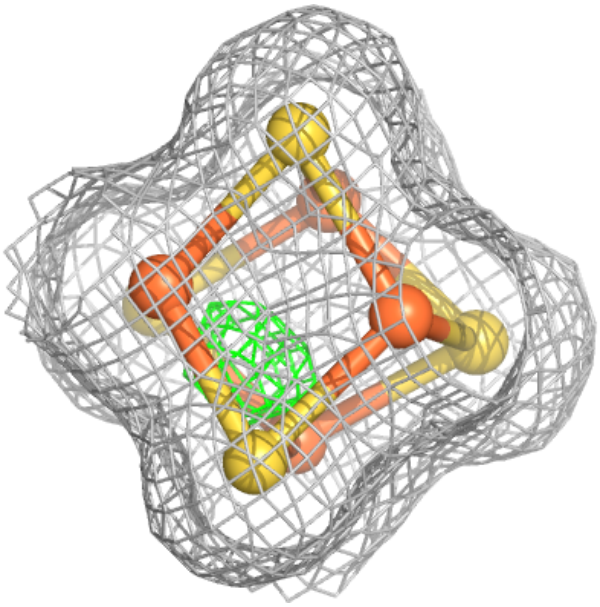


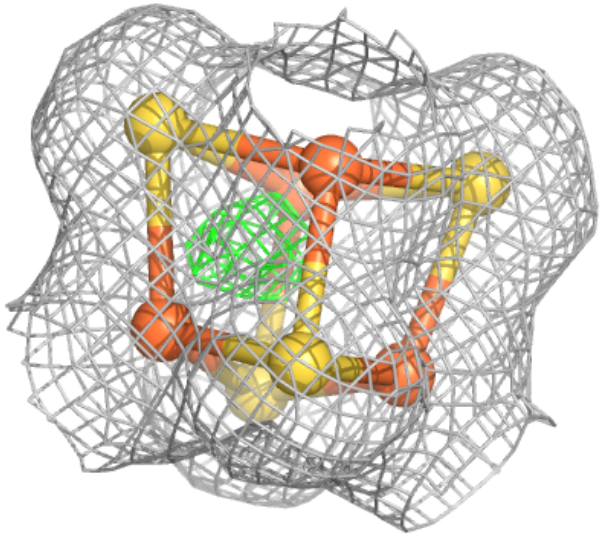


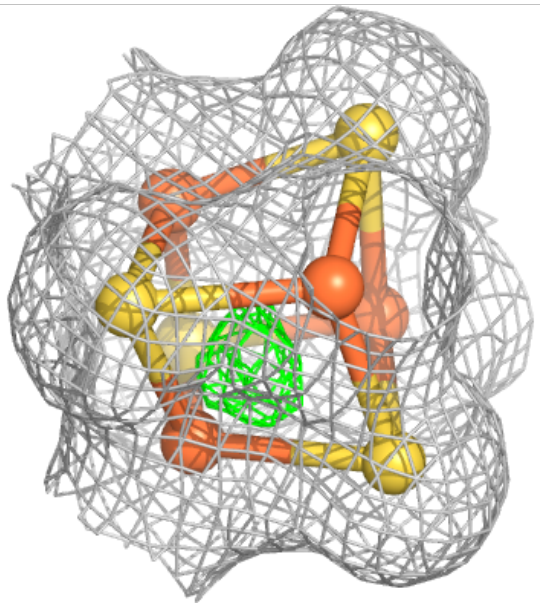


Electron density around SF4 B 1104:

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

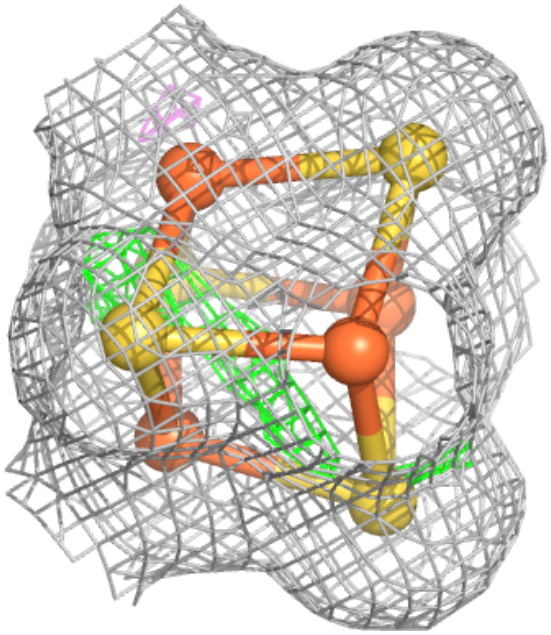


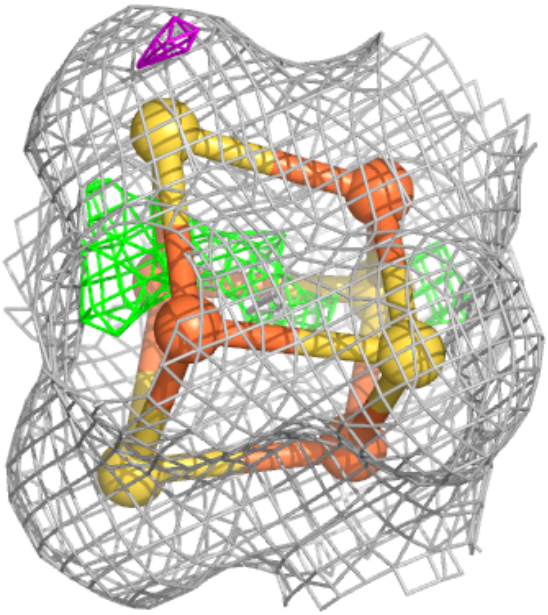


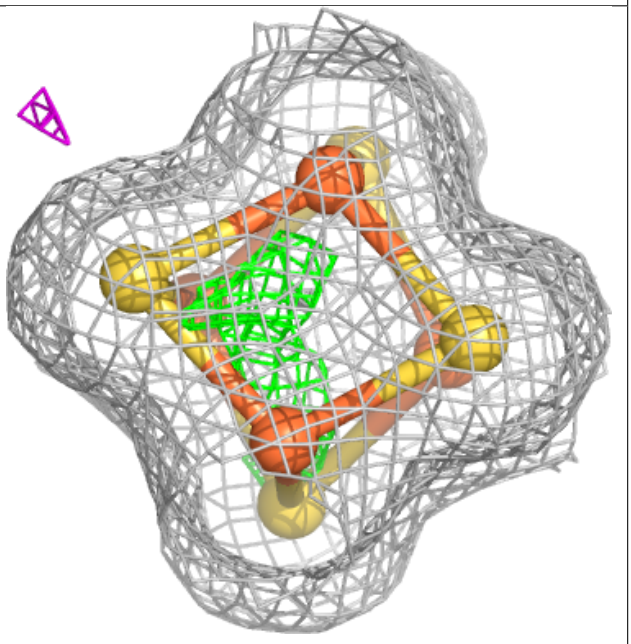


Electron density around SF4 B 1105:

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

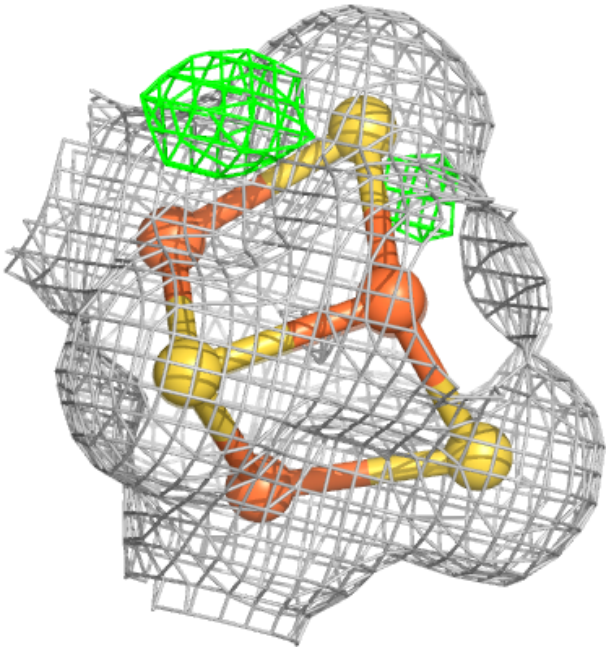


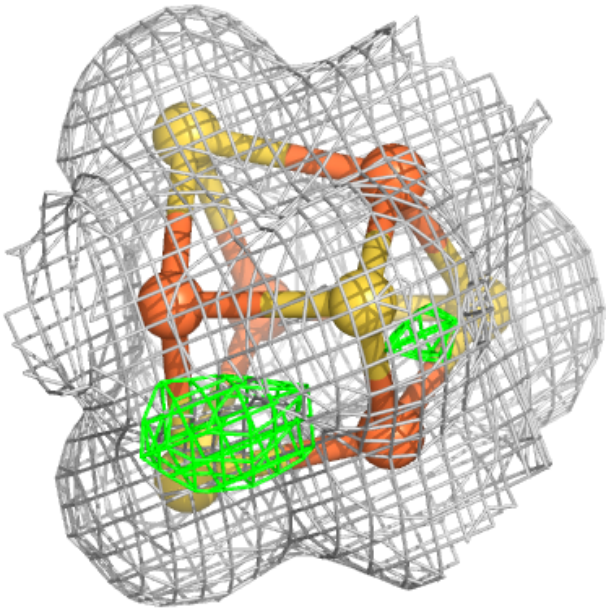


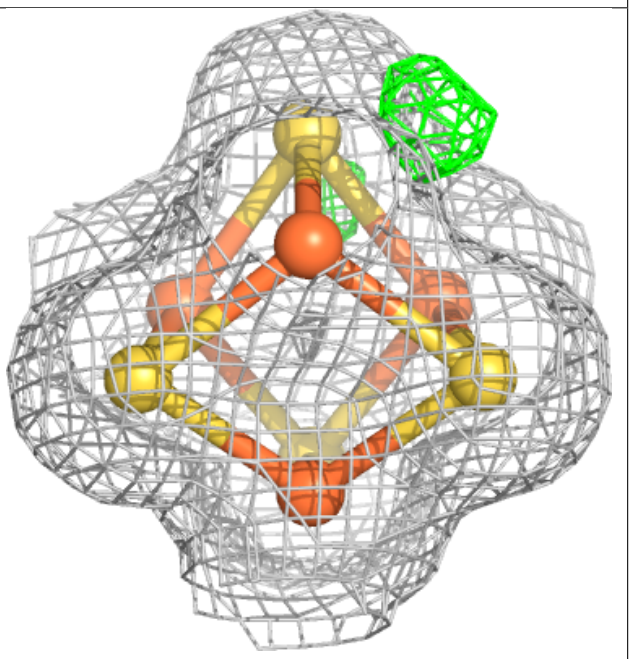


Electron density around SF4 C 1102:

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

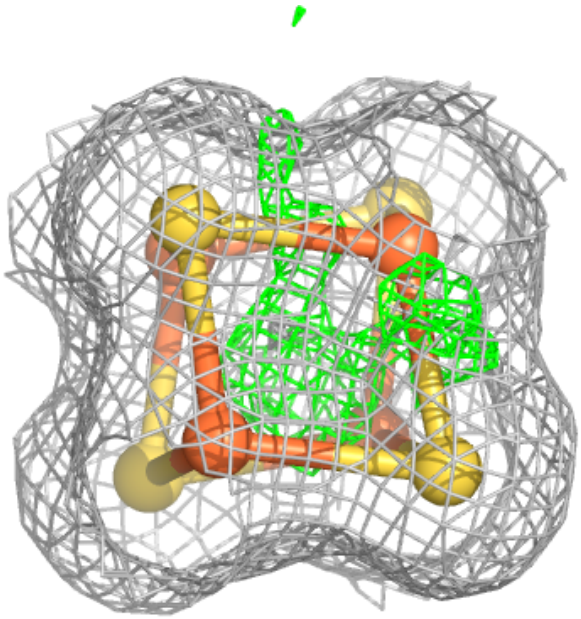


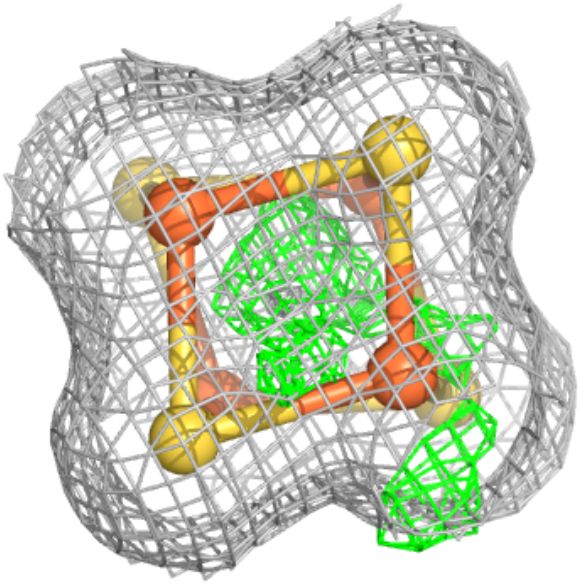


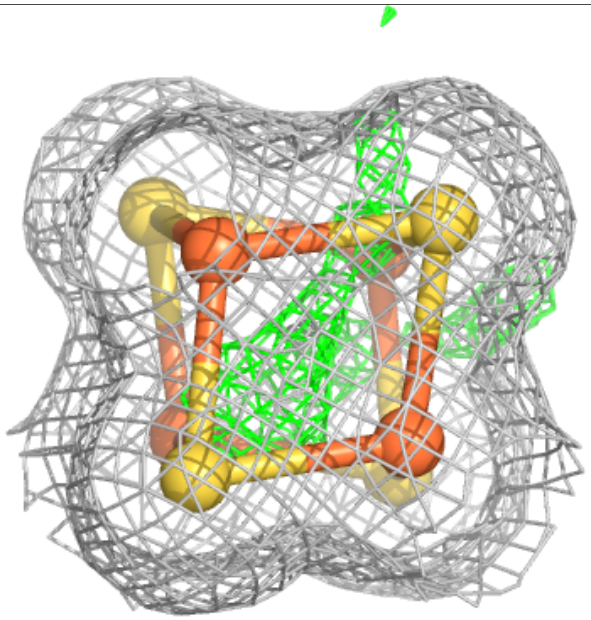


Electron density around SF4 C 1103:

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

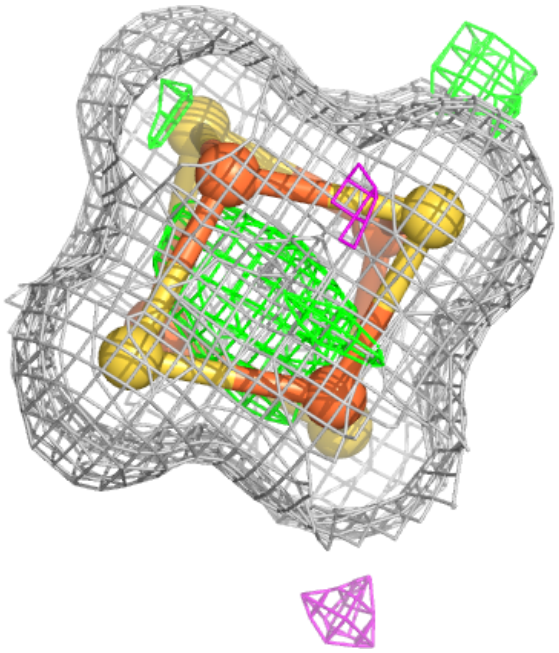


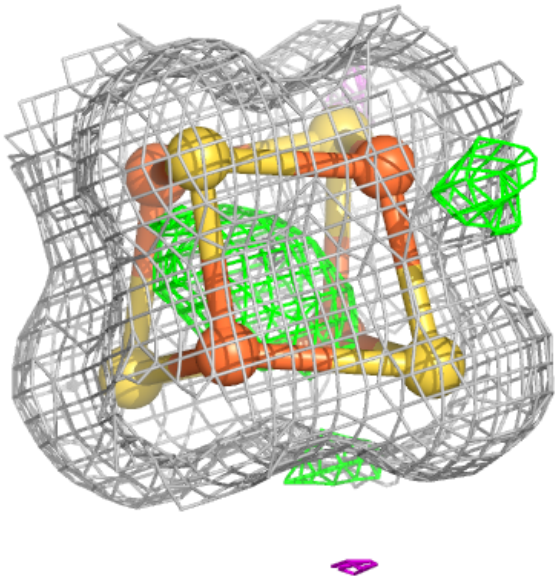


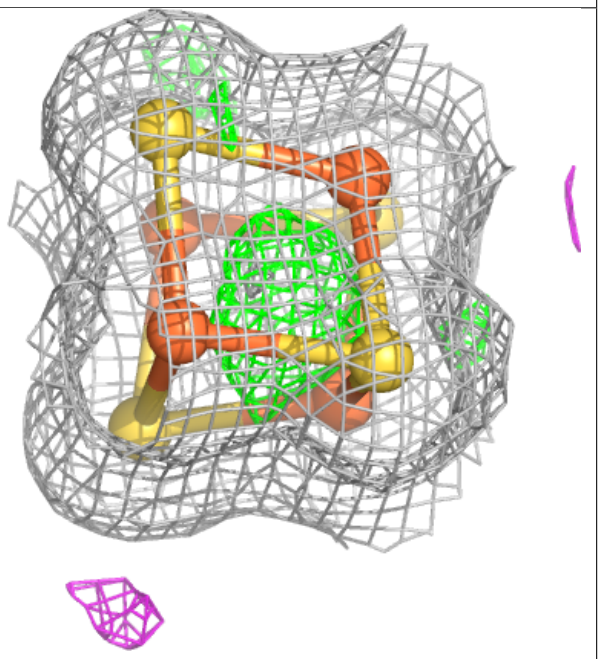


Electron density around SF4 C 1104:

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

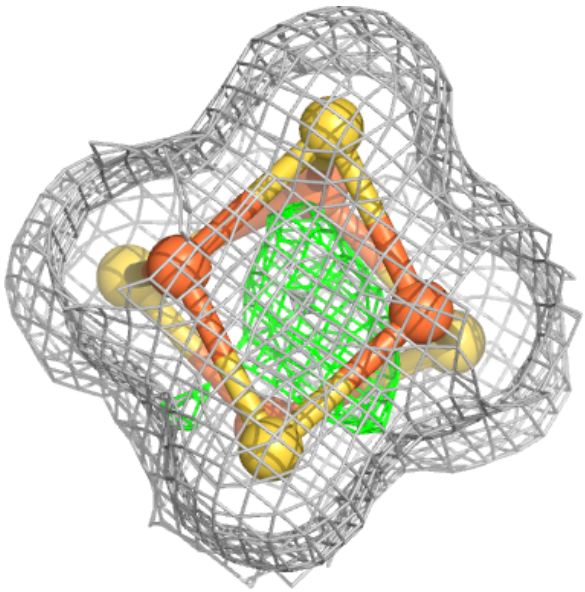


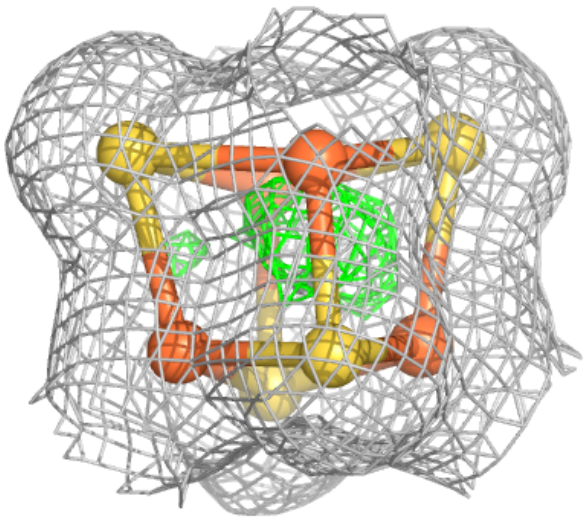


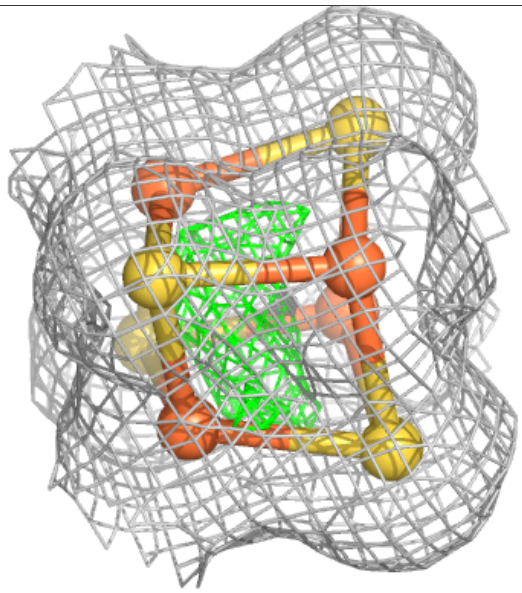


Electron density around SF4 A 1102:

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

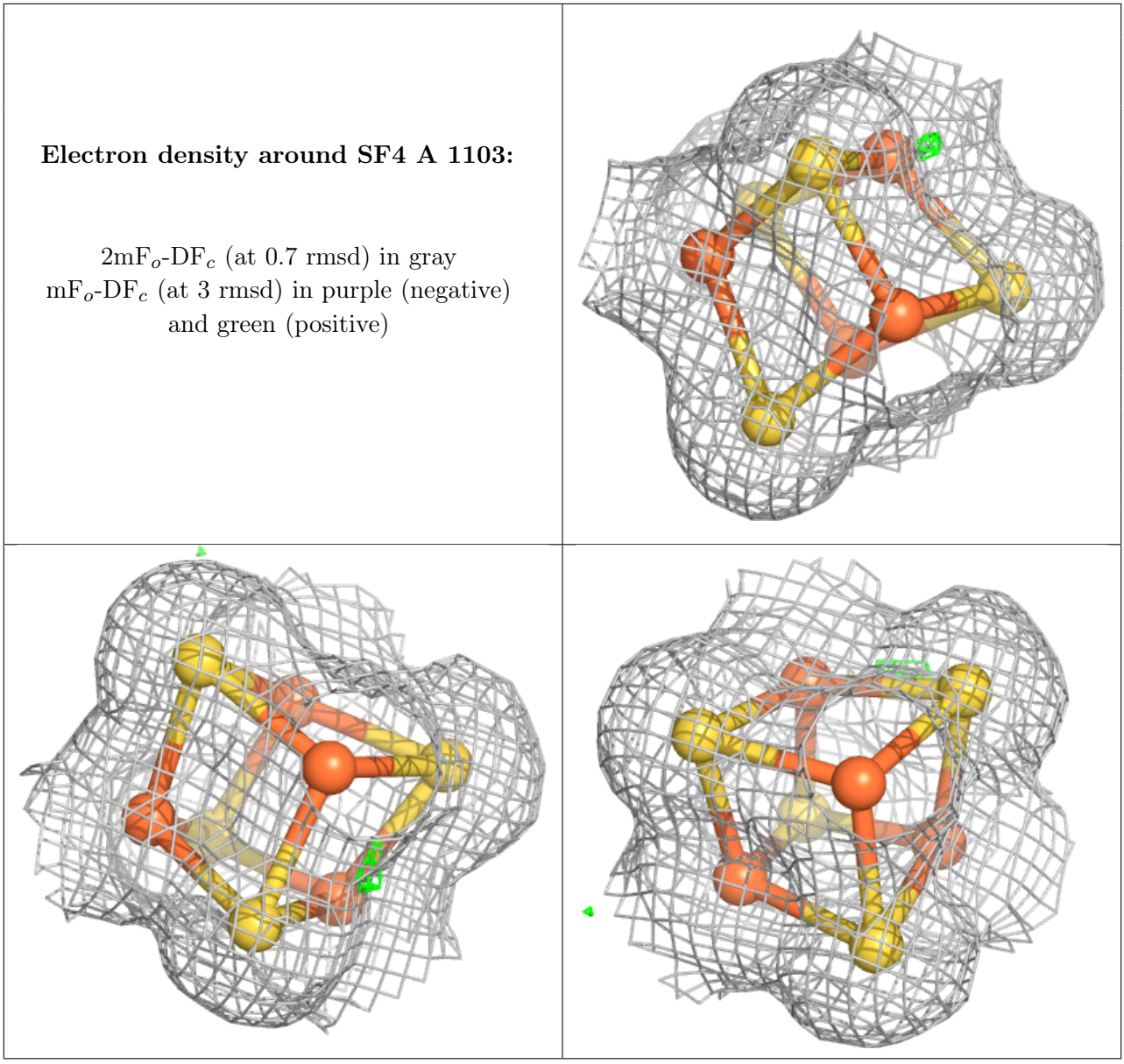






Electron density around SF4 A 1103:

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



6.5 Other polymers

There are no such residues in this entry.