wwPDB X-ray Structure Validation Summary 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)

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

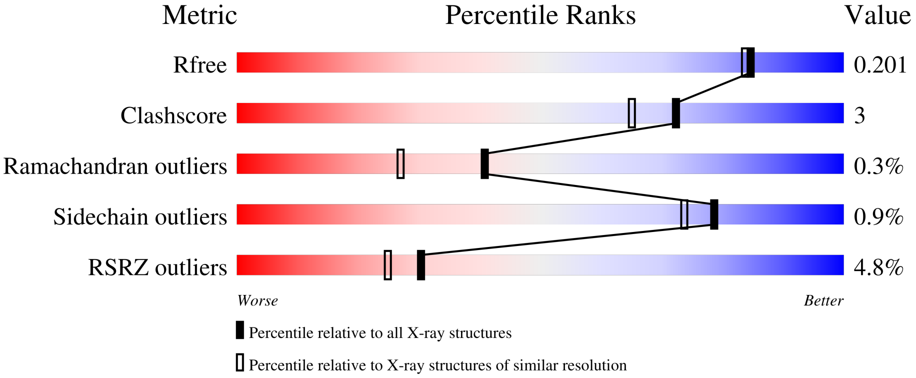
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

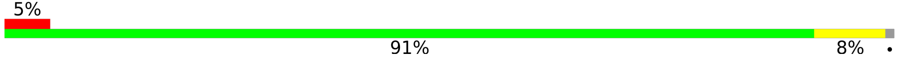
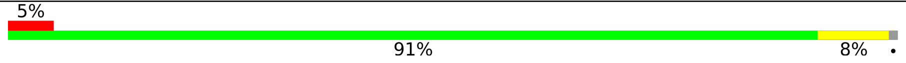
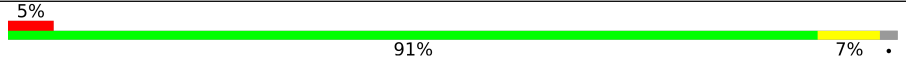
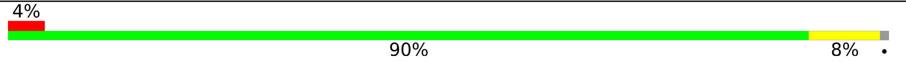
The reported resolution of this entry is 1.82 Å.

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	
1	B	1025	
1	C	1025	
1	D	1025	

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.

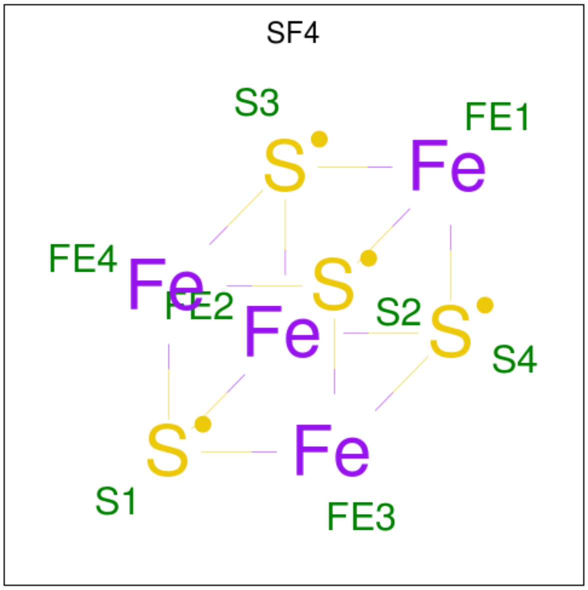
- Molecule 1 is a protein called Dihydropyrimidine dehydrogenase [NADP(+)].

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

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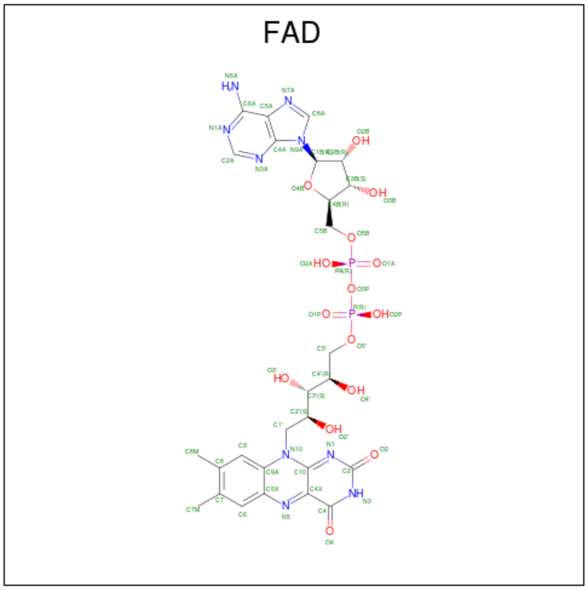
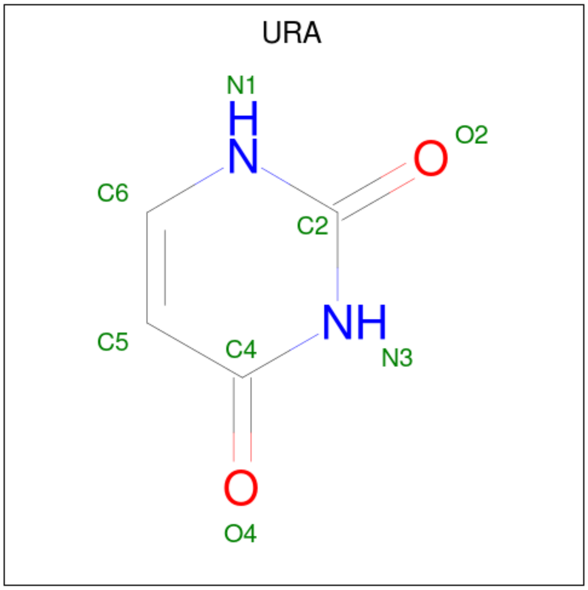
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Fe S 8 4 4	0	0
2	D	1	Total Fe S 8 4 4	0	0

- 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).



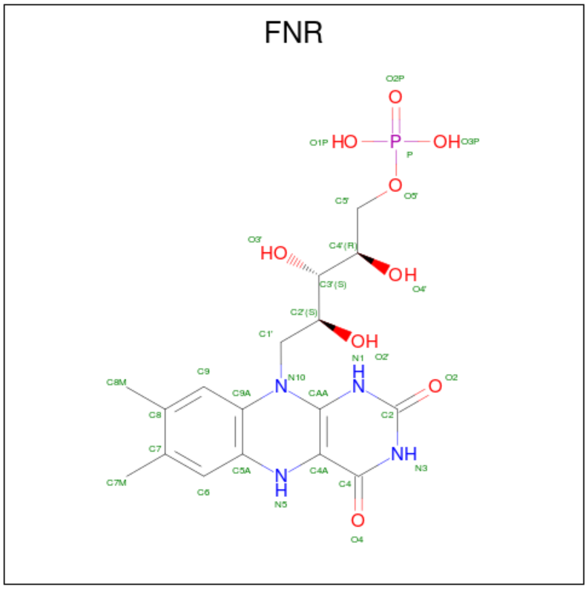
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 53 27 9 15 2	0	0
3	B	1	Total C N O P 53 27 9 15 2	0	0
3	C	1	Total C N O P 53 27 9 15 2	0	0
3	D	1	Total C N O P 53 27 9 15 2	0	0

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



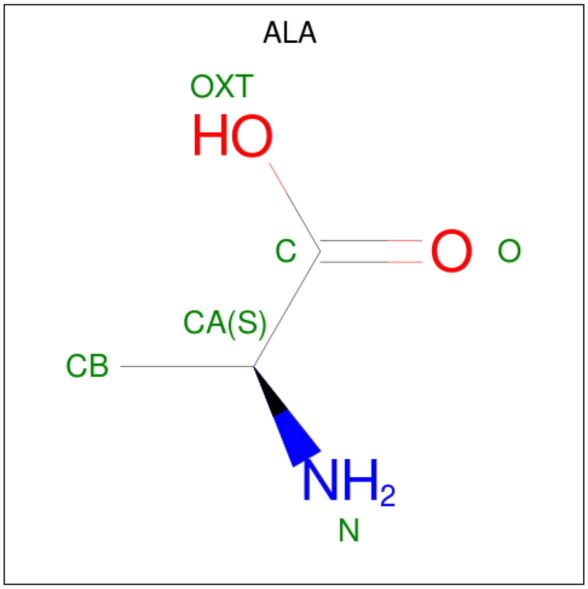
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 8 4 2 2	0	0
4	B	1	Total C N O 8 4 2 2	0	0
4	C	1	Total C N O 8 4 2 2	0	0
4	D	1	Total C N O 8 4 2 2	0	0

- 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).



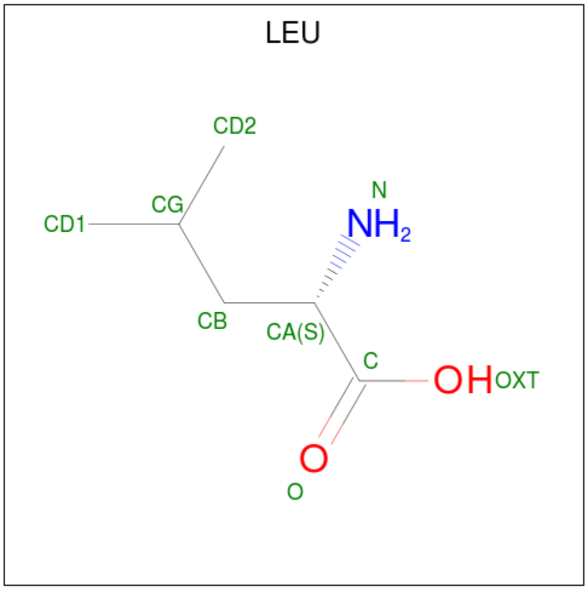
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 31 17 4 9 1	0	0
5	B	1	Total C N O P 31 17 4 9 1	0	0
5	C	1	Total C N O P 31 17 4 9 1	0	0
5	D	1	Total C N O P 31 17 4 9 1	0	0

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



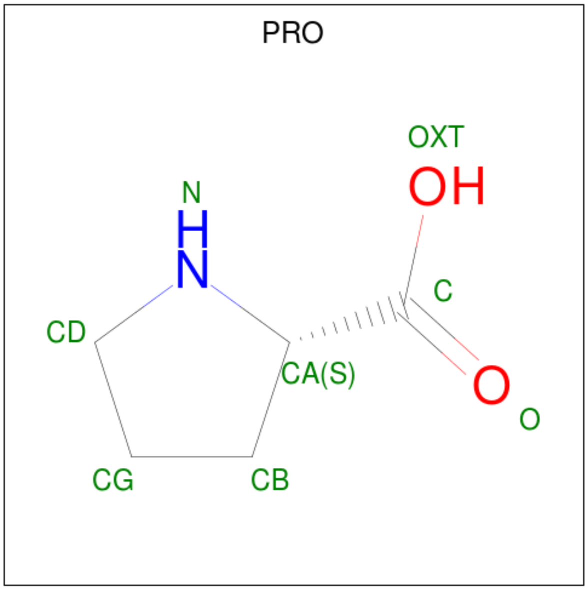
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 5 3 1 1	0	0
6	D	1	Total C N O 5 3 1 1	0	0

- 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.

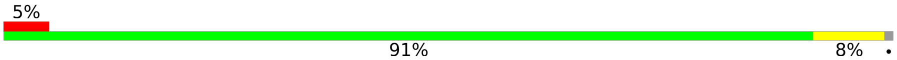
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	676	Total O 676 676	0	0
9	B	606	Total O 606 606	0	0
9	C	688	Total O 688 688	0	0
9	D	660	Total O 660 660	0	0

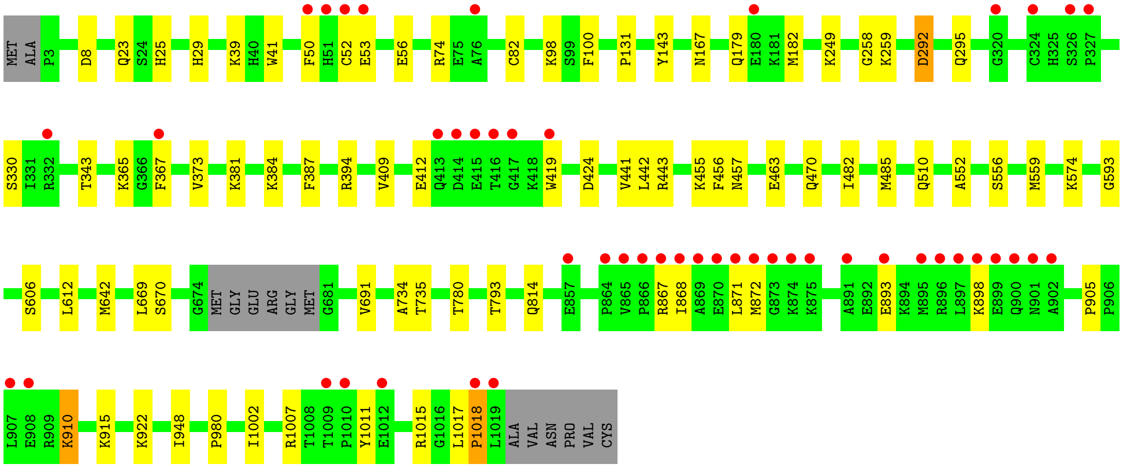
3 Residue-property plots ⓘ

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(+)]

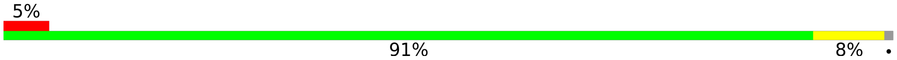
Chain A:

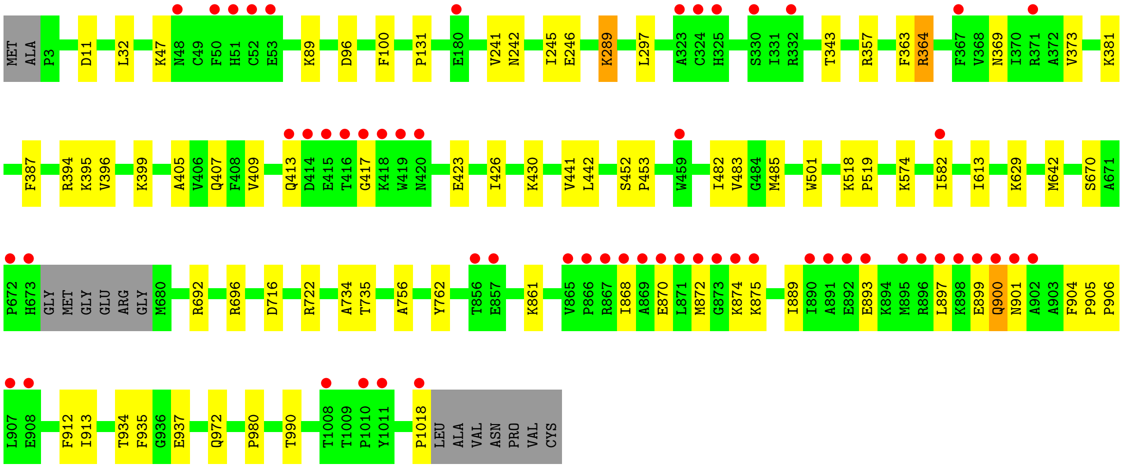




- Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]

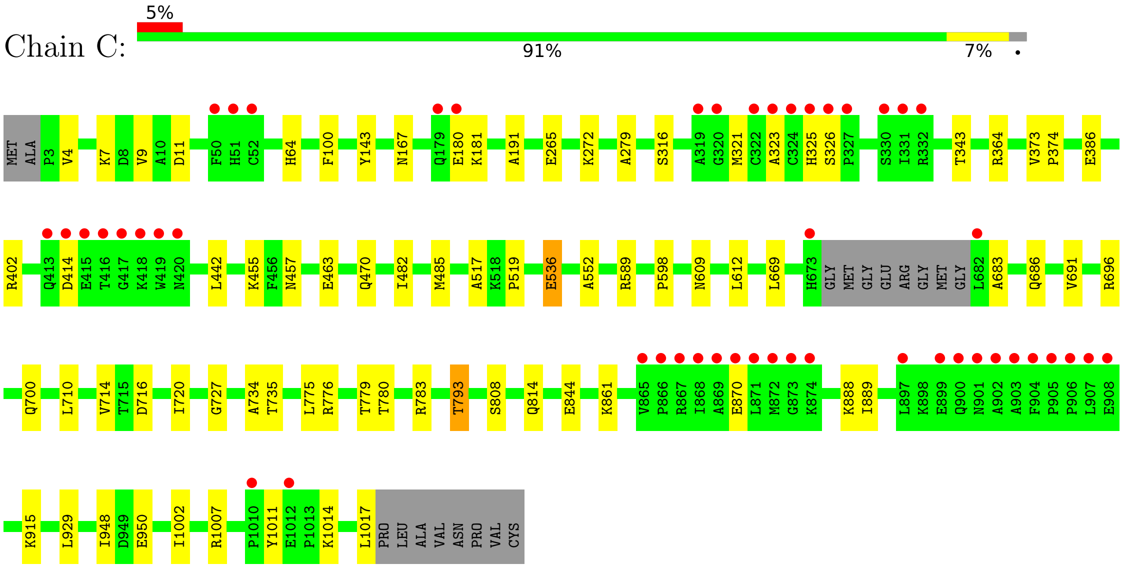
Chain B:





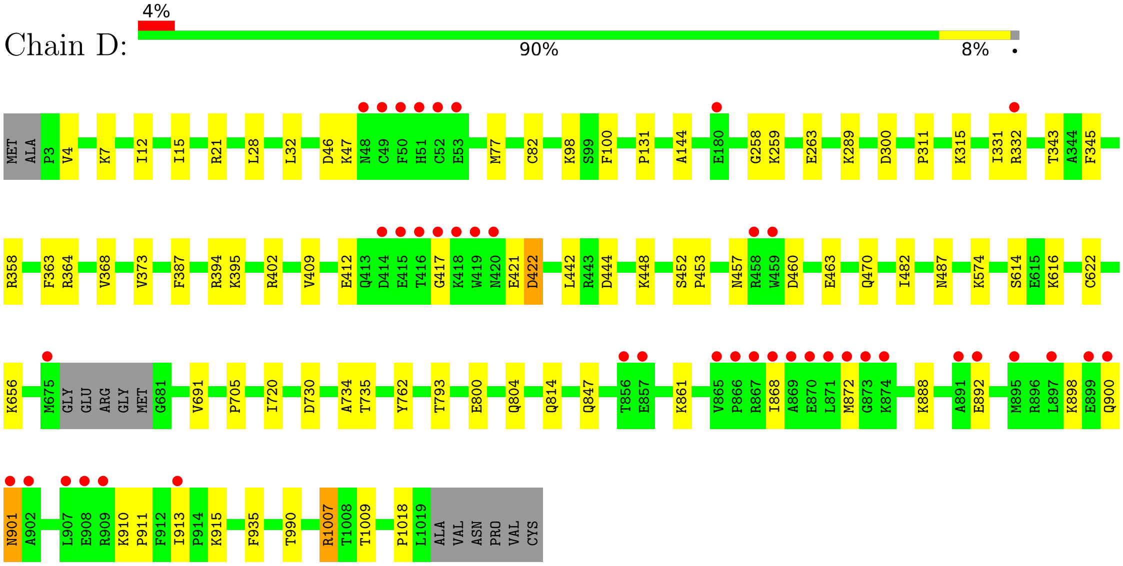
- Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]

Chain C:



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

Chain D:



4 Data and refinement statistics ⓘ

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.*

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[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.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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 ⓘ

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.

The worst 5 of 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

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 ⓘ

5.3.1 Protein backbone ⓘ

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

5 of 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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	364	ARG
1	D	487	ASN
1	C	888	LYS
1	D	1007[B]	ARG
1	D	363	PHE

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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#\vert Z\vert > 2$	Counts	RMSZ	$\#\vert Z\vert > 2$
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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 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

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

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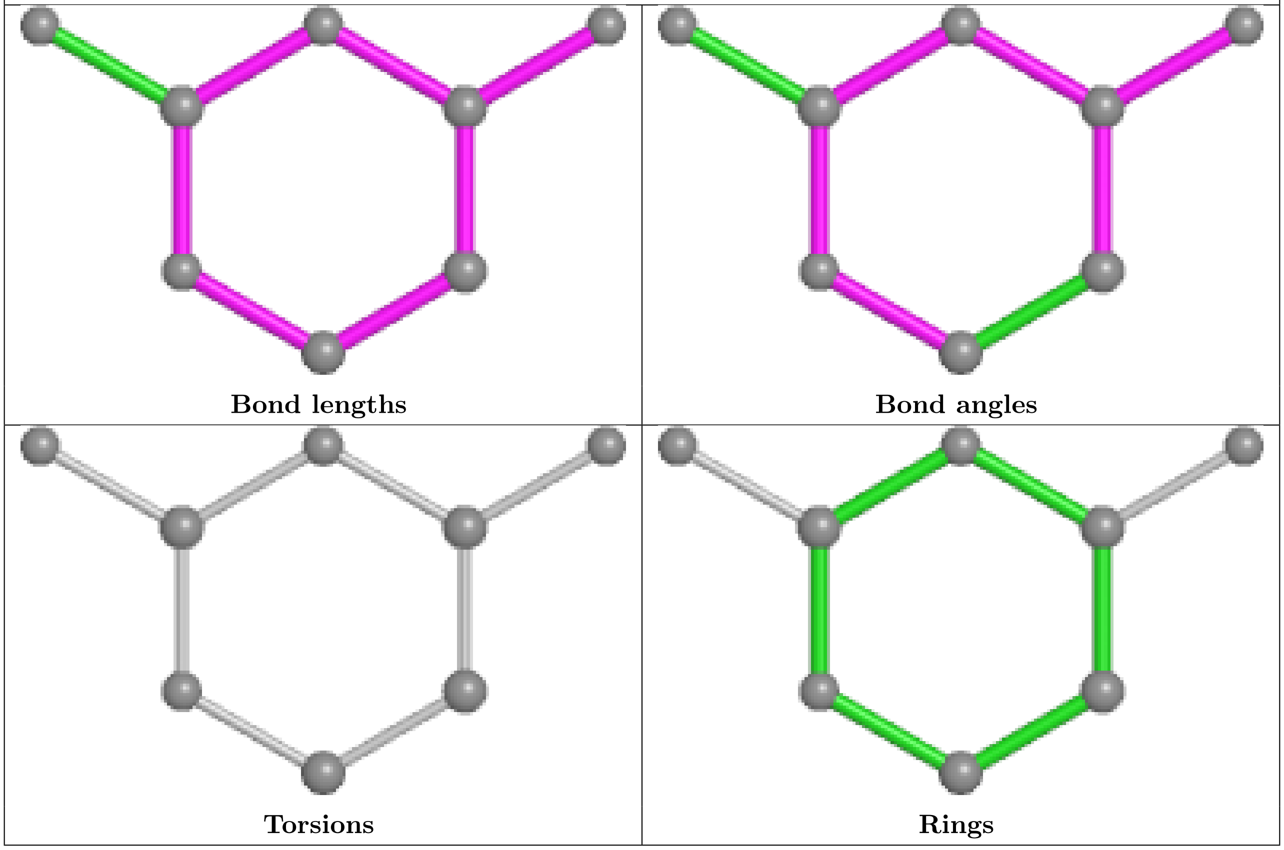
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1107	FNR	3	0
3	C	1106	FAD	1	0
6	D	1102	ALA	1	0
6	A	1108	ALA	2	0
8	C	1101	PRO	1	0
5	D	1109	FNR	1	0
3	B	1106	FAD	1	0
3	D	1107	FAD	1	0
5	C	1108	FNR	1	0
3	A	1105	FAD	1	0

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



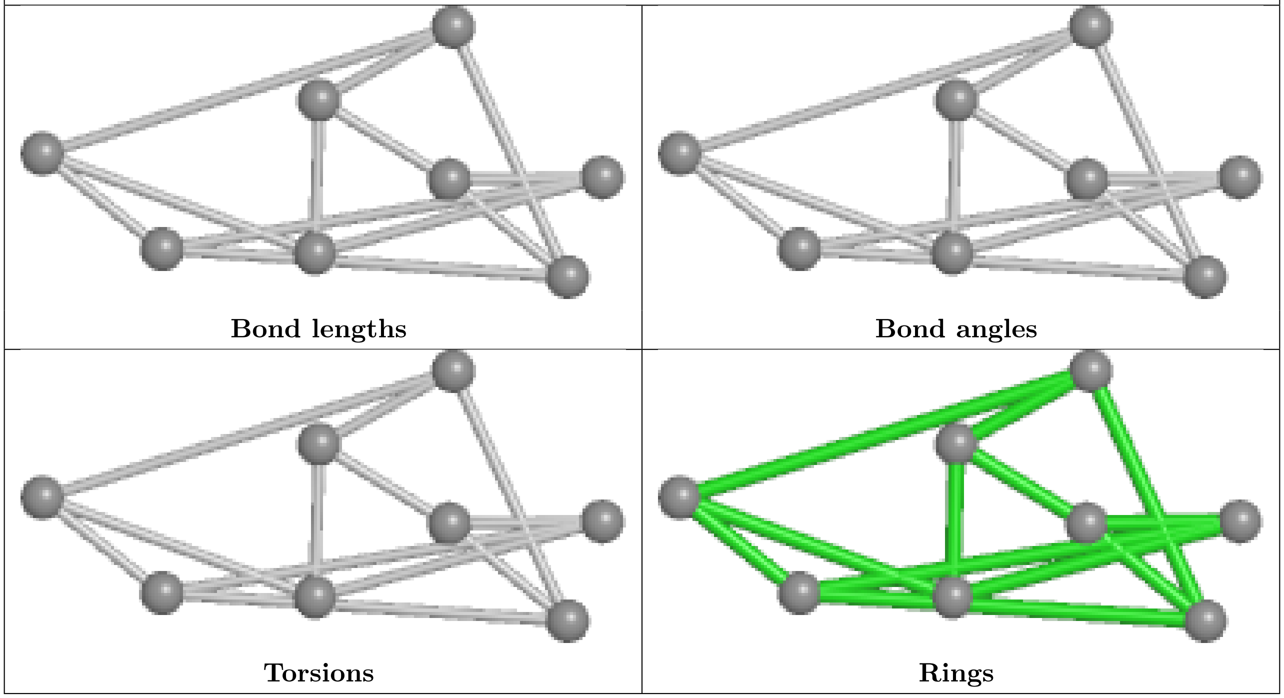
Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 A 1103



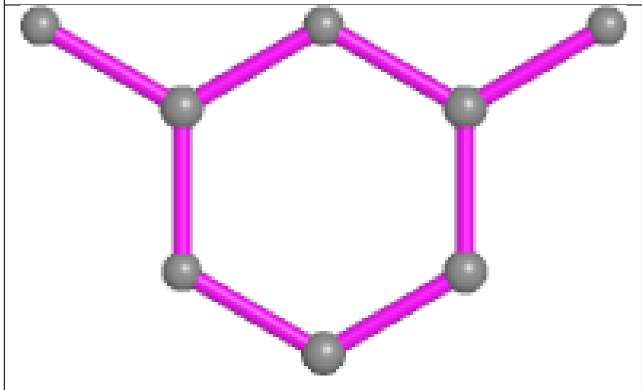
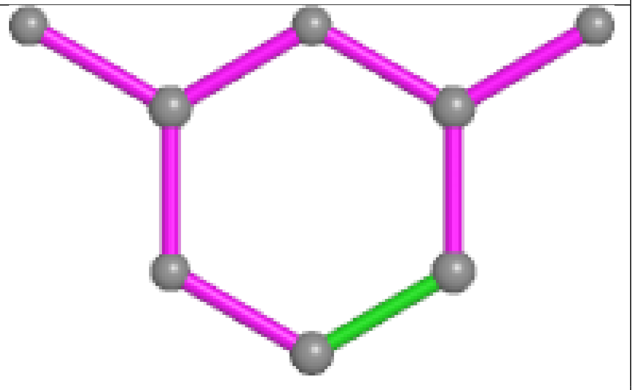
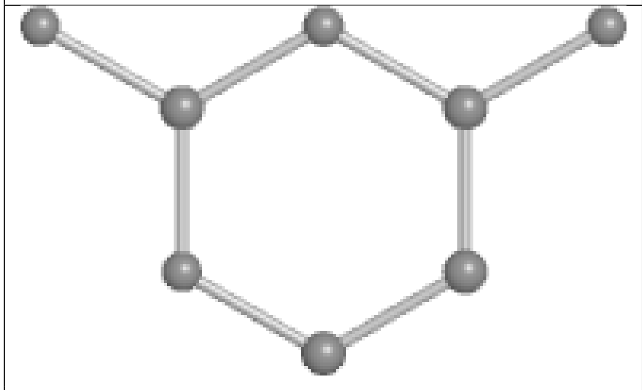
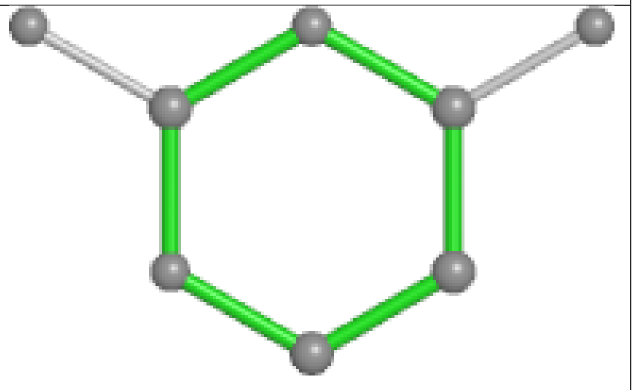
Bond lengths

Bond angles

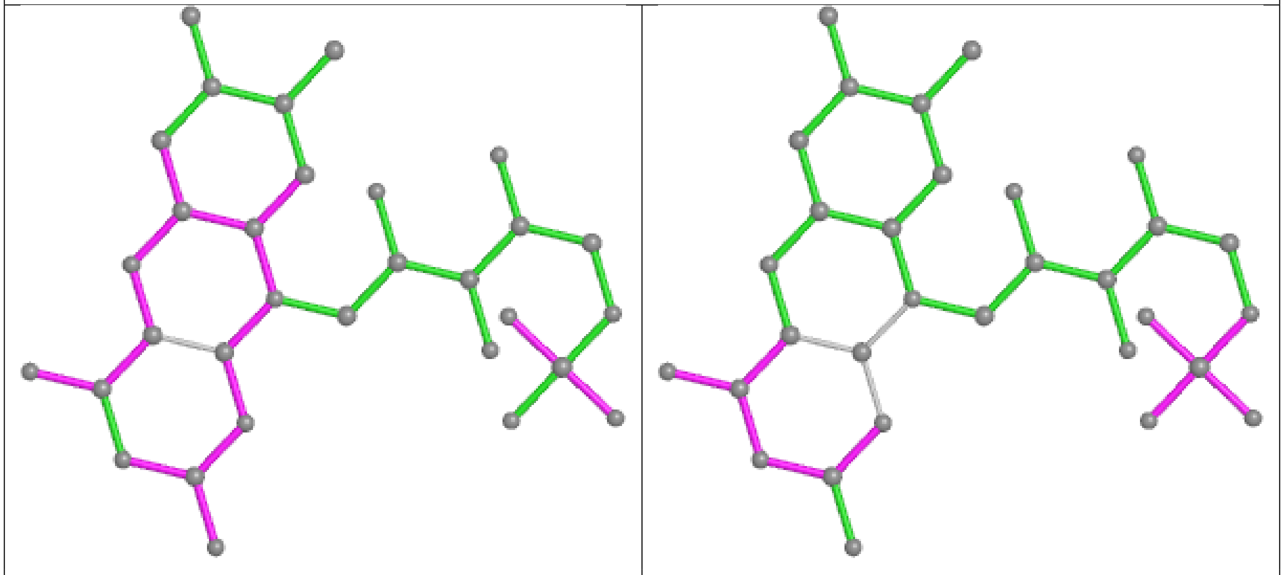
Torsions

Rings

Ligand URA A 1106

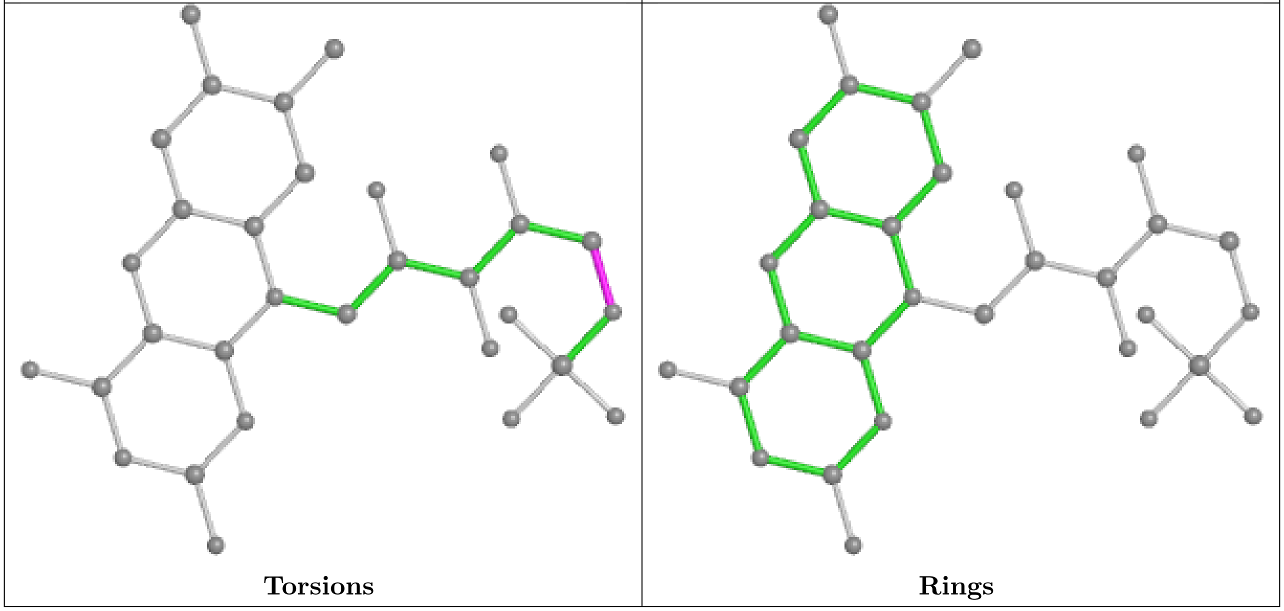
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand FNR B 1108



Bond lengths

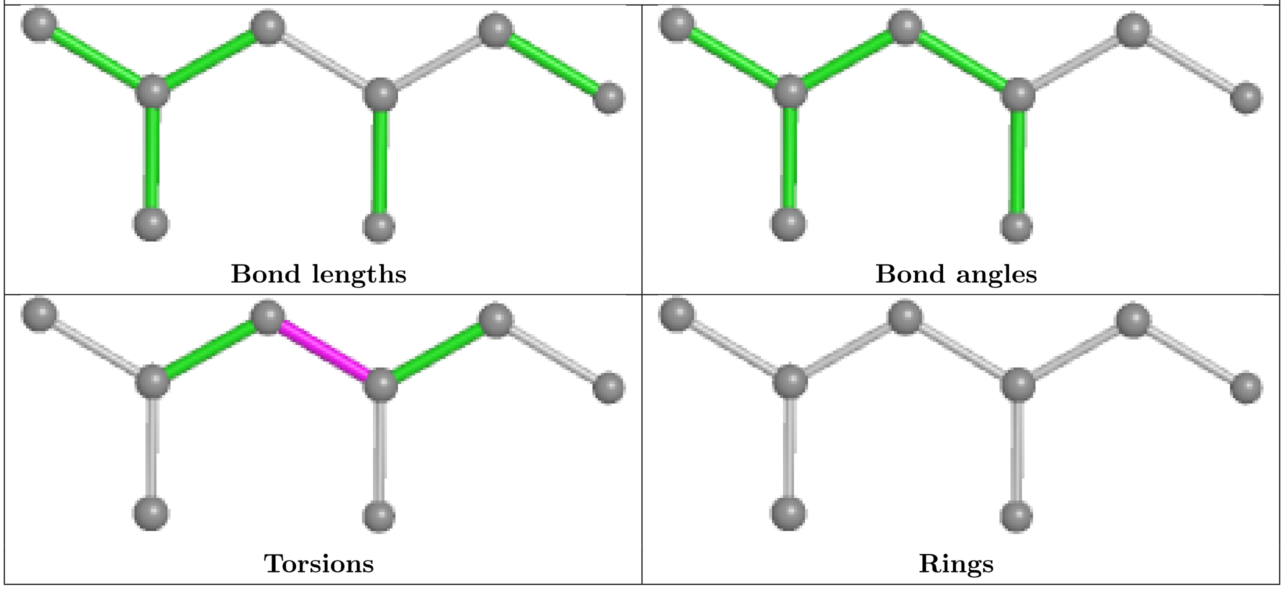
Bond angles



Torsions

Rings

Ligand LEU B 1101



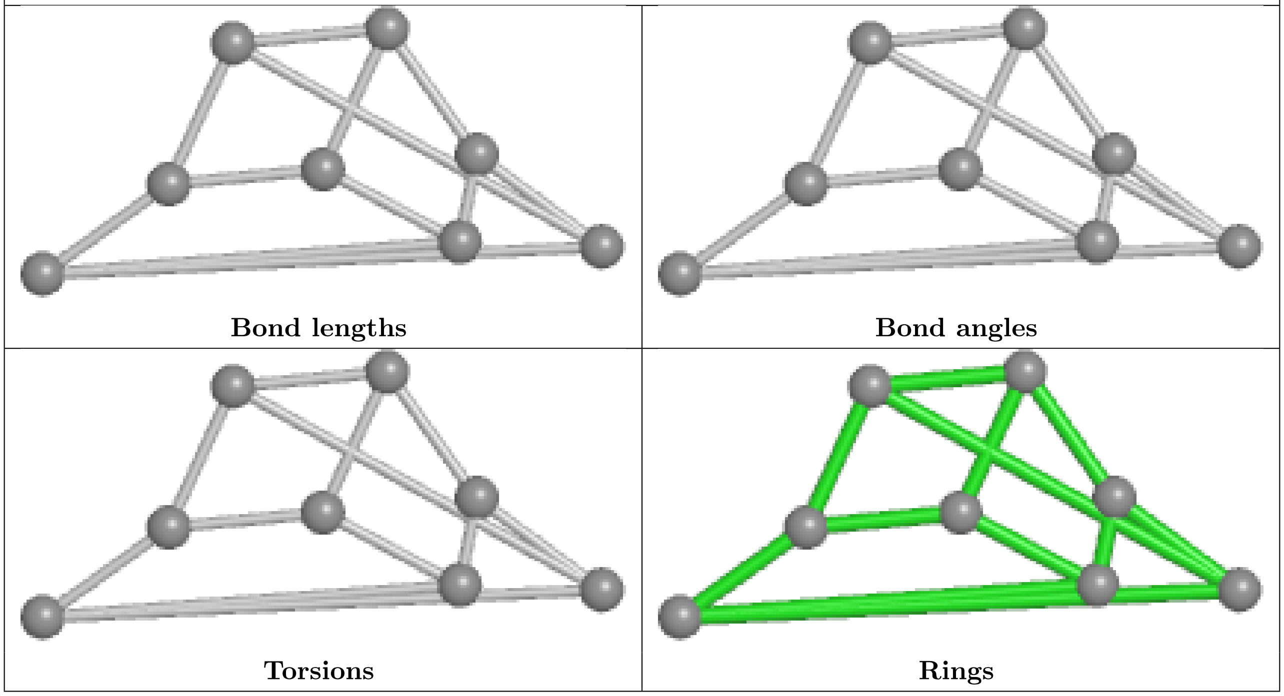
Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 D 1106



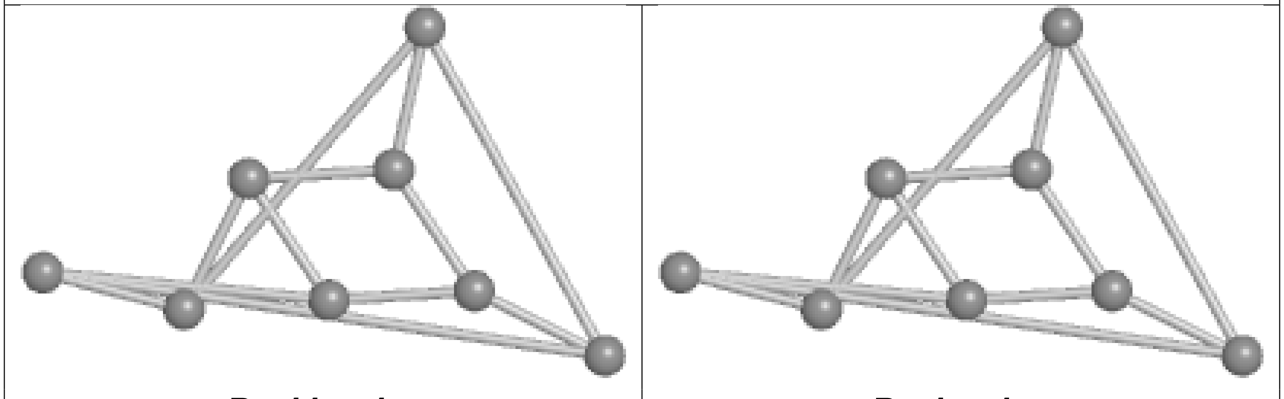
Bond lengths

Bond angles

Torsions

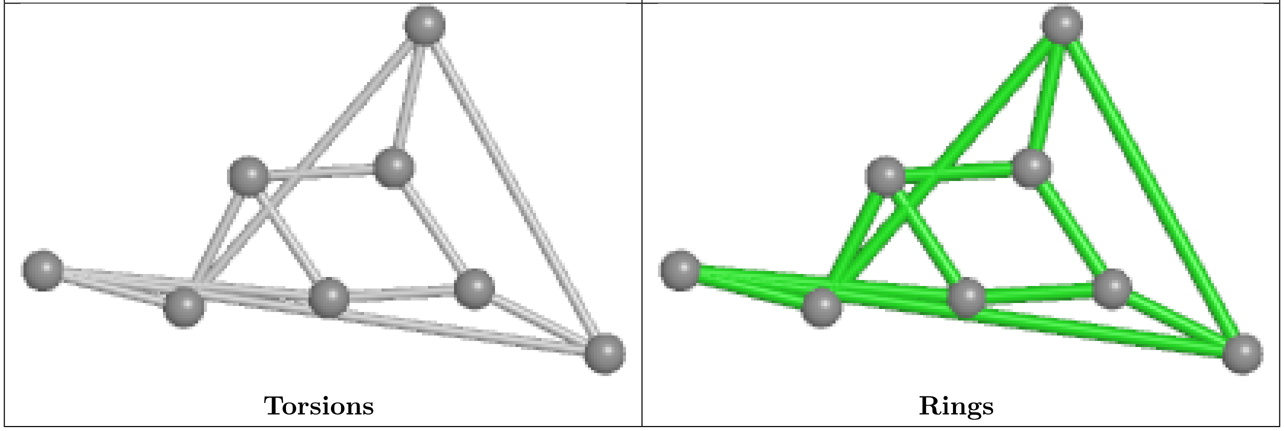
Rings

Ligand SF4 B 1105



Bond lengths

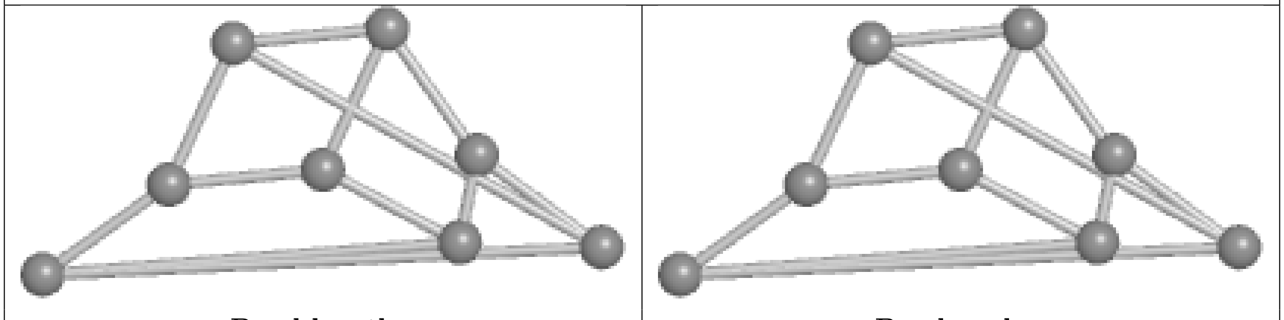
Bond angles



Torsions

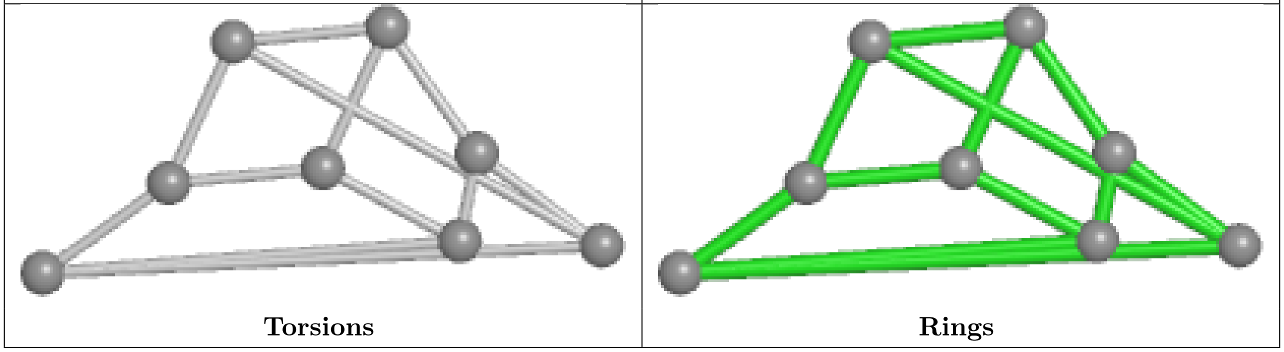
Rings

Ligand SF4 D 1104



Bond lengths

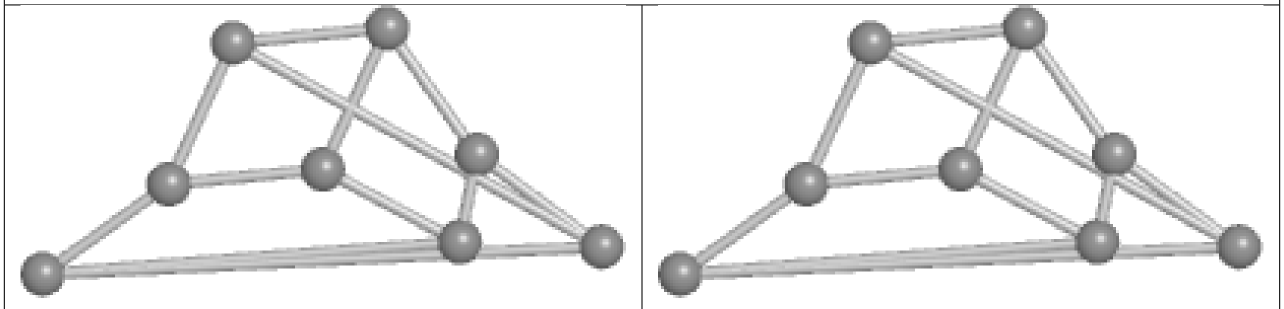
Bond angles



Torsions

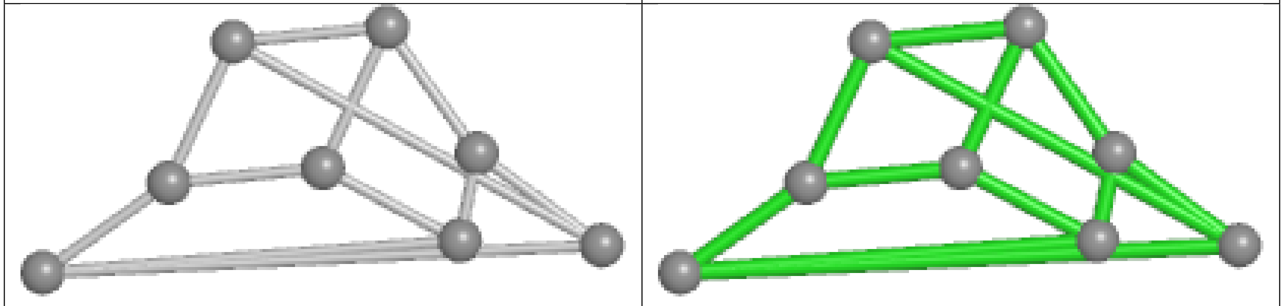
Rings

Ligand SF4 D 1103



Bond lengths

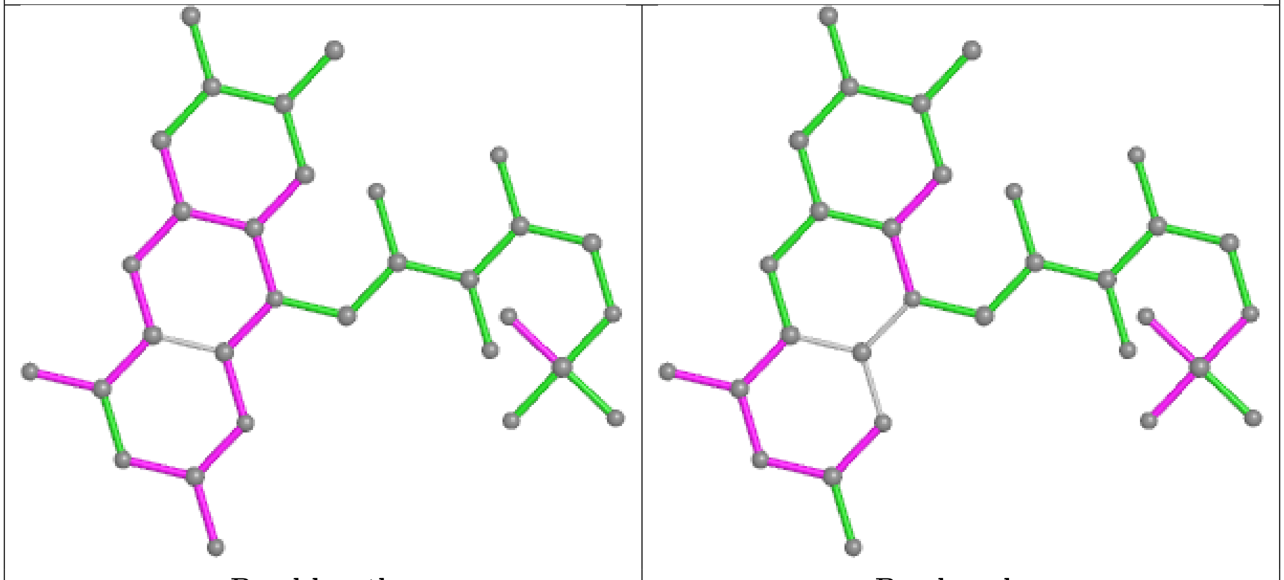
Bond angles



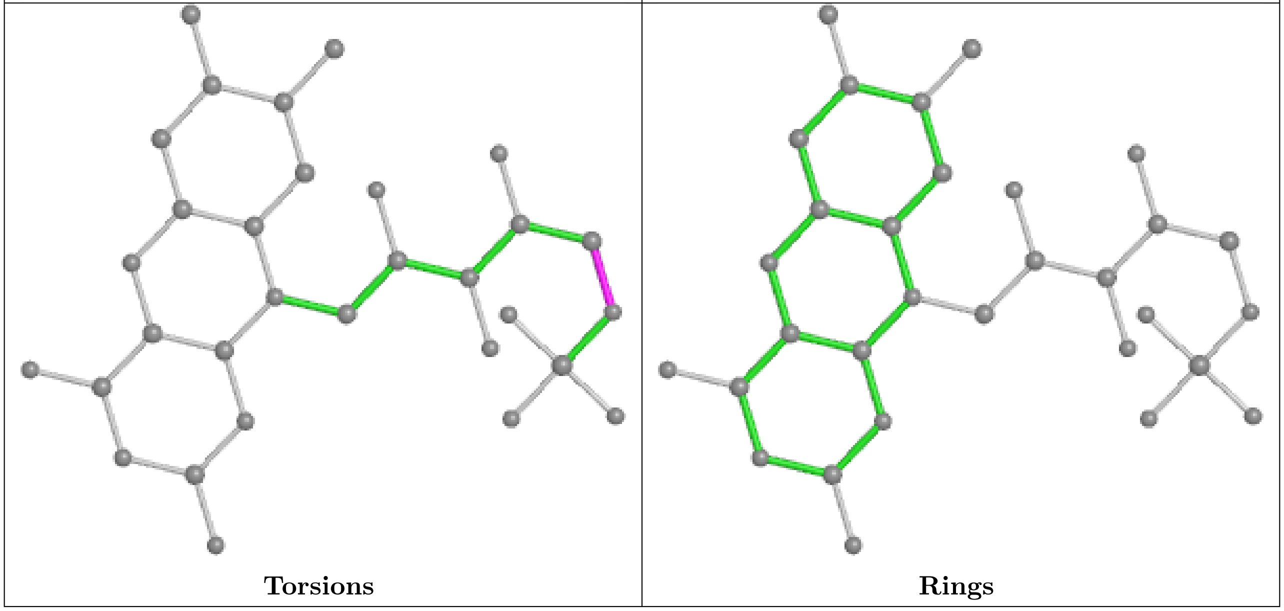
Torsions

Rings

Ligand FNR A 1107

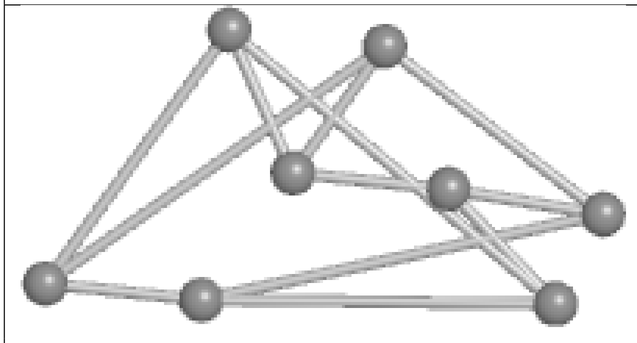


Bond lengths **Bond angles**

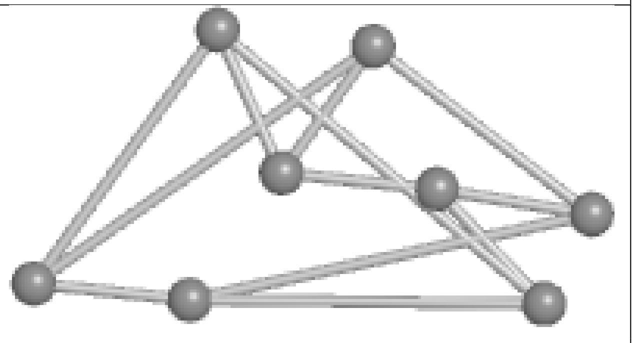


Torsions **Rings**

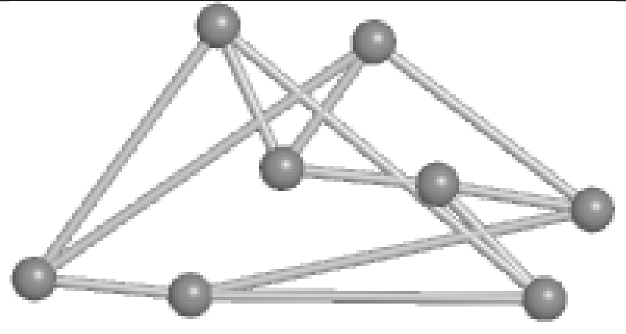
Ligand SF4 C 1103



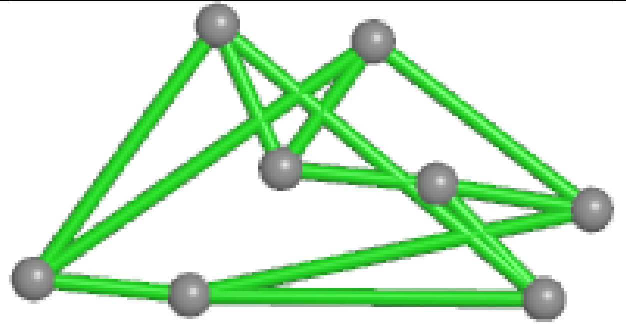
Bond lengths



Bond angles

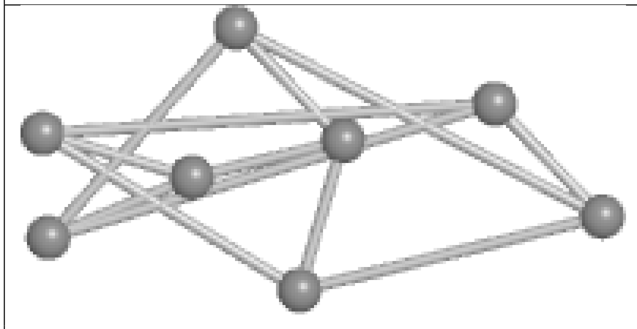


Torsions

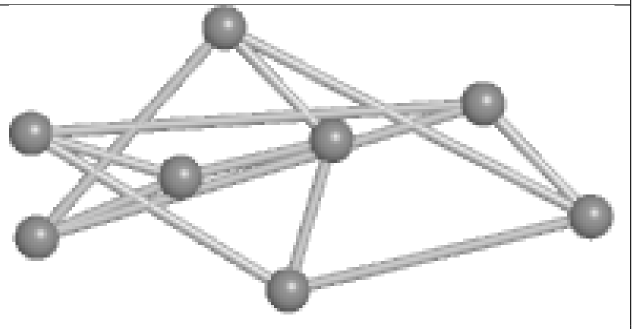


Rings

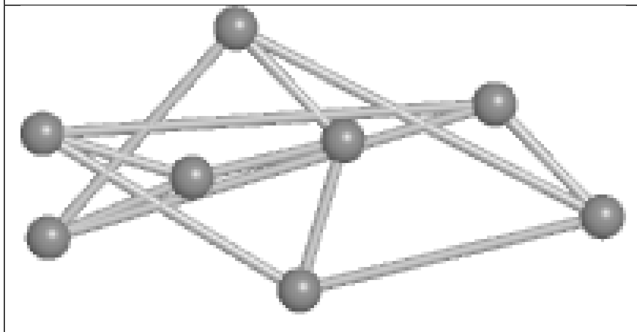
Ligand SF4 D 1105



Bond lengths



Bond angles



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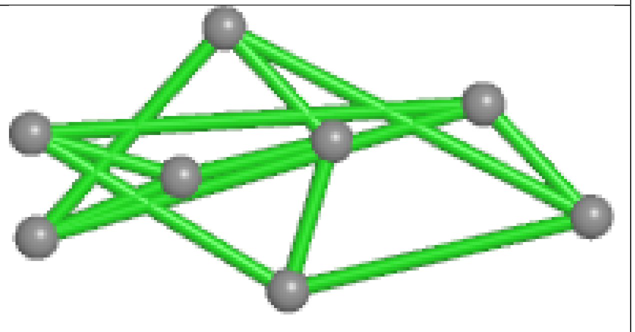
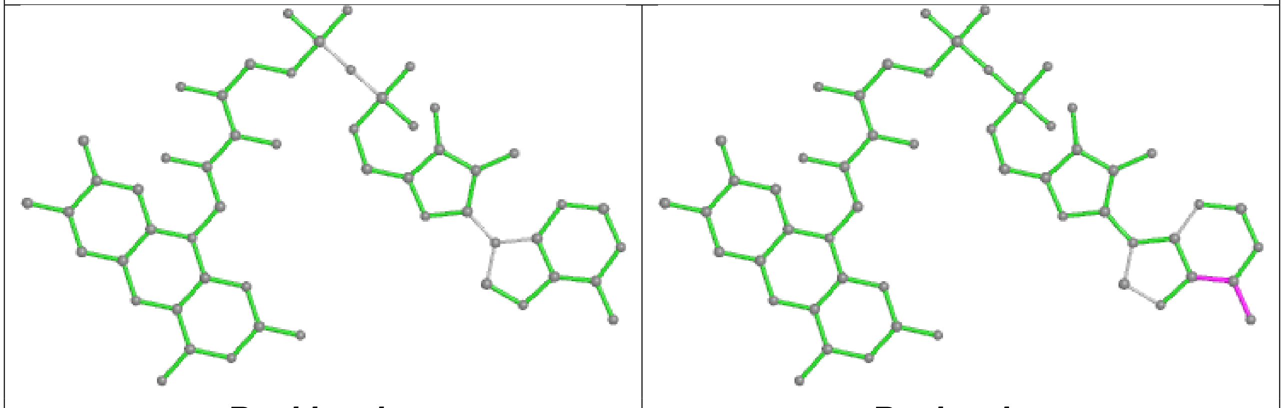
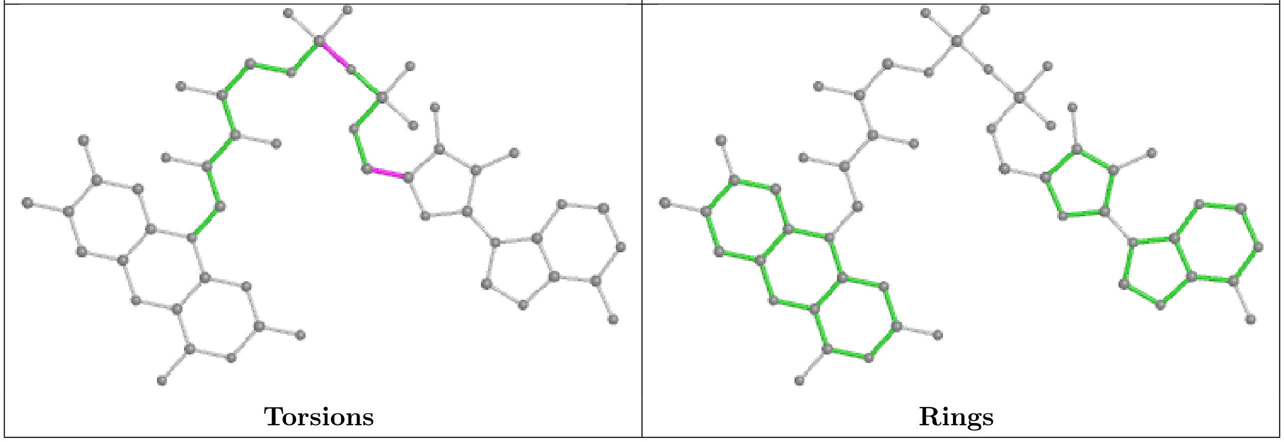


Rings

Ligand FAD C 1106

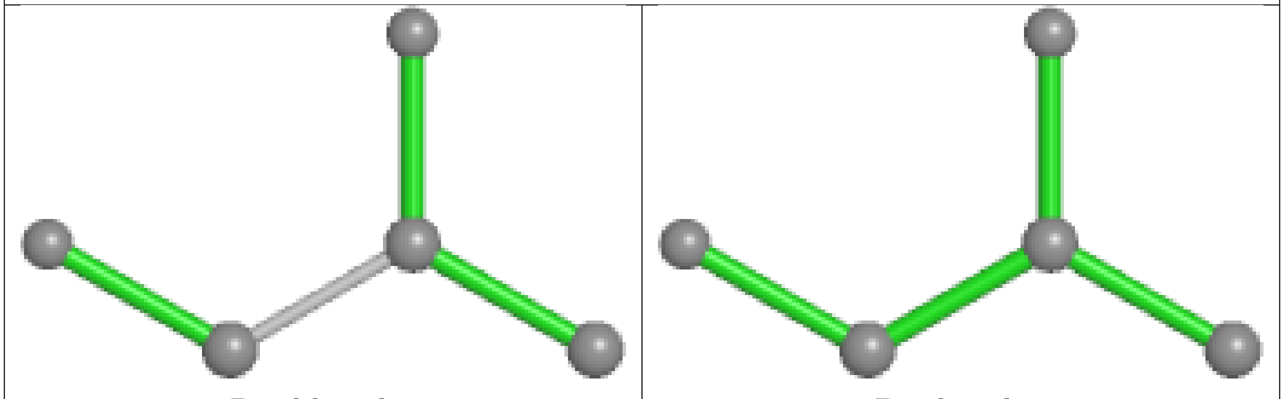


Bond lengths **Bond angles**



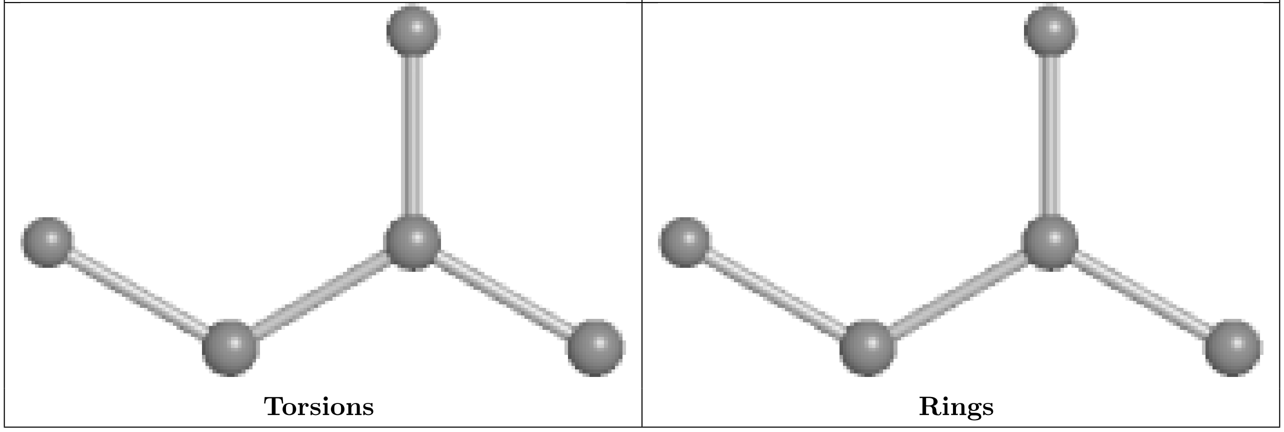
Torsions **Rings**

Ligand ALA D 1102



Bond lengths

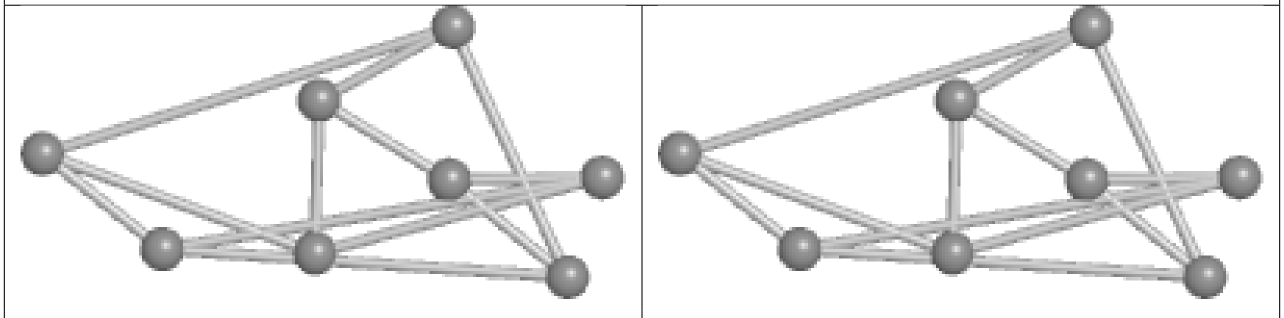
Bond angles



Torsions

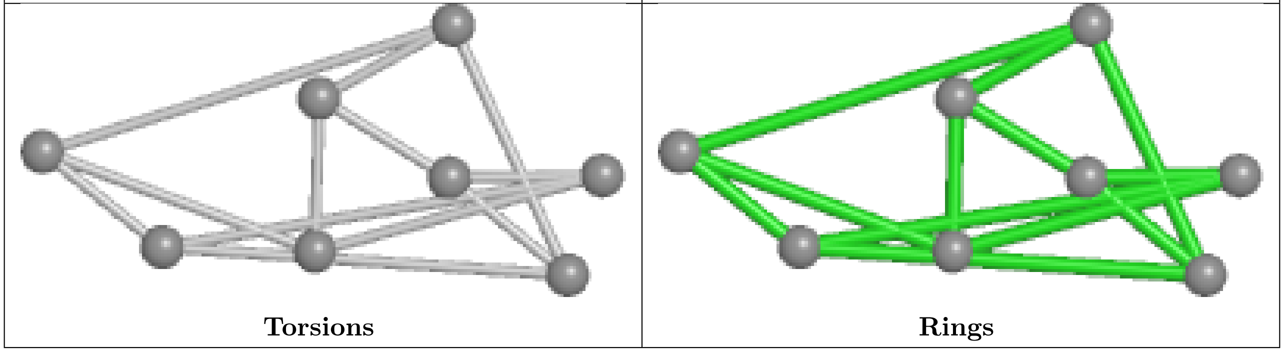
Rings

Ligand SF4 B 1104



Bond lengths

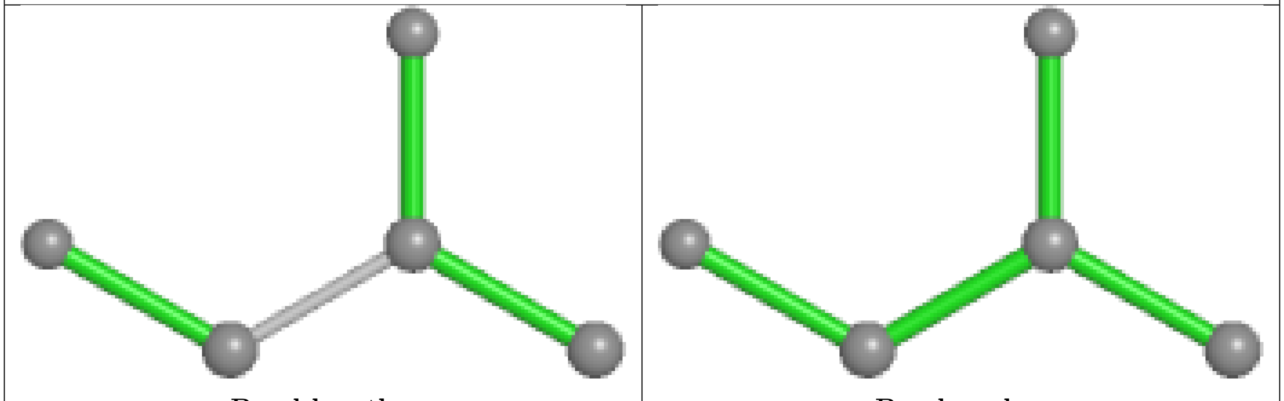
Bond angles



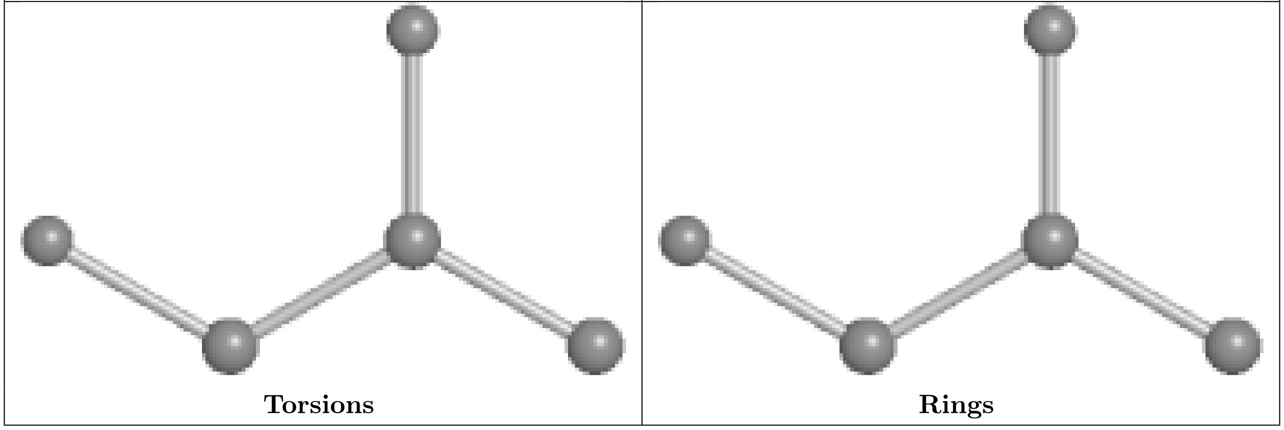
Torsions

Rings

Ligand ALA A 1108

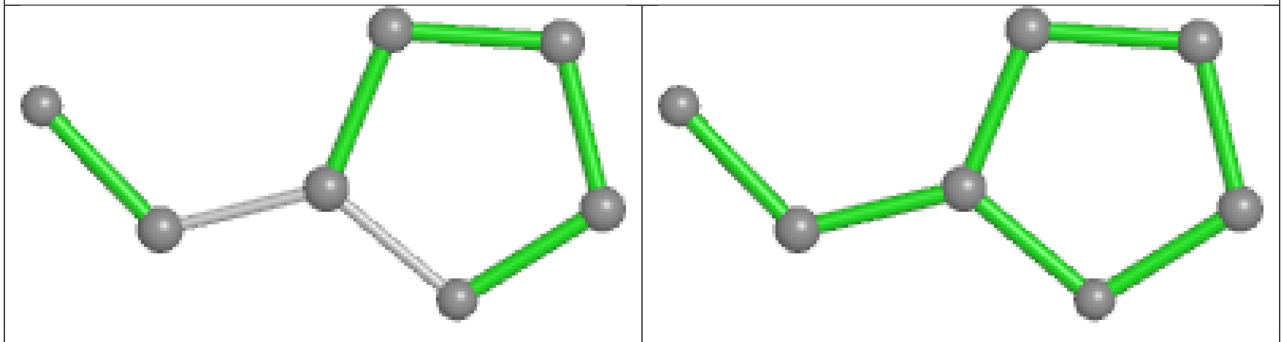


Bond lengths **Bond angles**

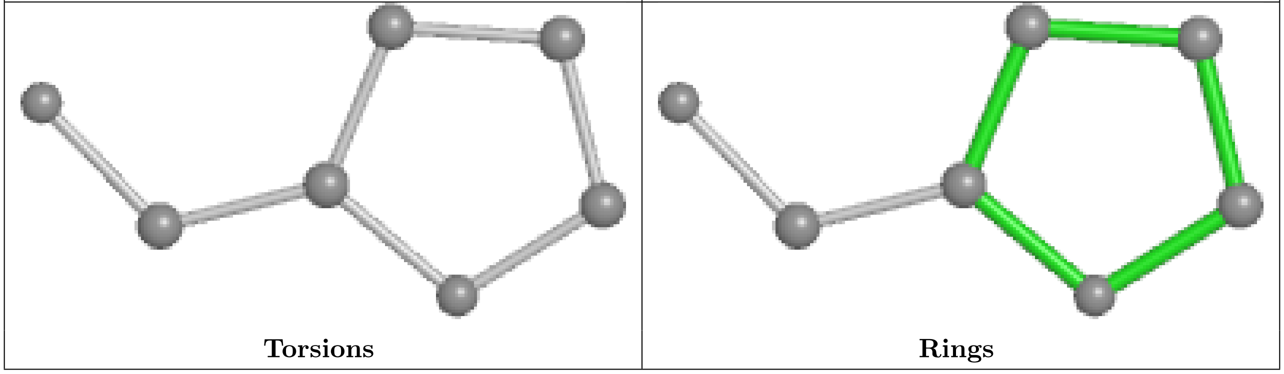


Torsions **Rings**

Ligand PRO C 1101

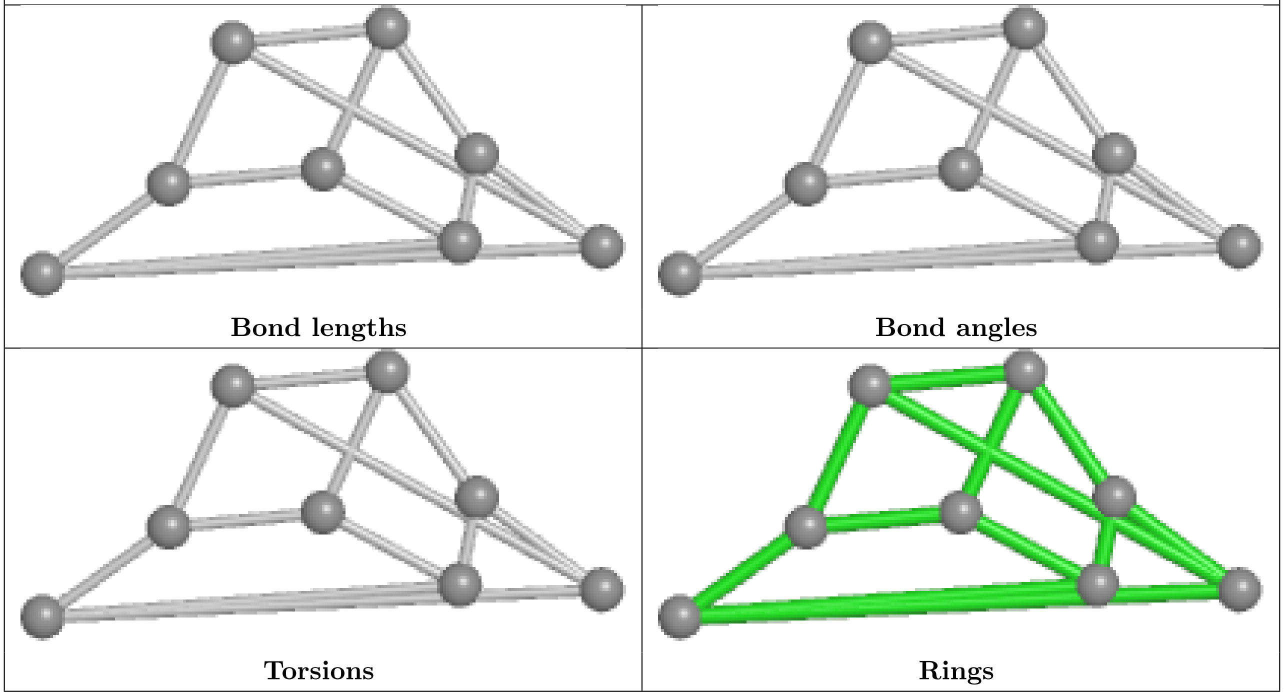


Bond lengths **Bond angles**



Torsions **Rings**

Ligand SF4 A 1102



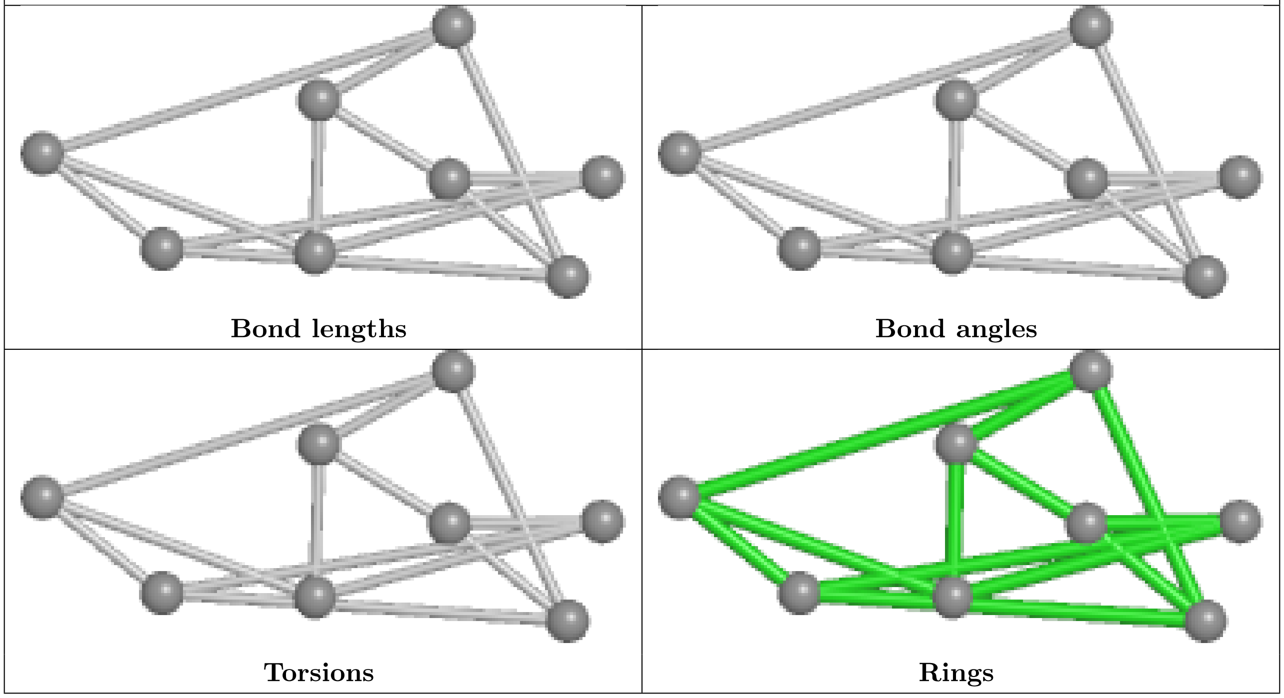
Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 A 1101



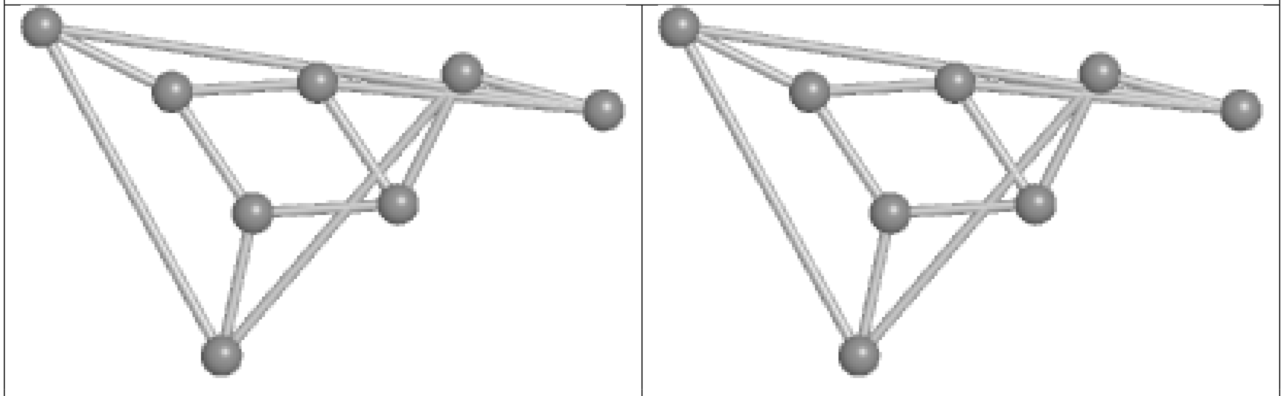
Bond lengths

Bond angles

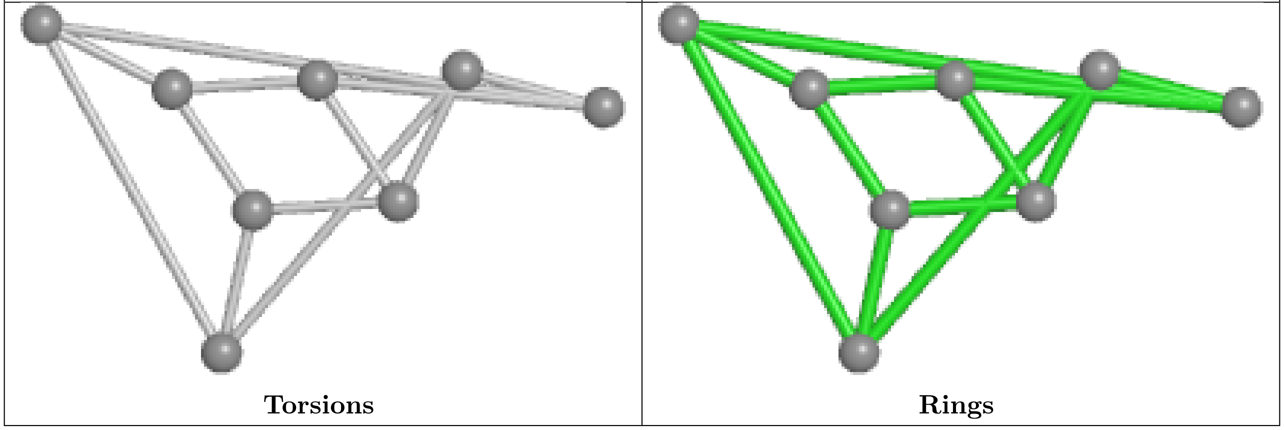
Torsions

Rings

Ligand SF4 A 1104

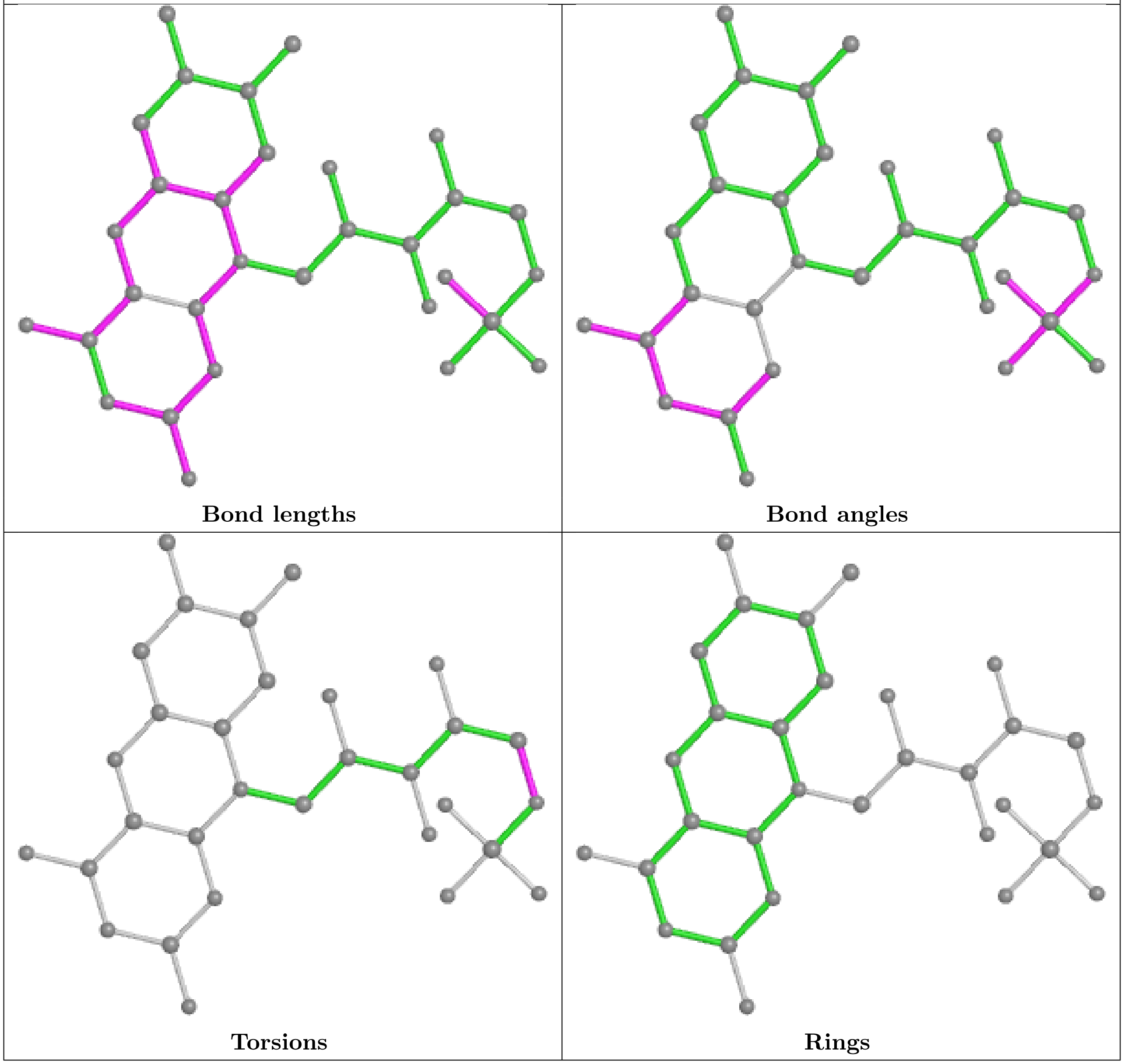


Bond lengths **Bond angles**



Torsions **Rings**

Ligand FNR D 1109



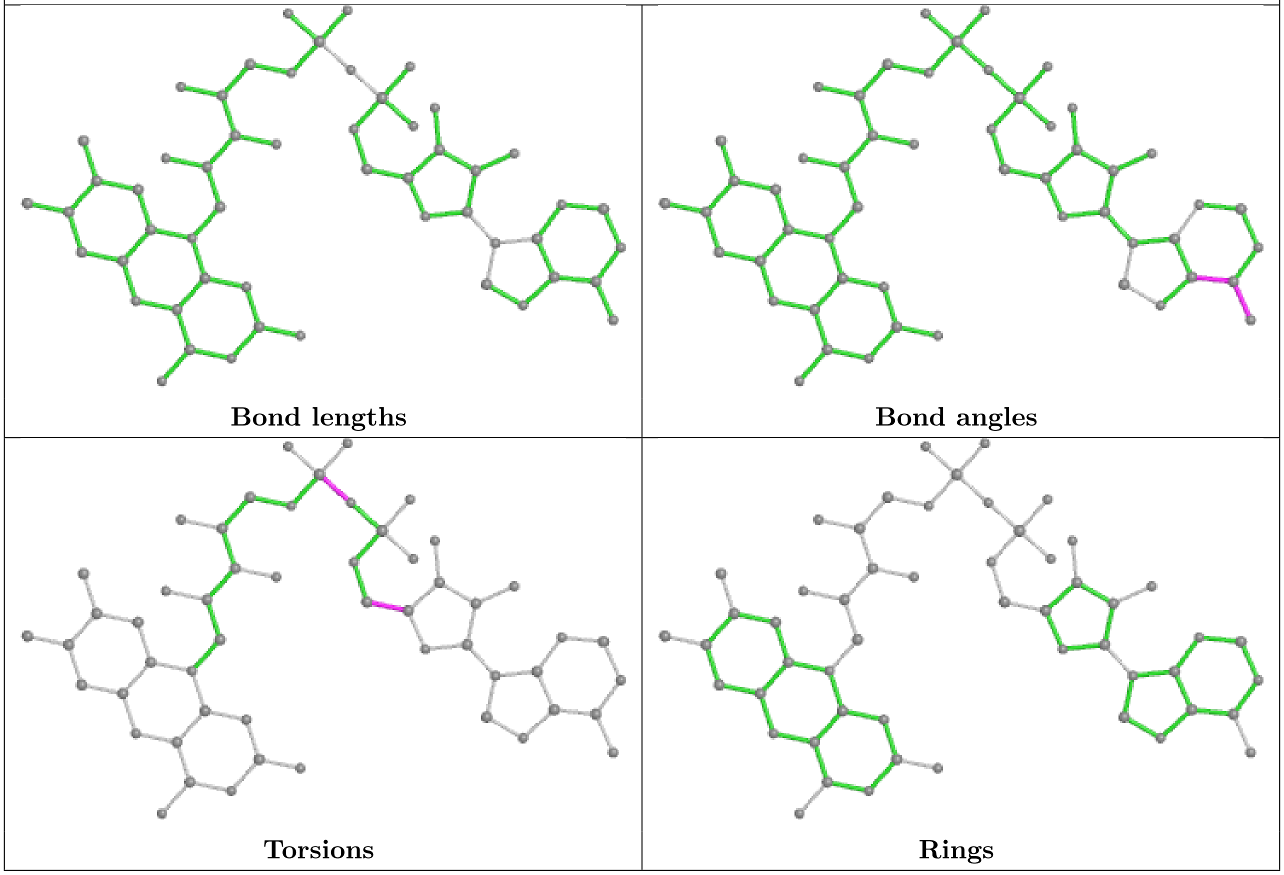
Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 1106



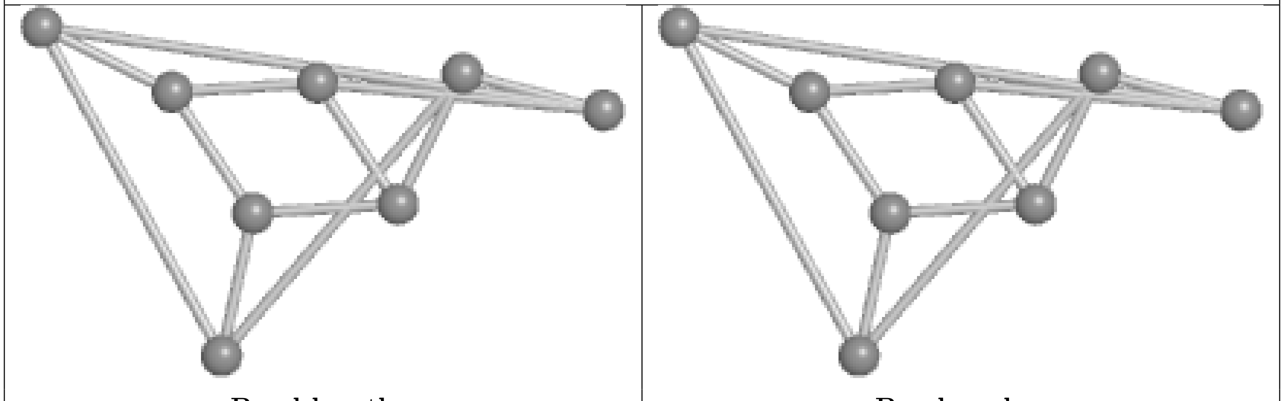
Bond lengths

Bond angles

Torsions

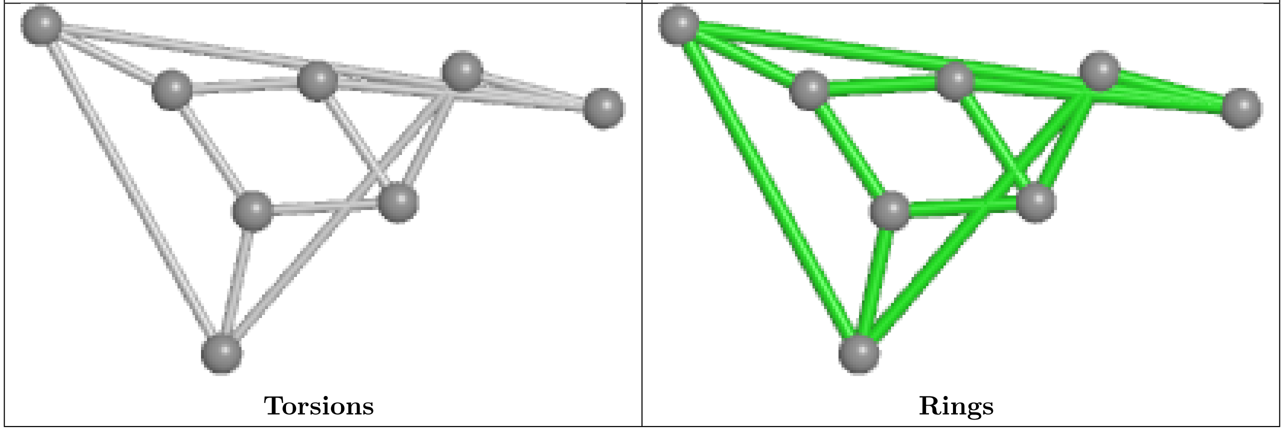
Rings

Ligand SF4 C 1102



Bond lengths

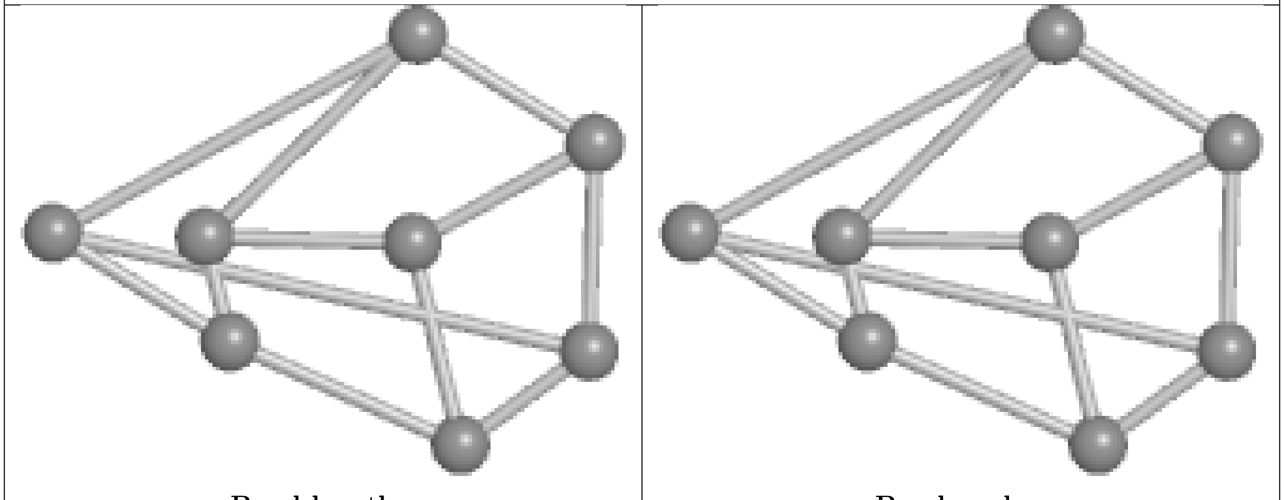
Bond angles



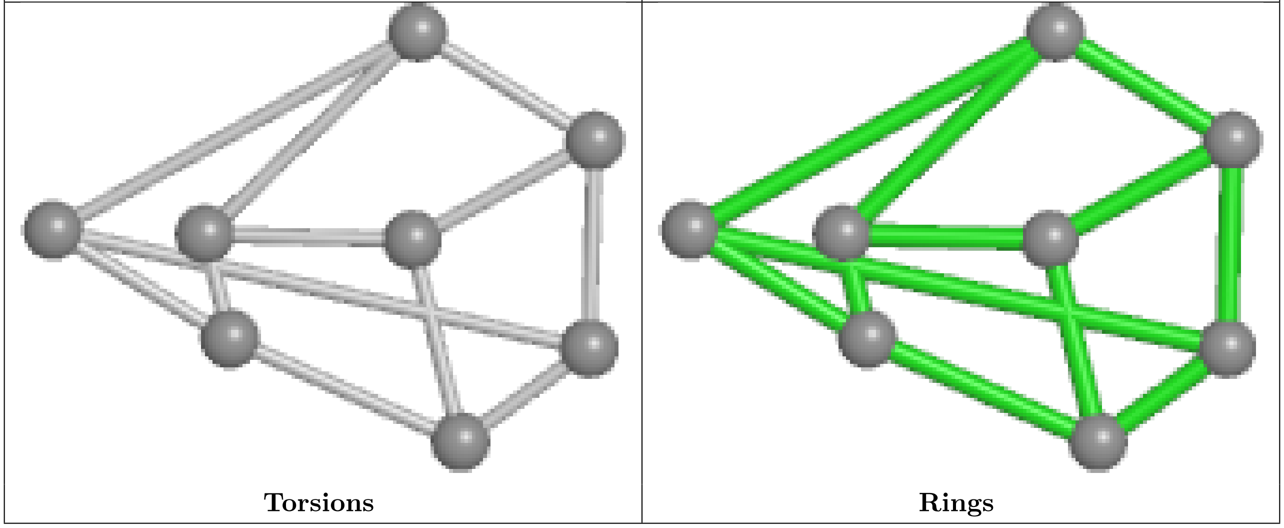
Torsions

Rings

Ligand SF4 C 1104

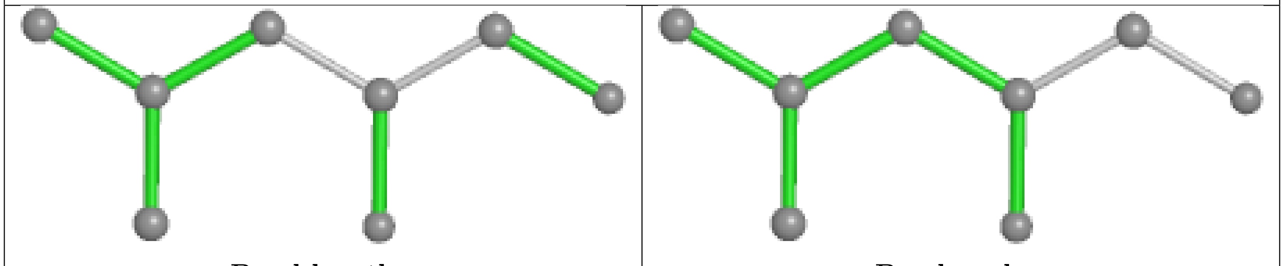


Bond lengths **Bond angles**

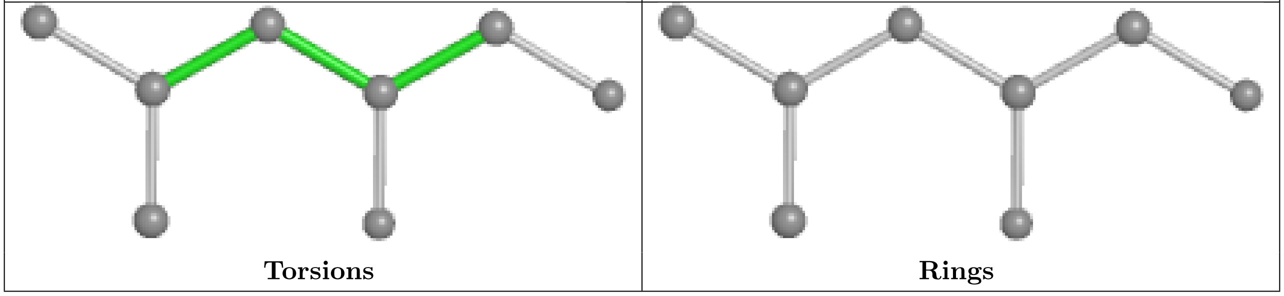


Torsions **Rings**

Ligand LEU D 1101

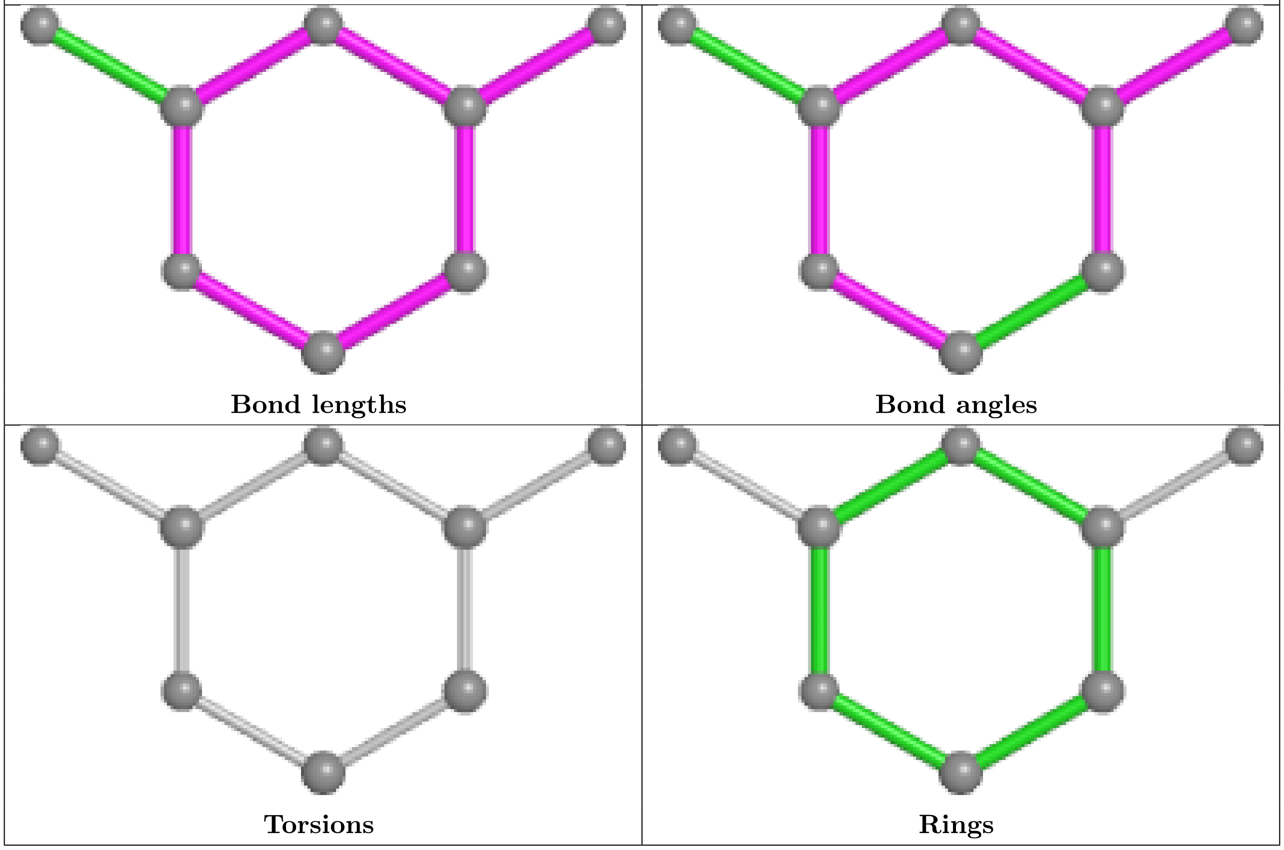


Bond lengths **Bond angles**

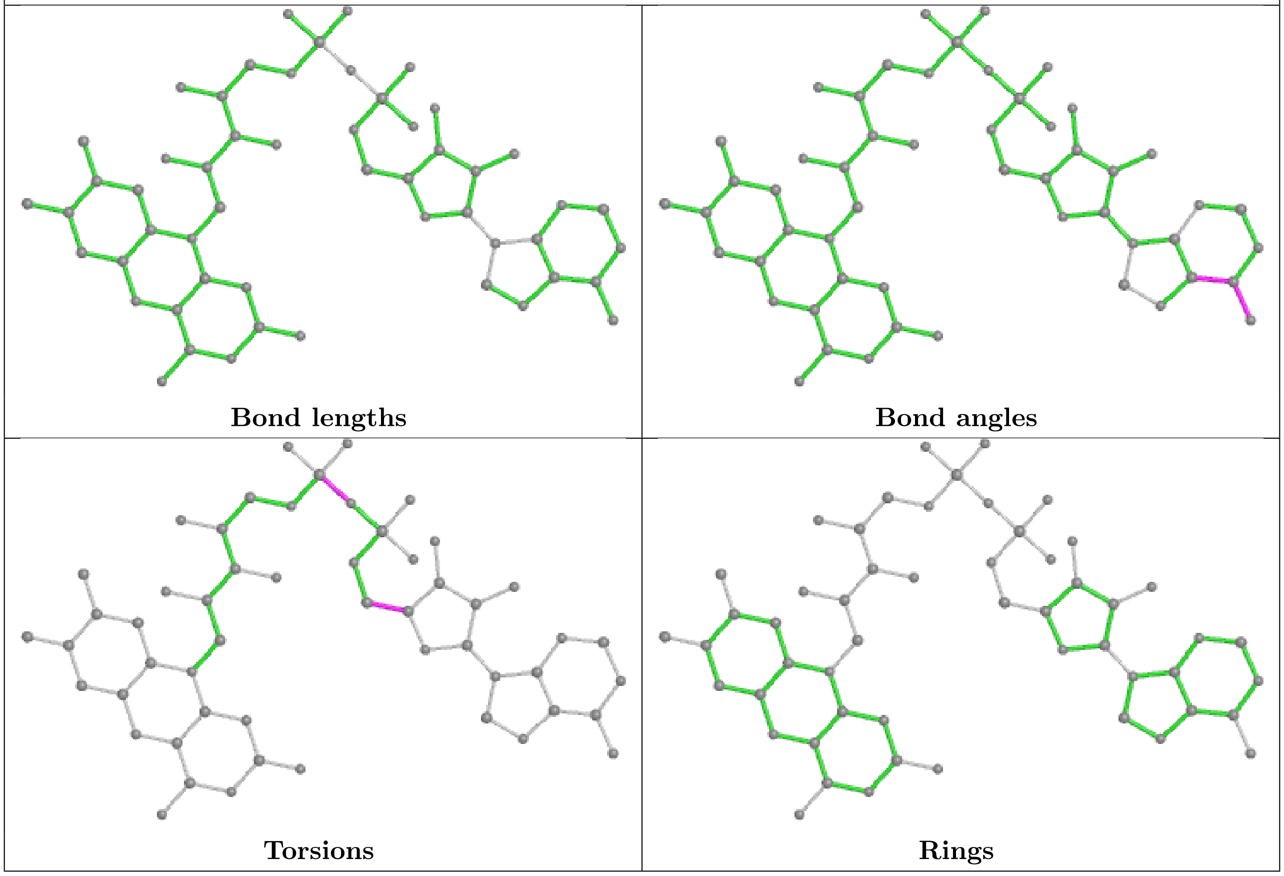


Torsions **Rings**

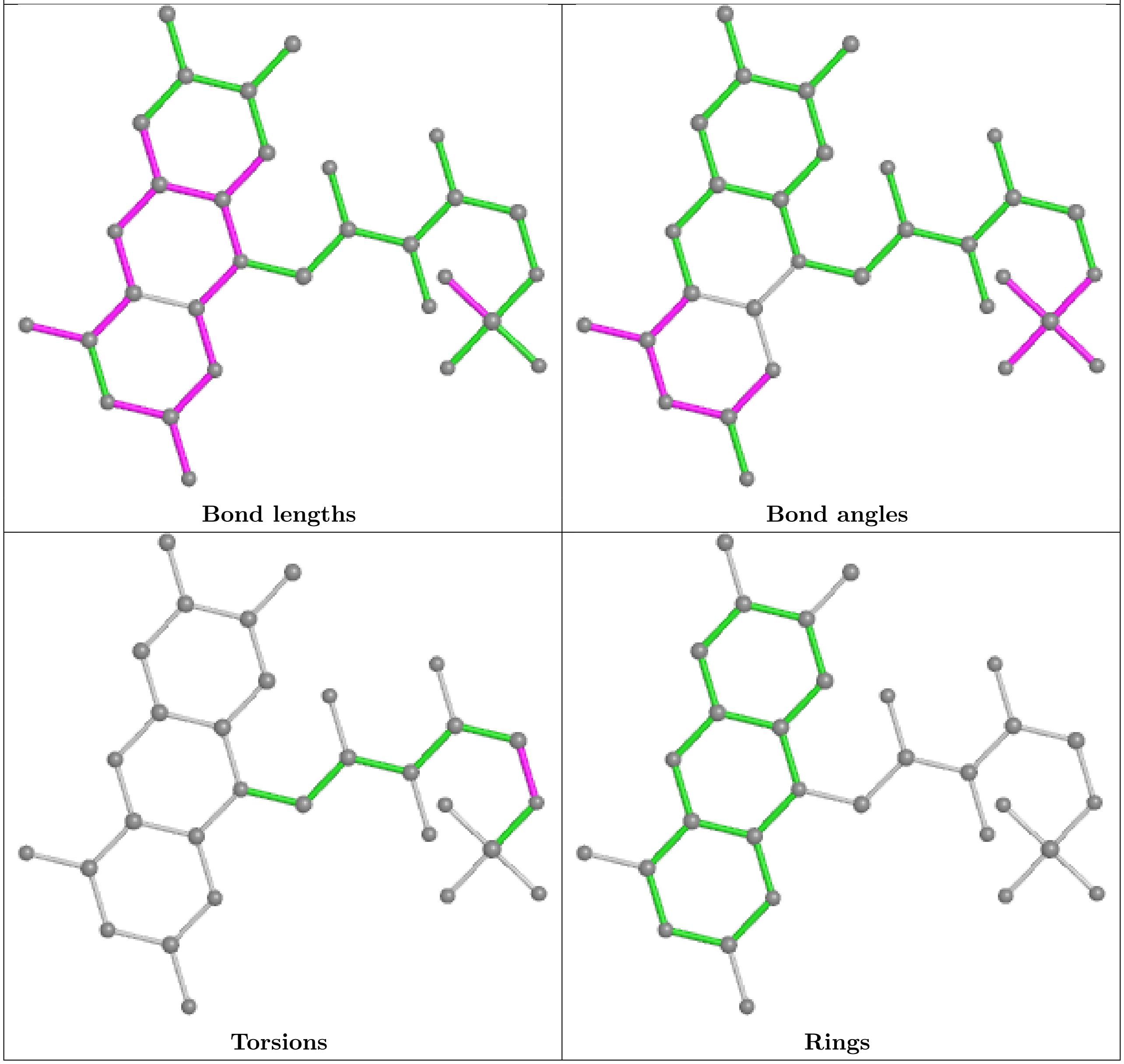
Ligand URA D 1108



Ligand FAD D 1107



Ligand FNR C 1108



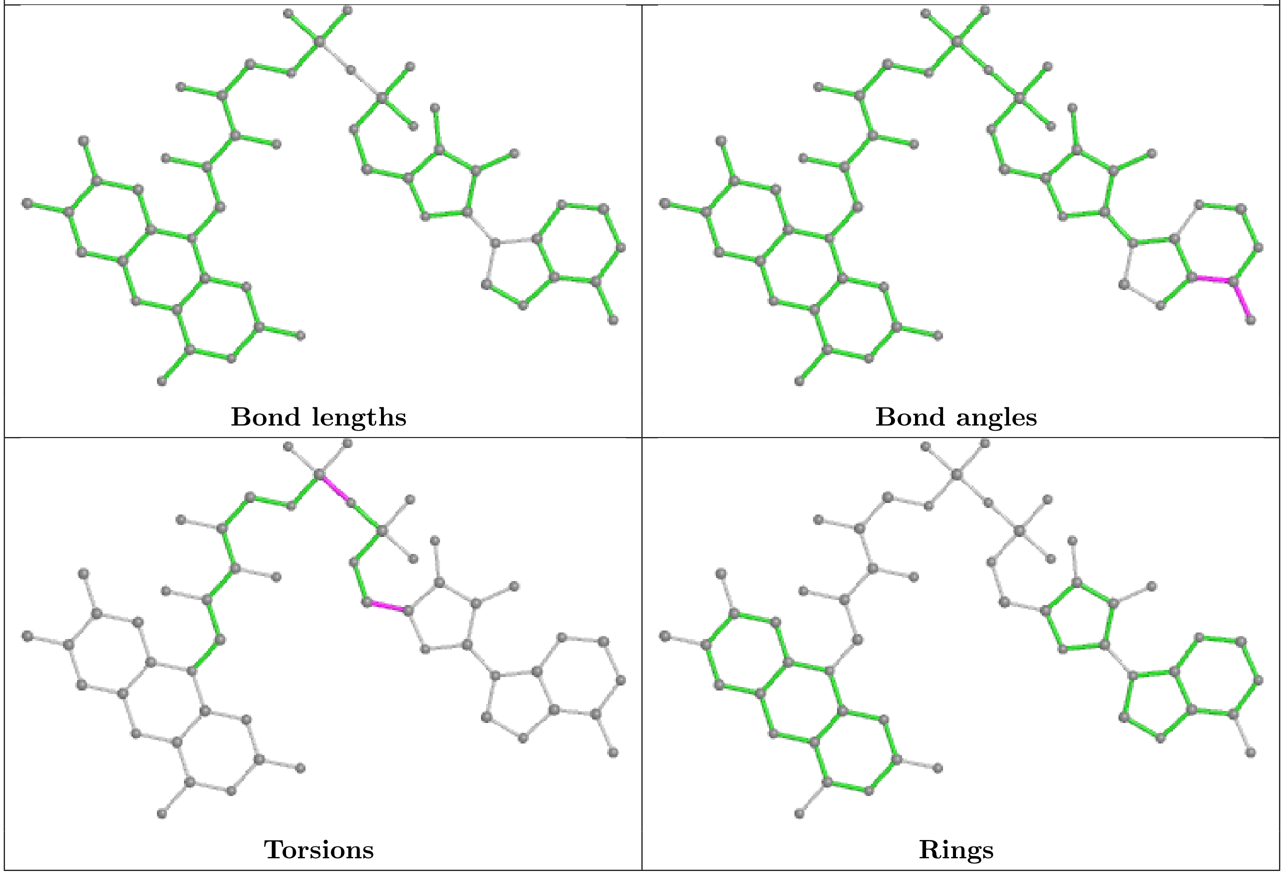
Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 1105



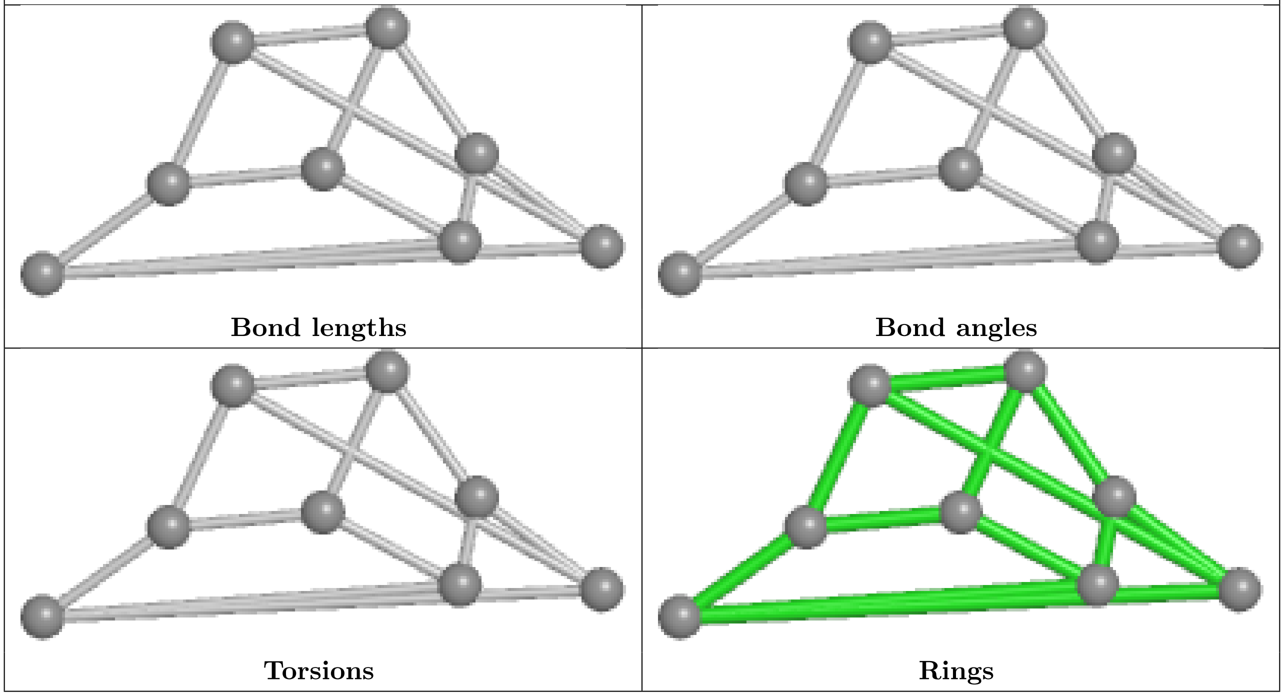
Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 B 1103



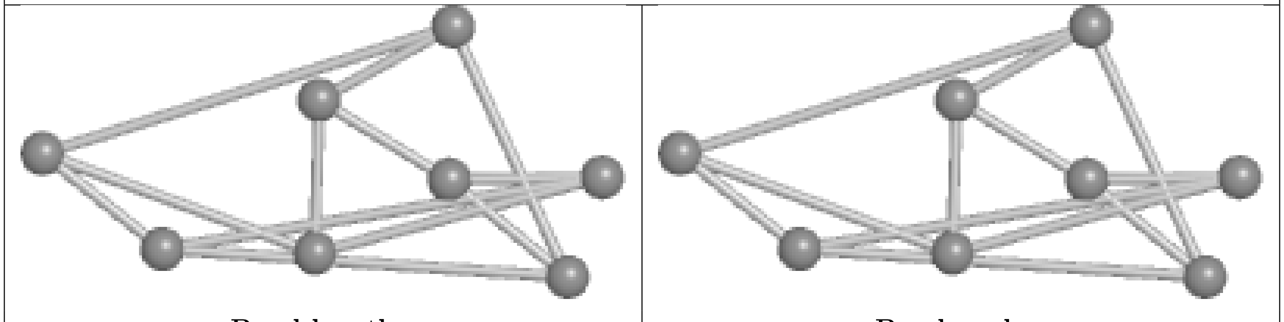
Bond lengths

Bond angles

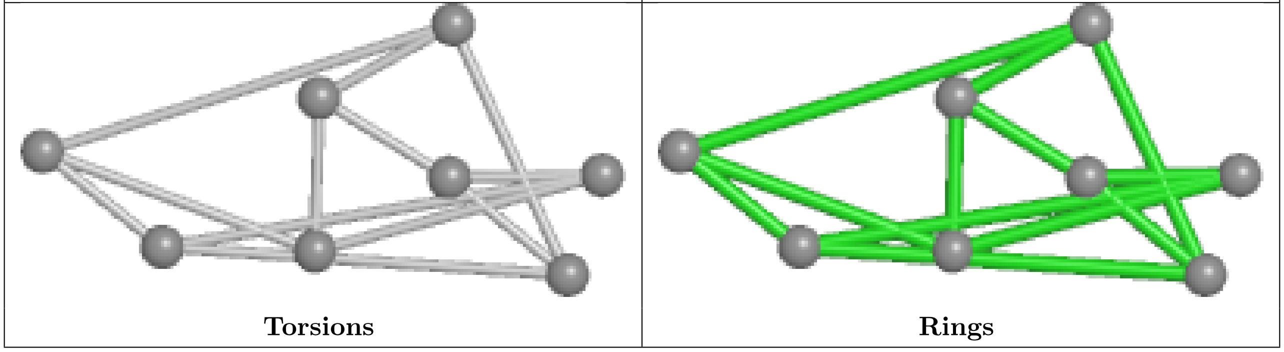
Torsions

Rings

Ligand SF4 B 1102

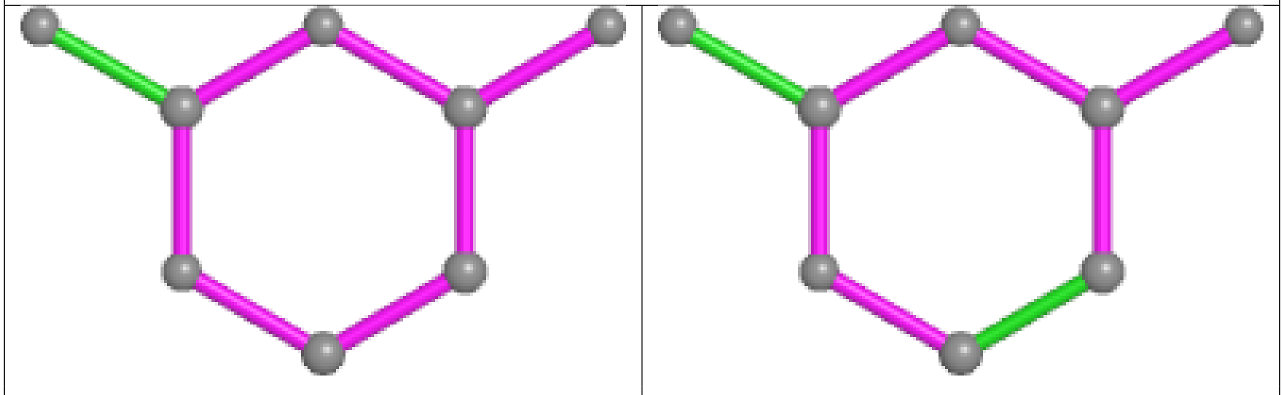


Bond lengths **Bond angles**

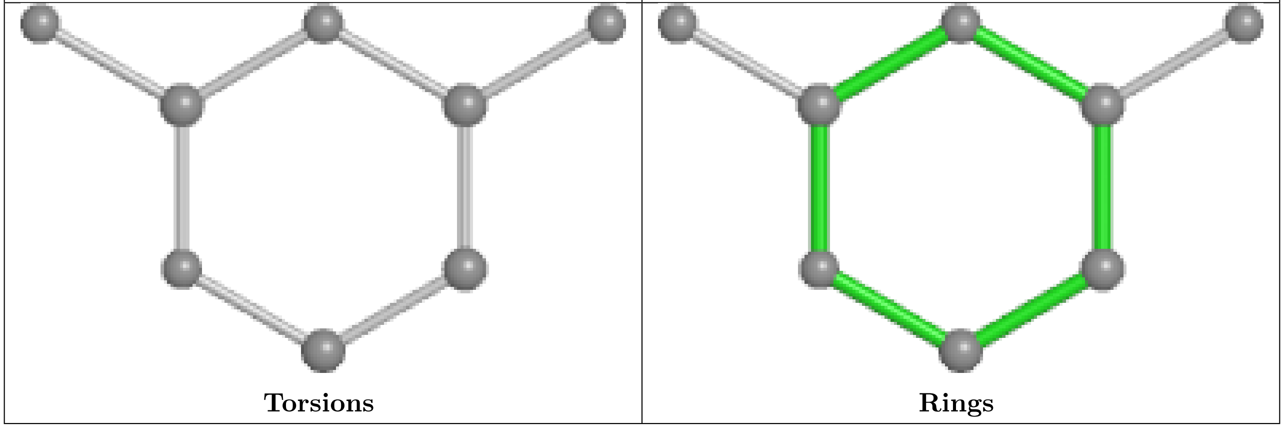


Torsions **Rings**

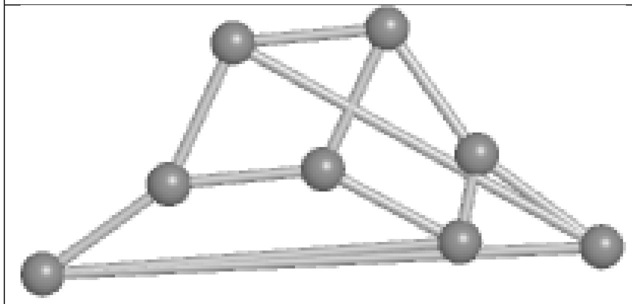
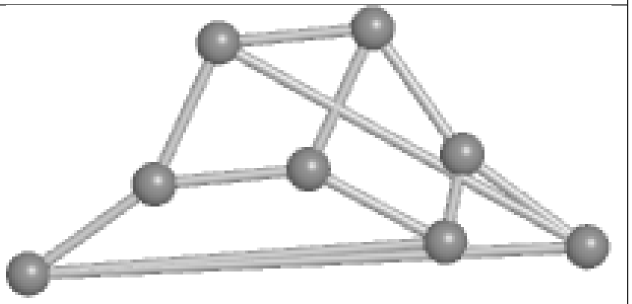
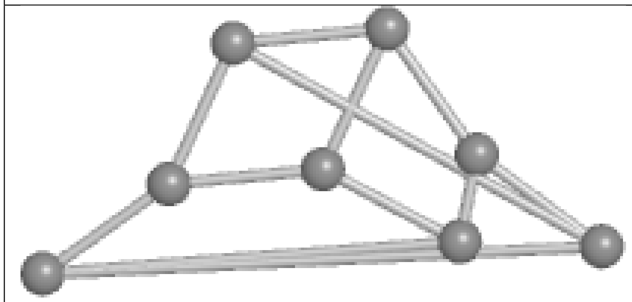
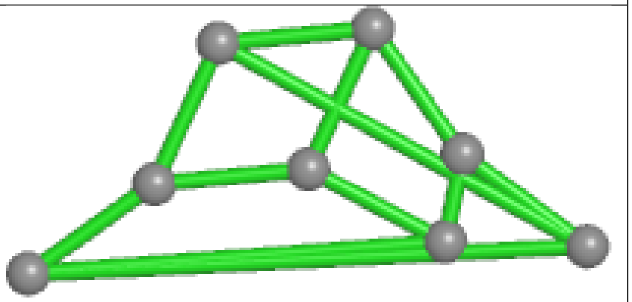
Ligand URA B 1107



Bond lengths **Bond angles**



Torsions **Rings**

Ligand SF4 C 1105	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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

The worst 5 of 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

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

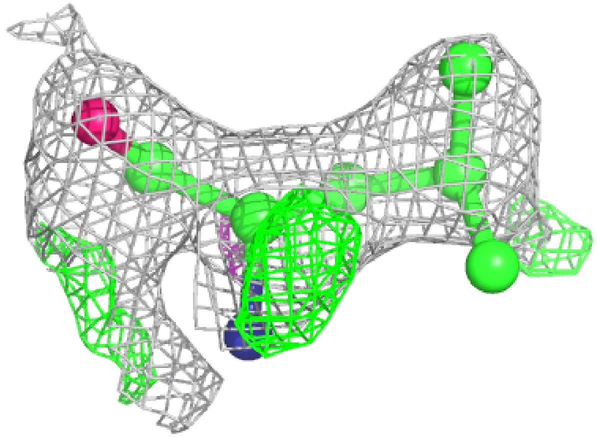
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

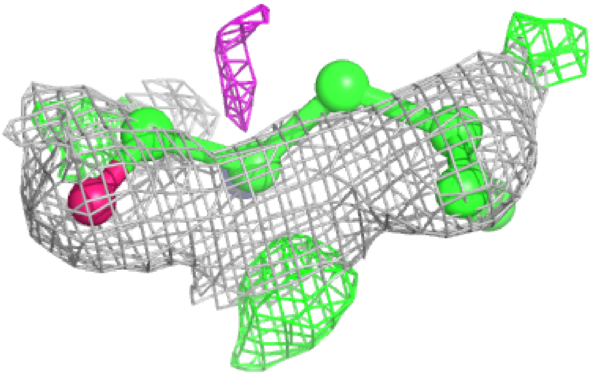
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
7	LEU	B	1101	8/9	0.70	0.35	47,61,70,72	0
6	ALA	A	1108	5/6	0.72	0.31	58,65,68,69	0
6	ALA	D	1102	5/6	0.79	0.22	54,62,66,71	0
8	PRO	C	1101	7/8	0.79	0.28	52,59,62,64	0
7	LEU	D	1101	8/9	0.87	0.26	48,53,65,74	0
4	URA	B	1107	8/8	0.94	0.09	29,32,35,35	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
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

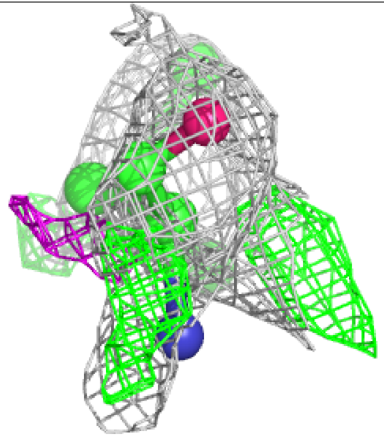
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

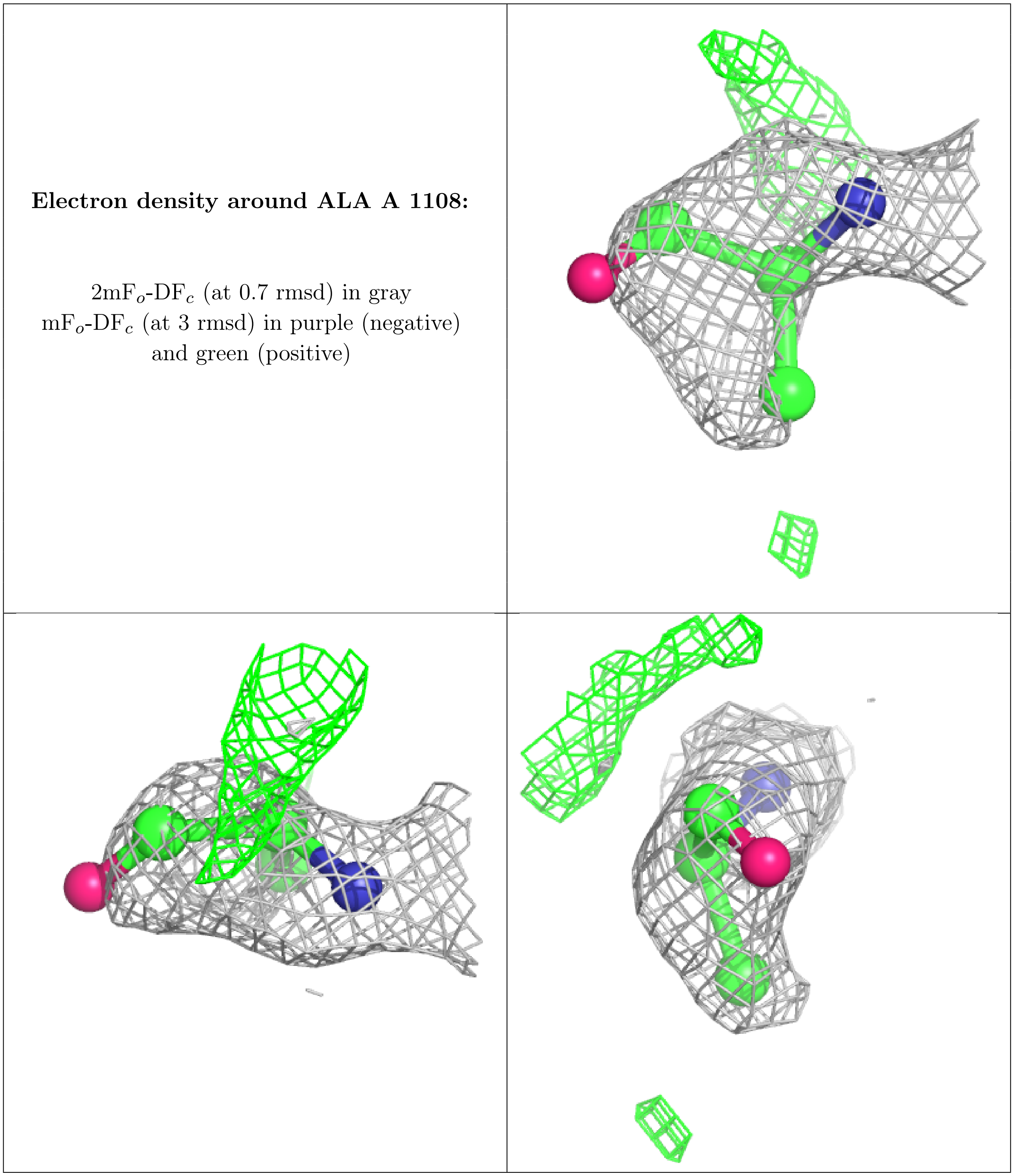


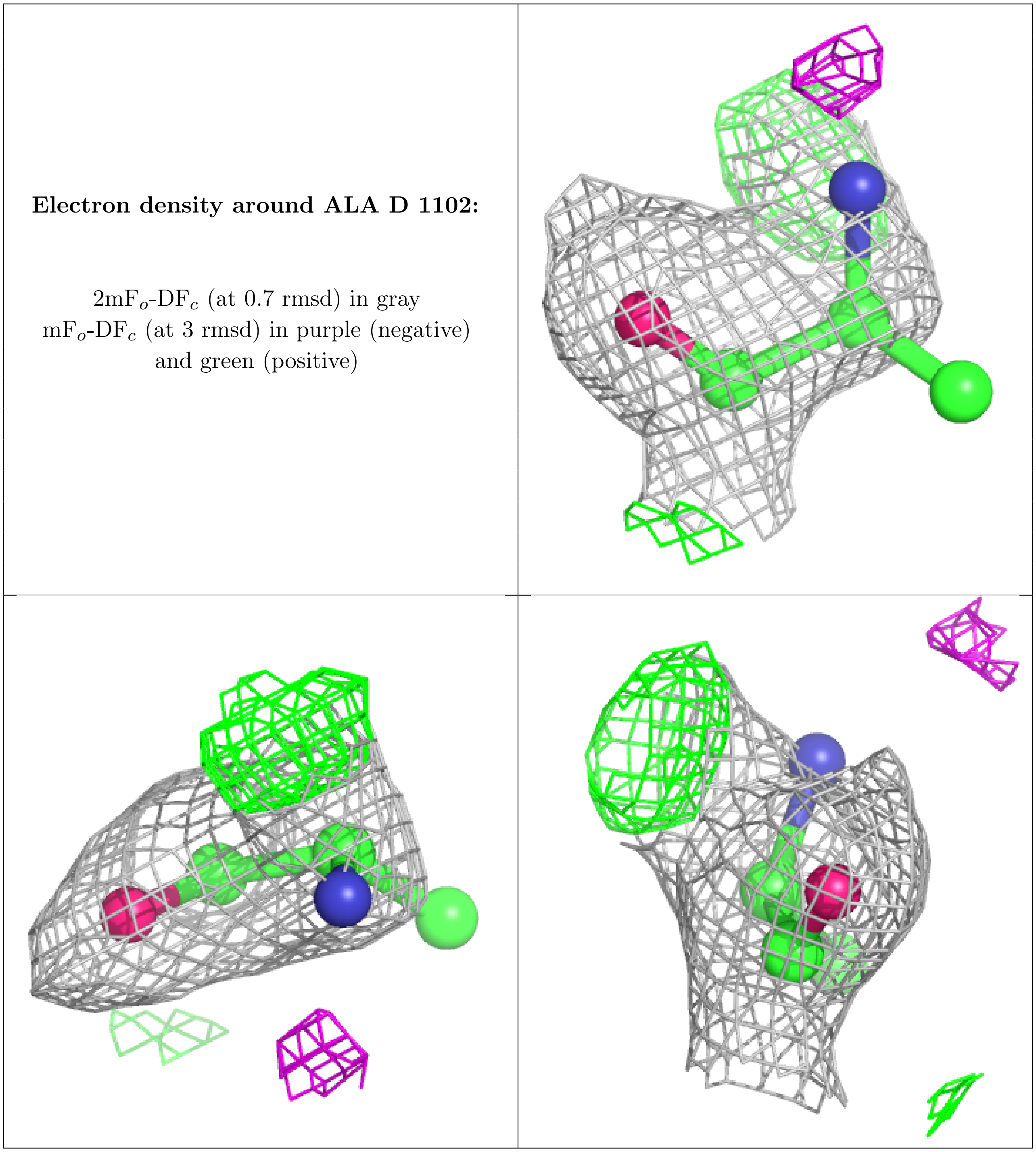




Electron density around ALA A 1108:

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



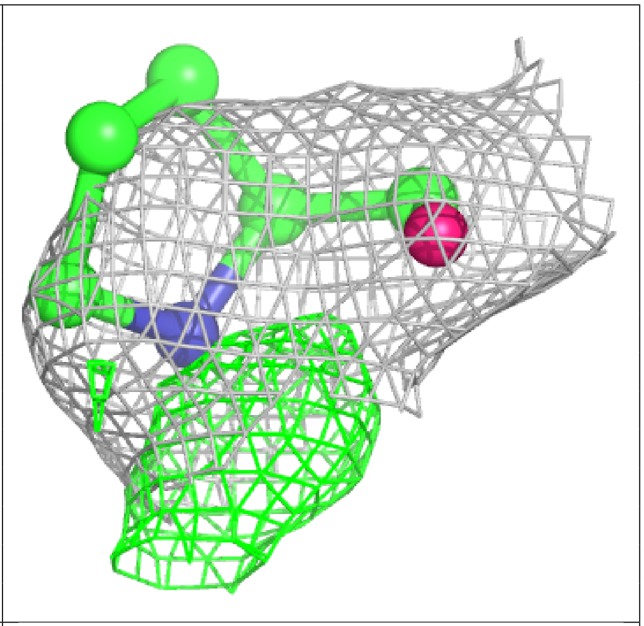


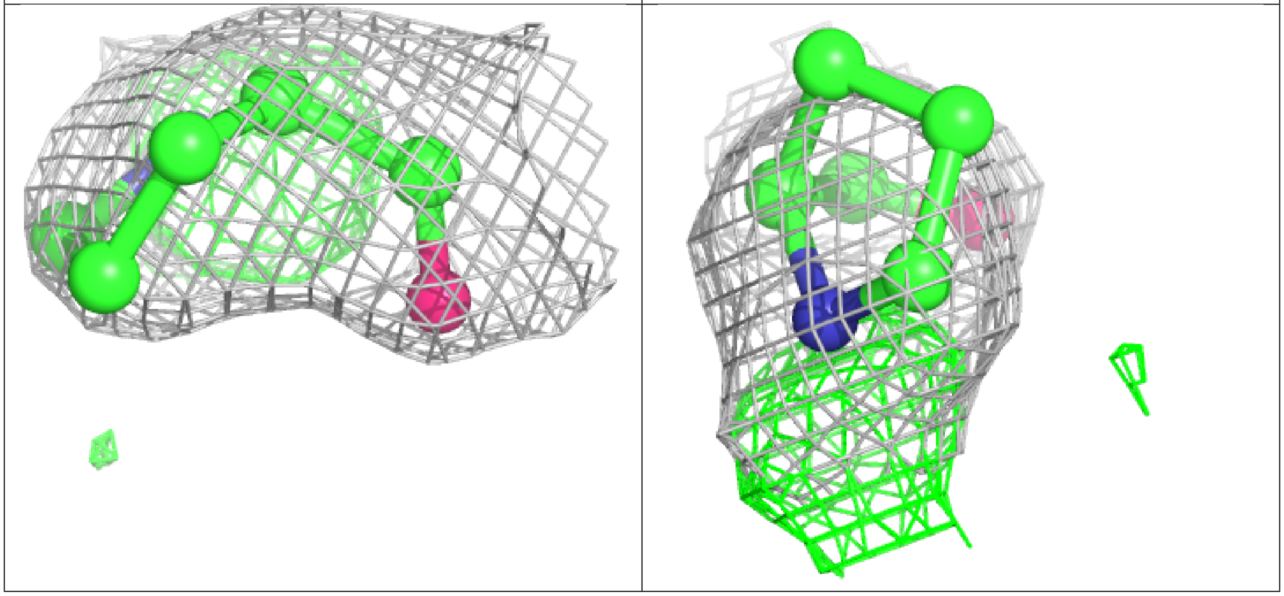
Electron density around ALA D 1102:

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:

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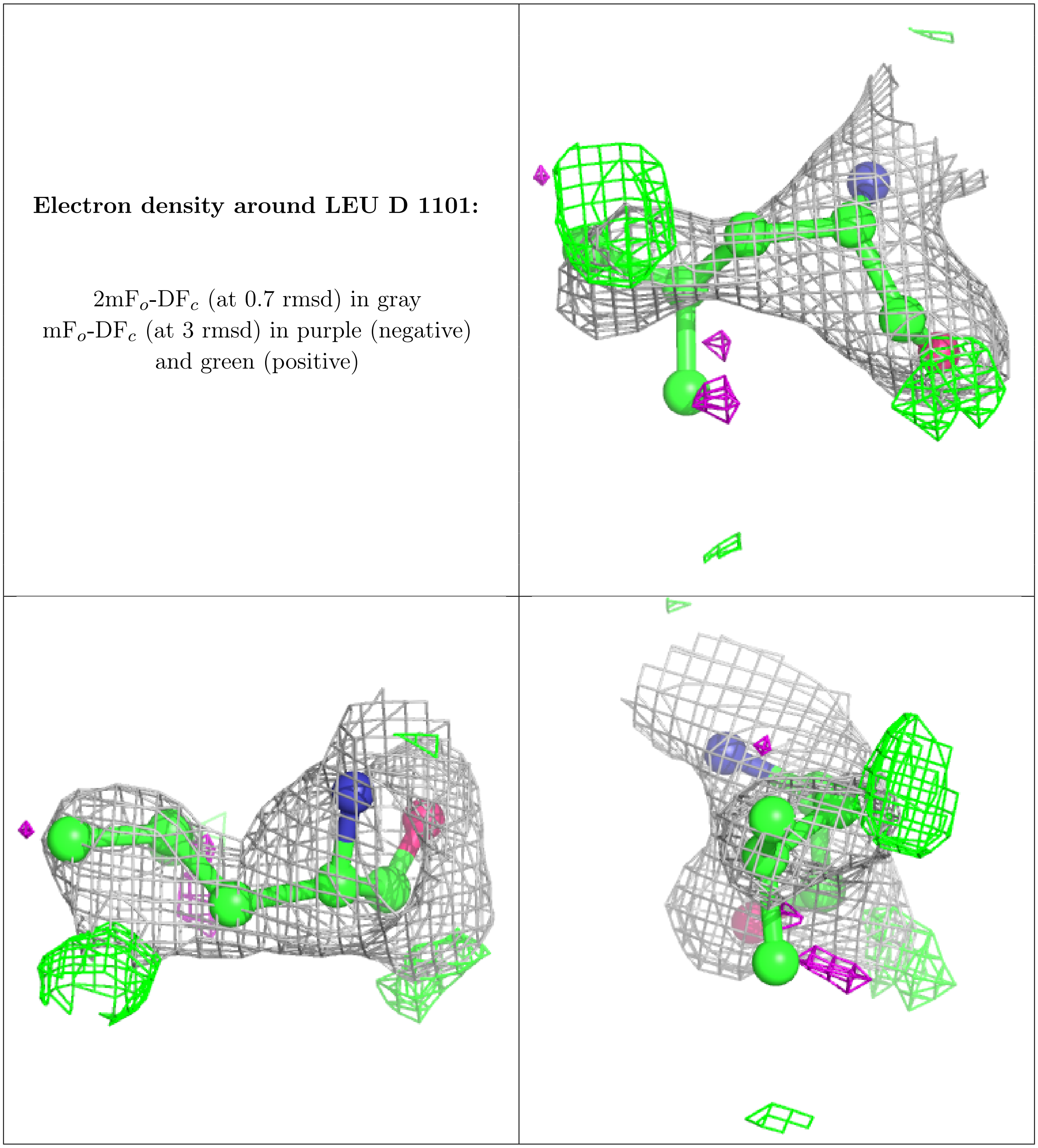
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around URA B 1107:

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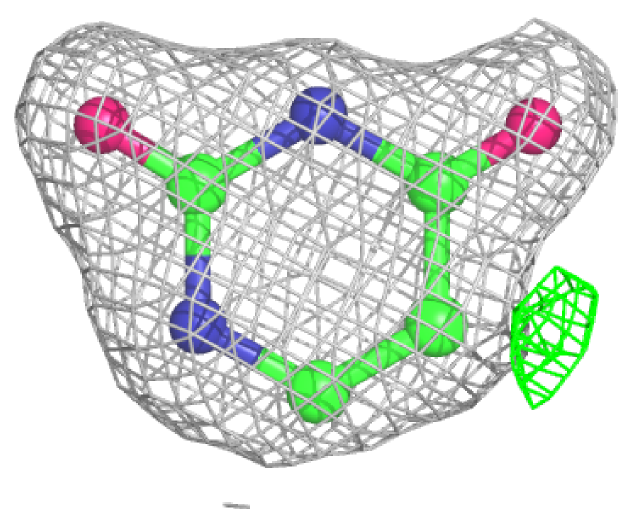
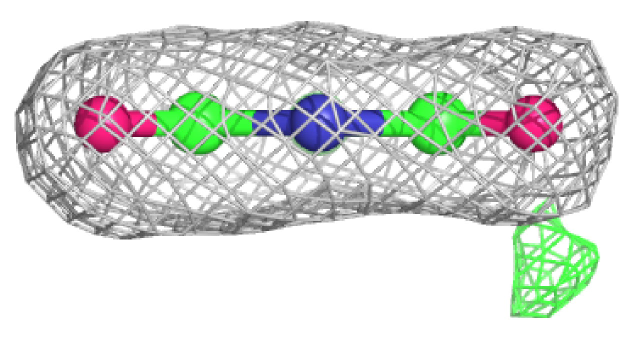
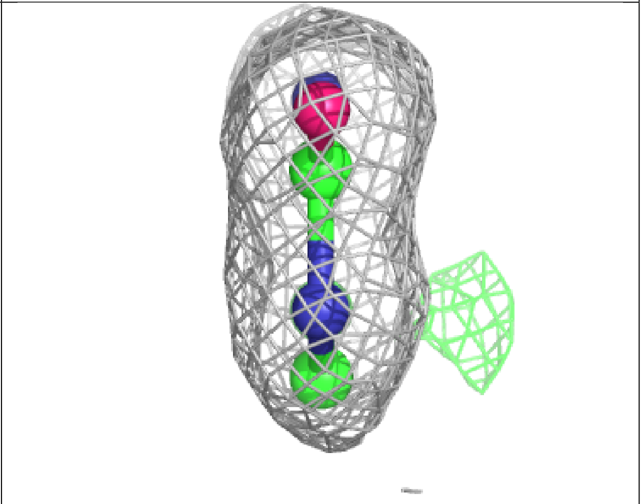
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

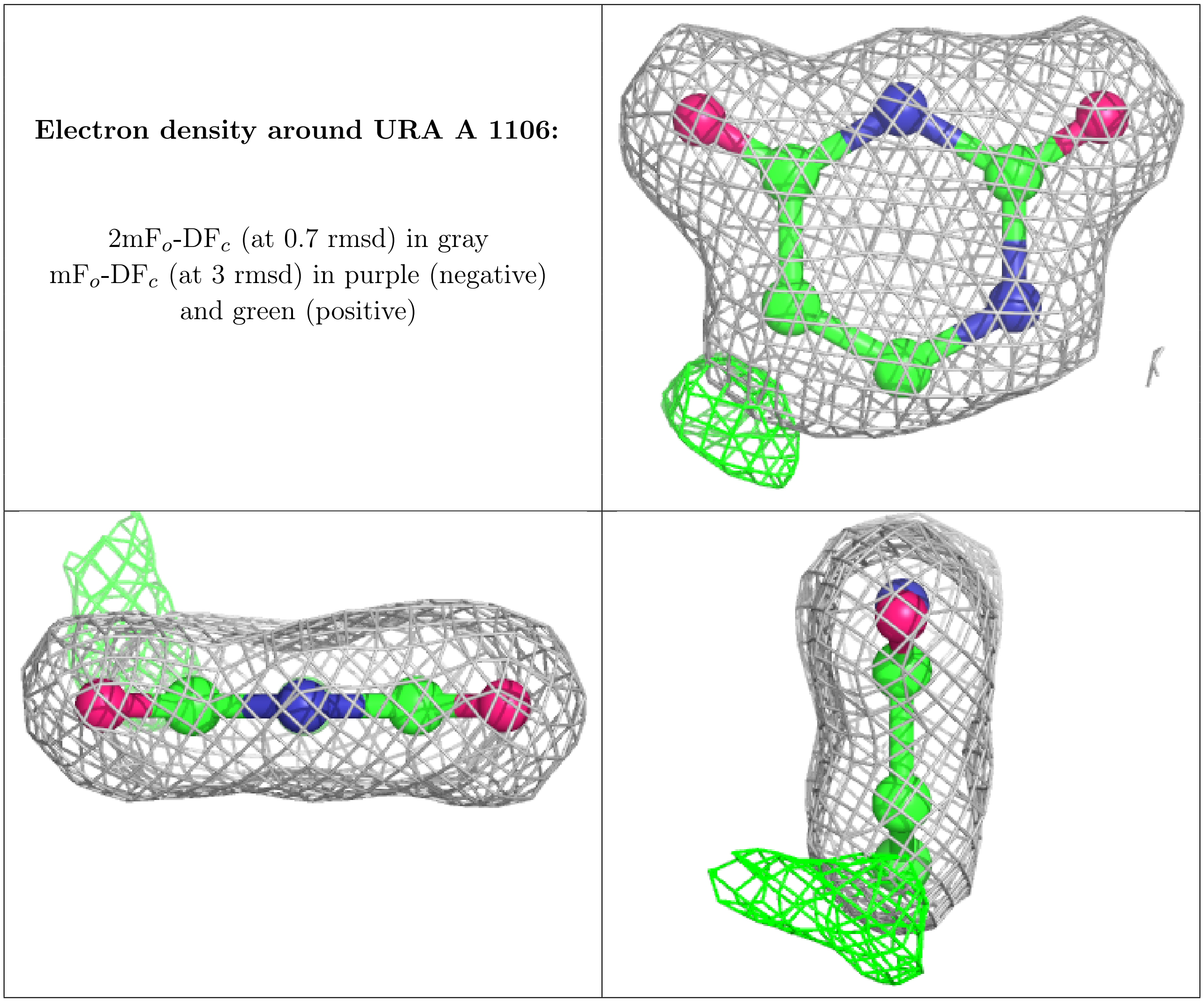






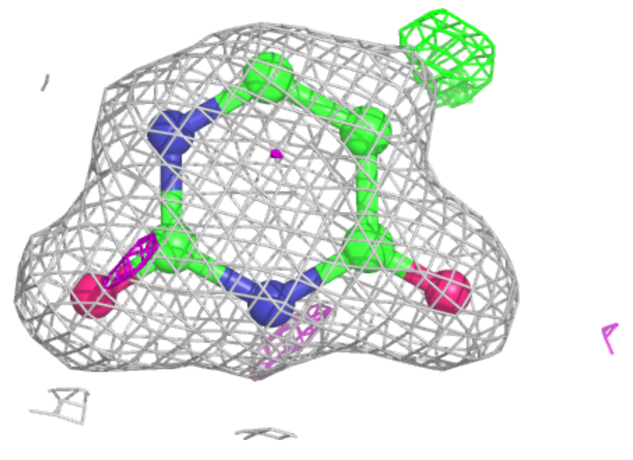
Electron density around URA A 1106:

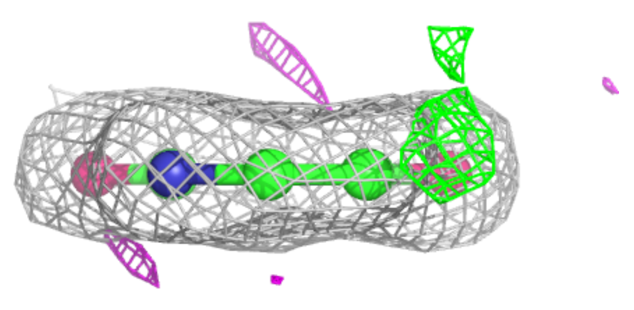
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

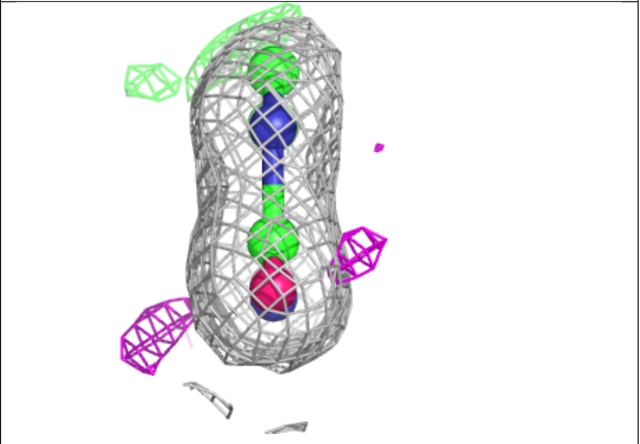


Electron density around URA D 1108:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

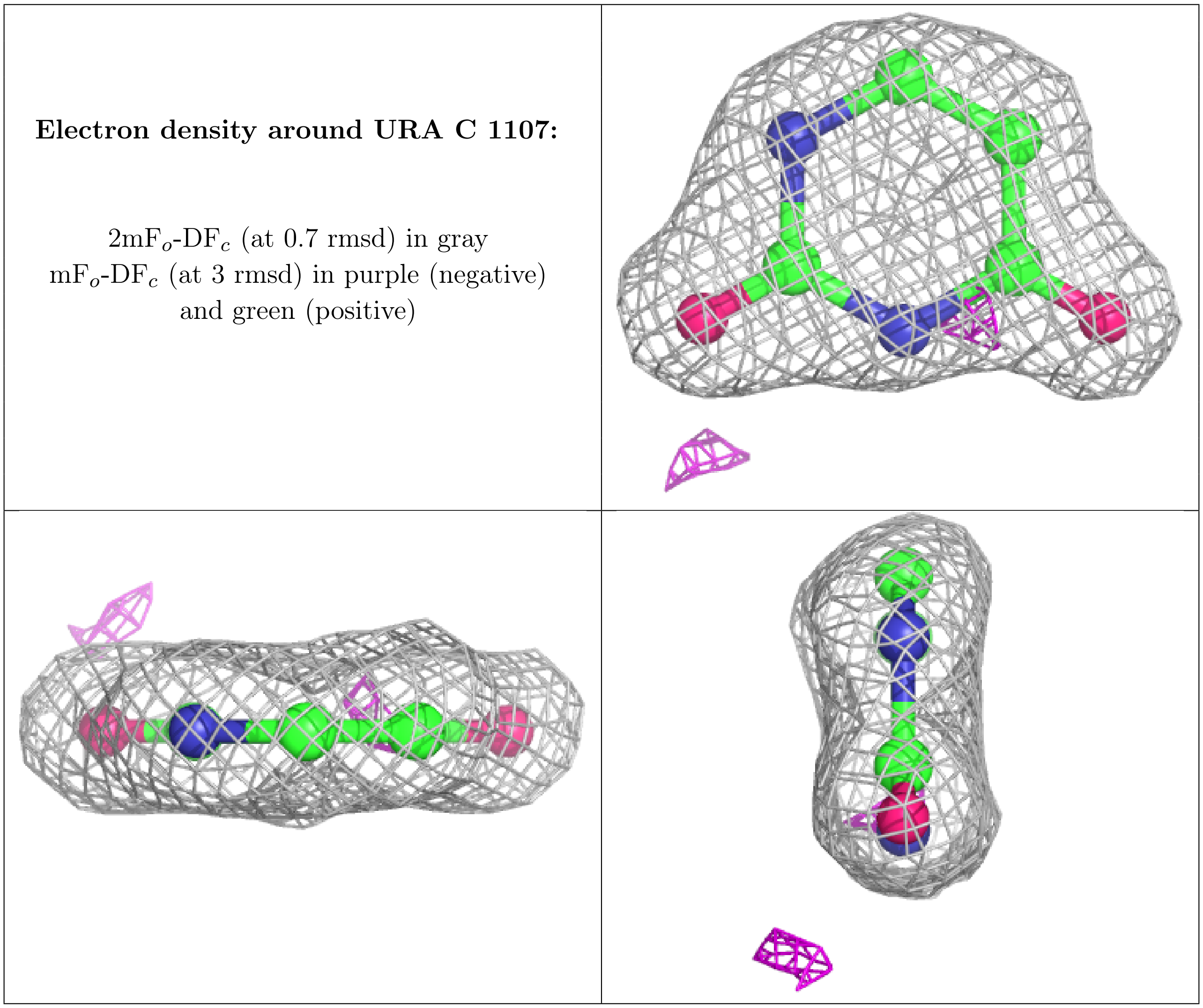






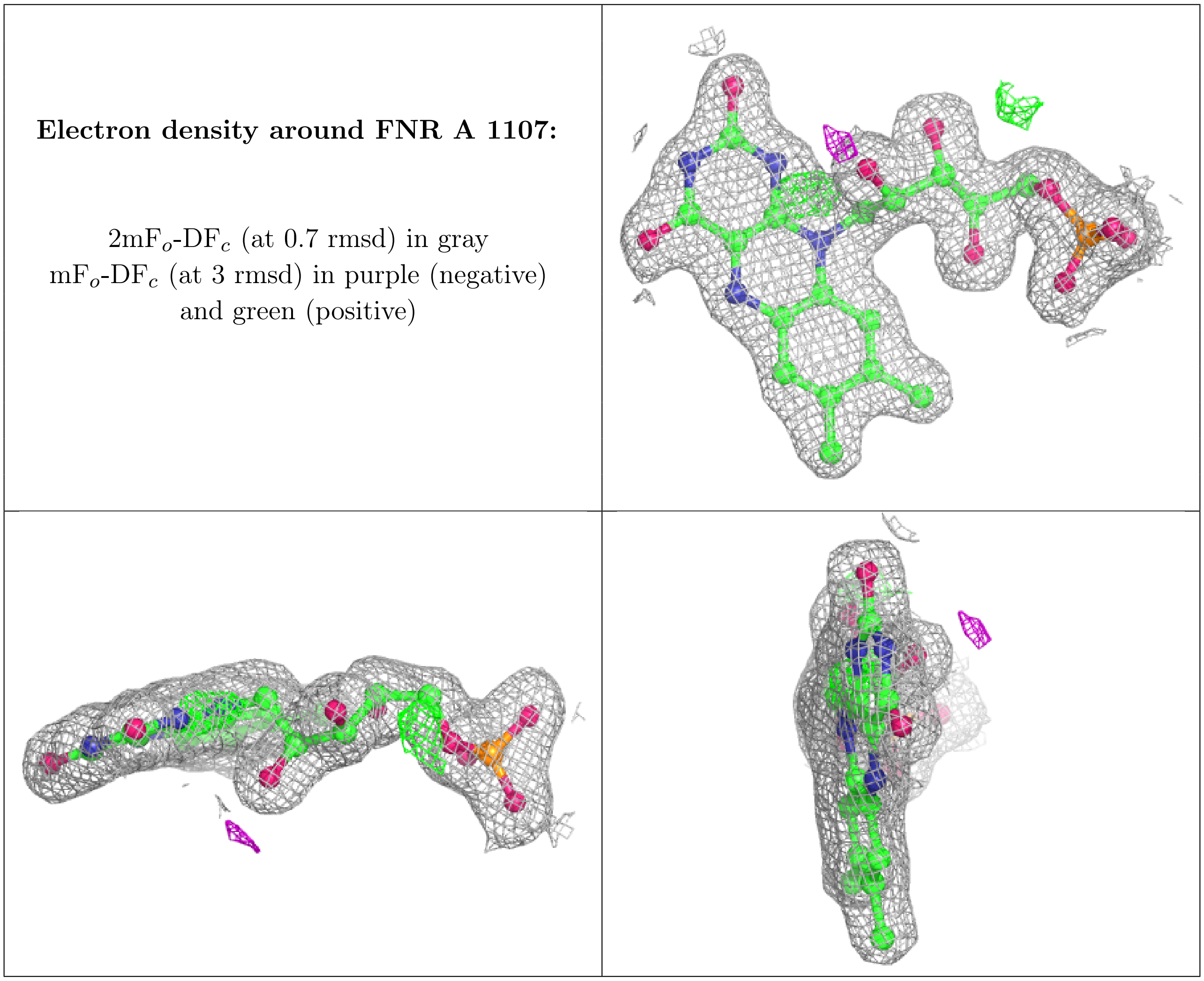
Electron density around URA C 1107:

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:

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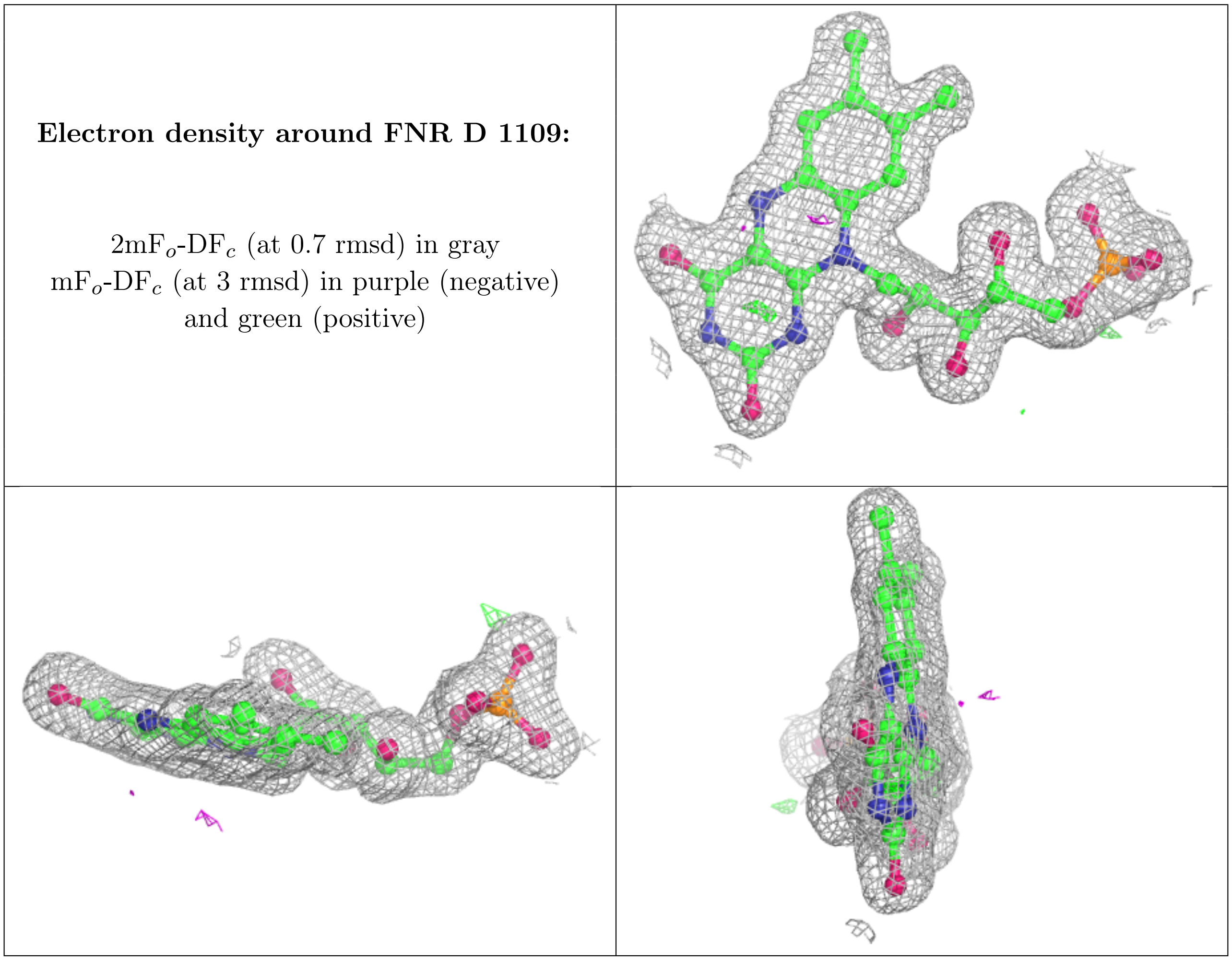
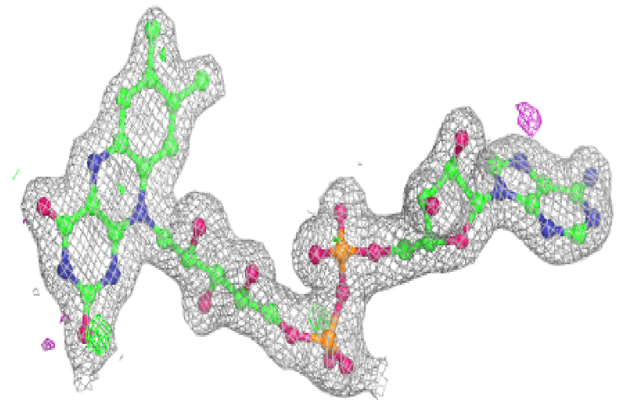
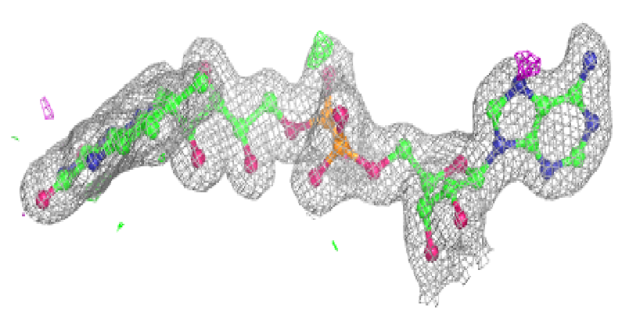
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

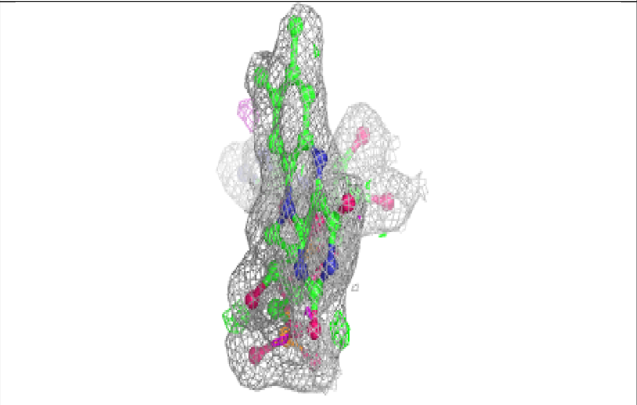


Electron density around FAD B 1106:

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

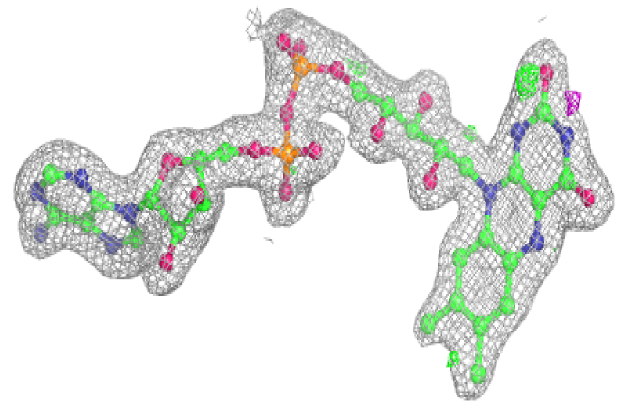


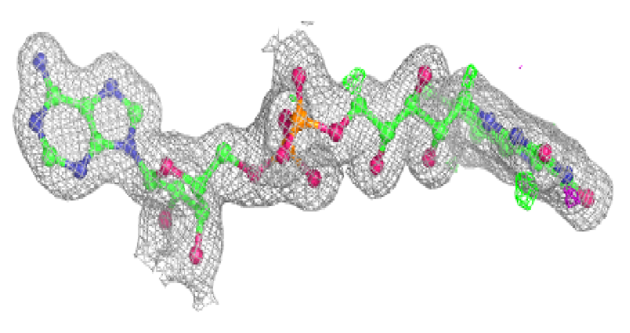


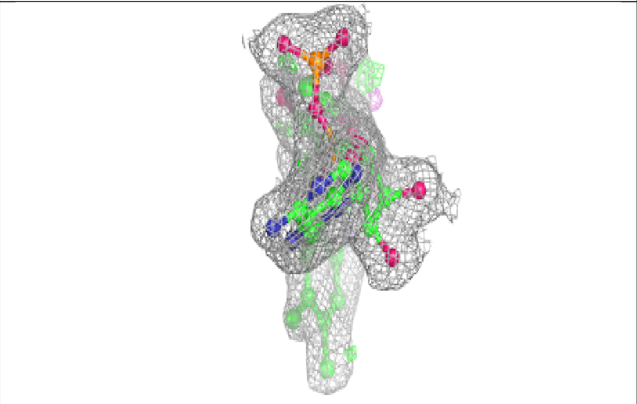


Electron density around FAD C 1106:

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

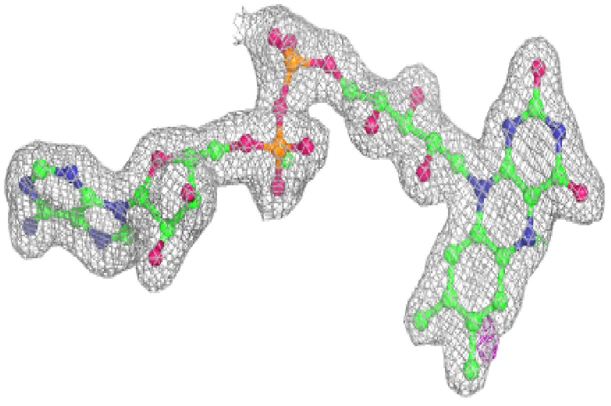


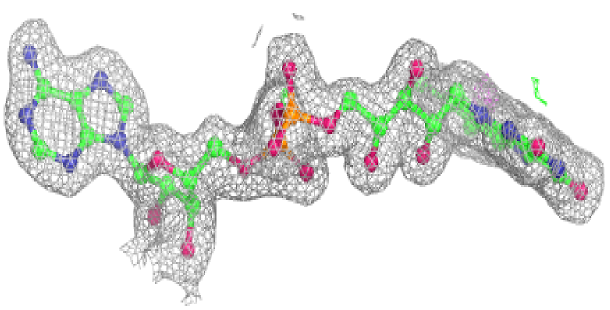


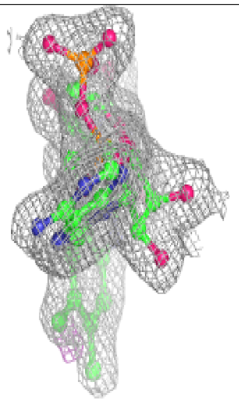


Electron density around FAD D 1107:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

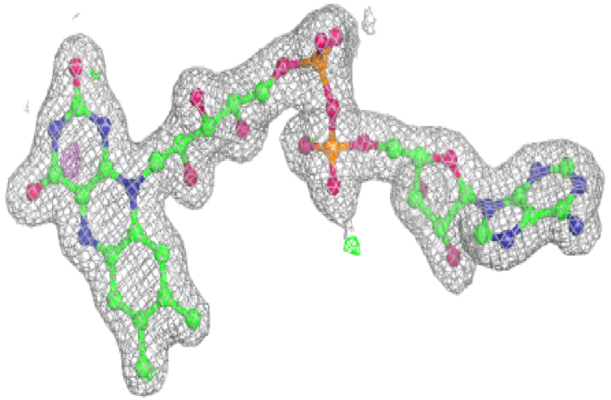


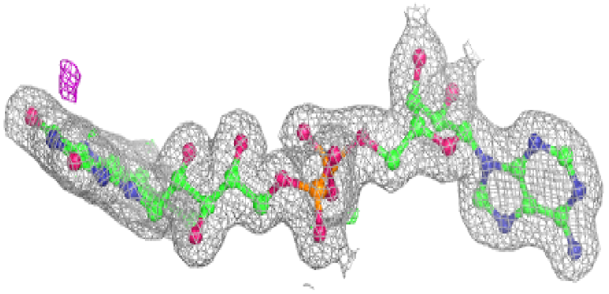


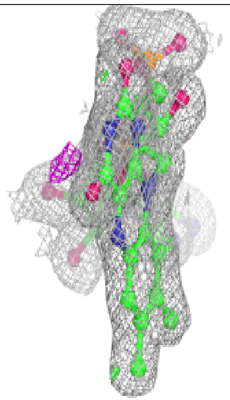


Electron density around FAD A 1105:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

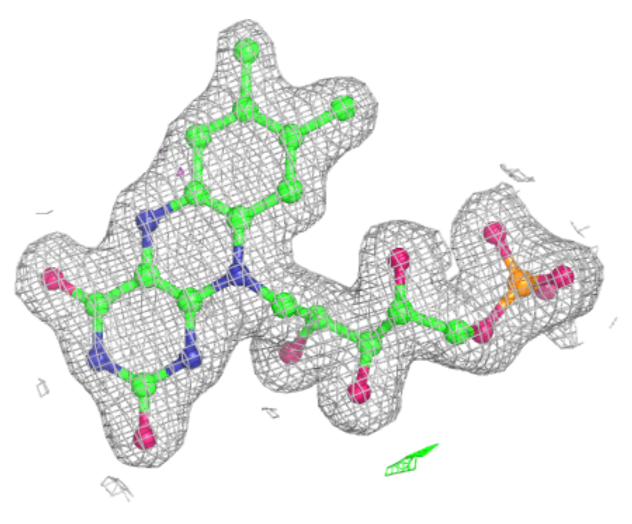


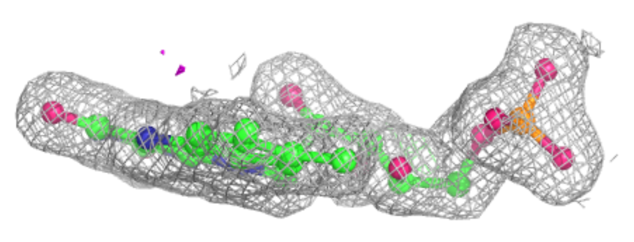


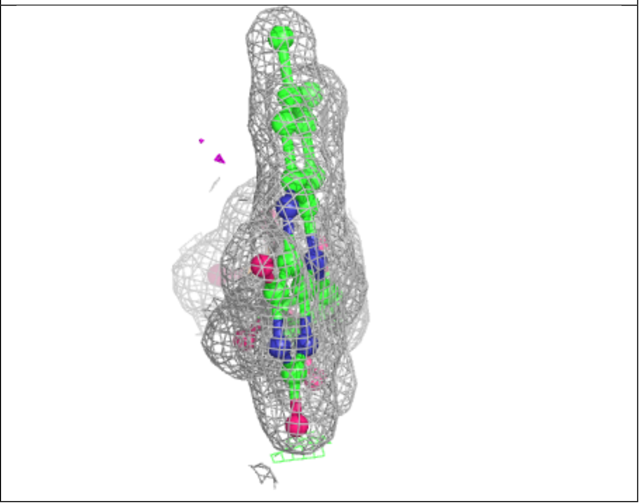


Electron density around FNR C 1108:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

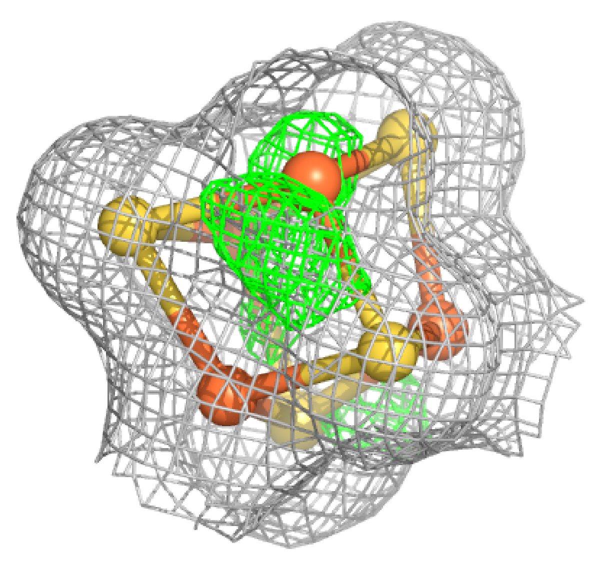


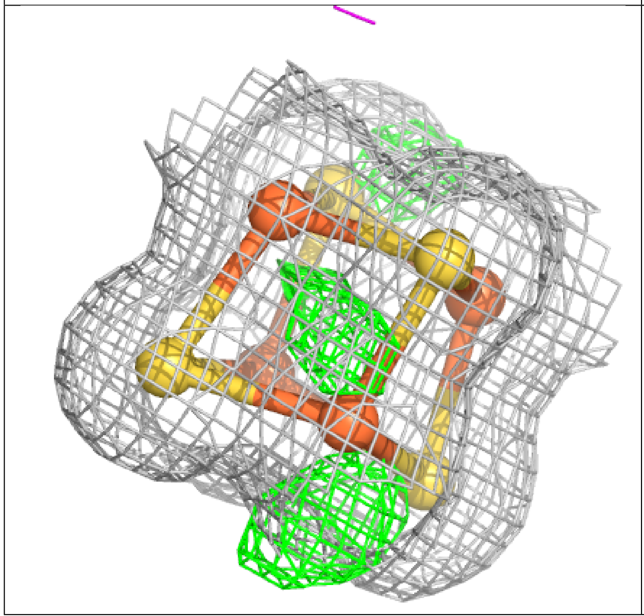


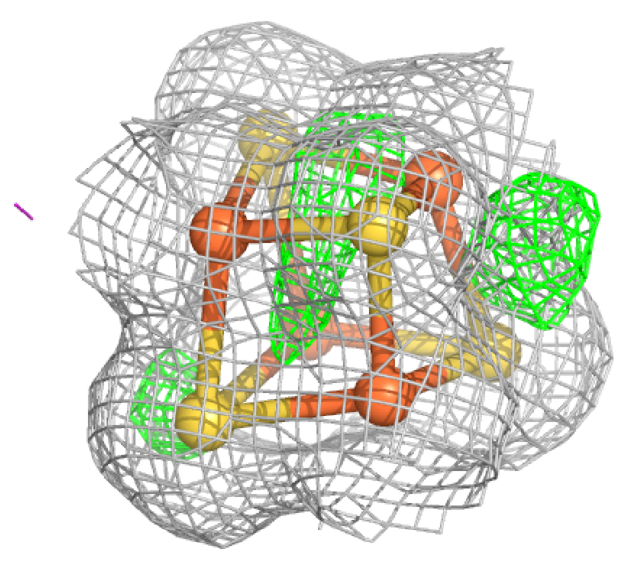


Electron density around SF4 D 1104:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

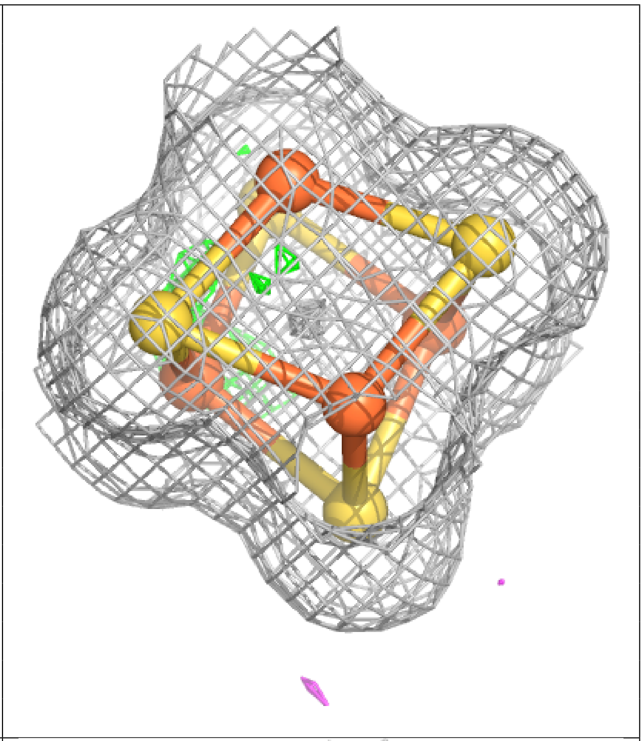


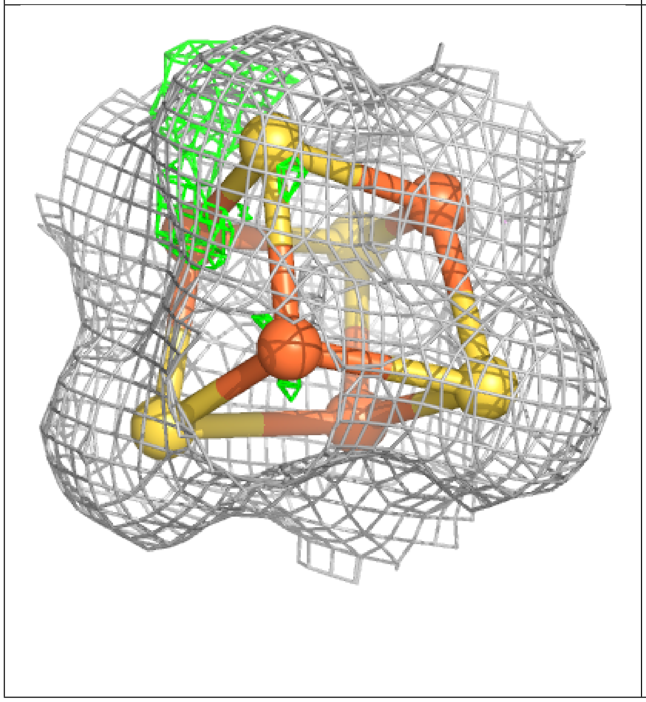


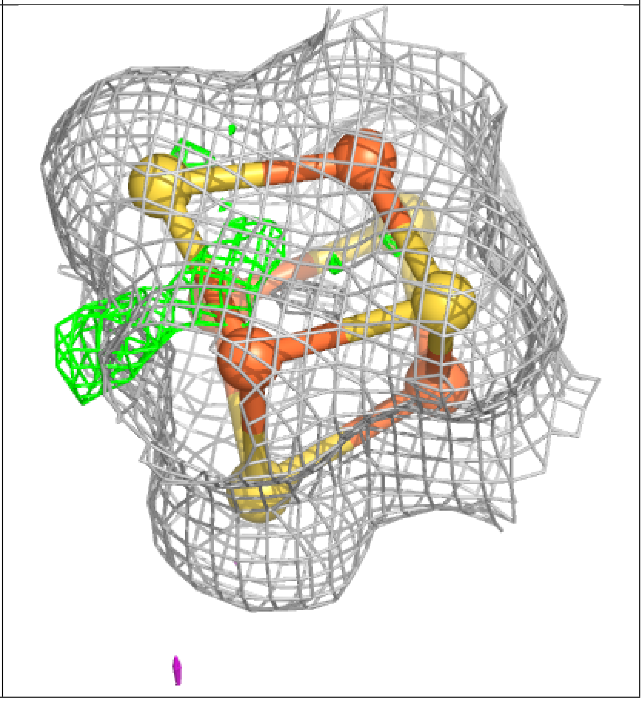


Electron density around SF4 D 1105:

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

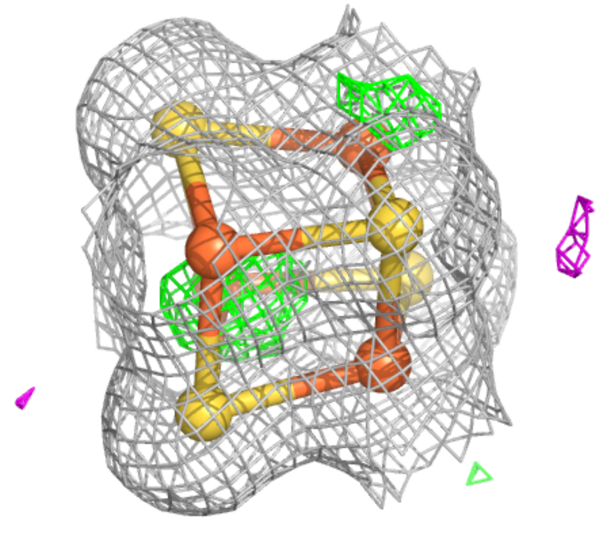


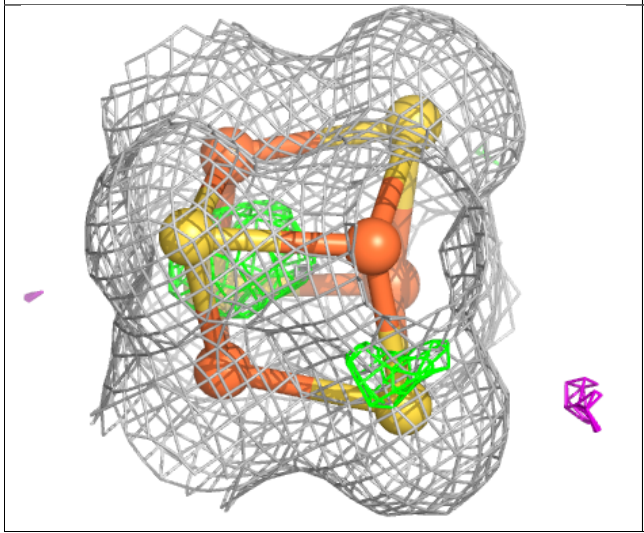


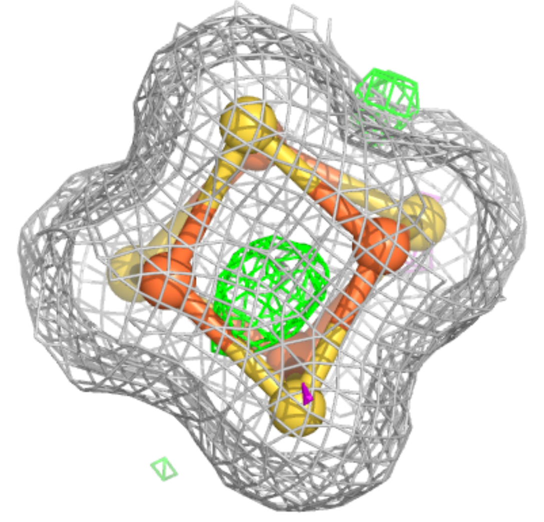


Electron density around SF4 D 1106:

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

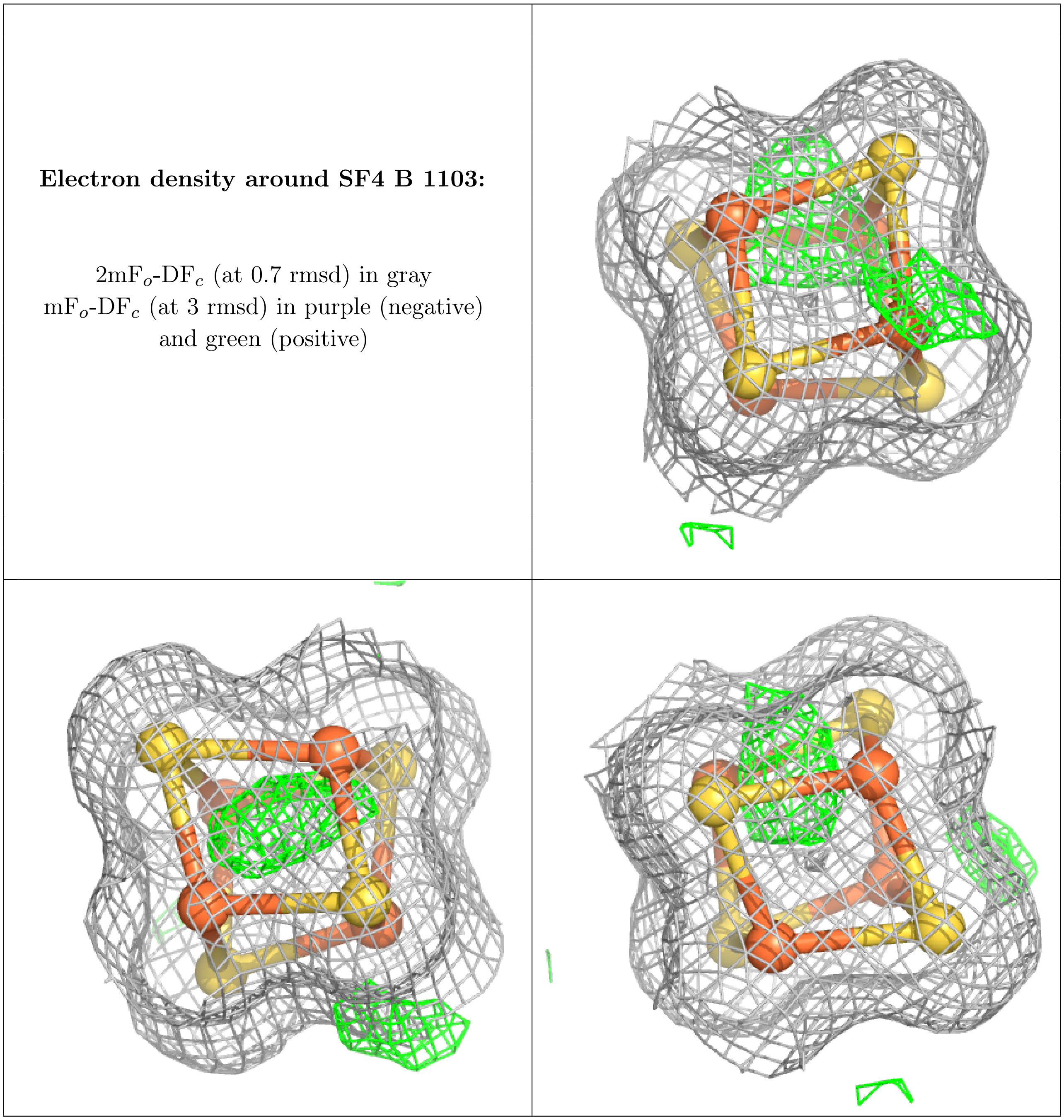


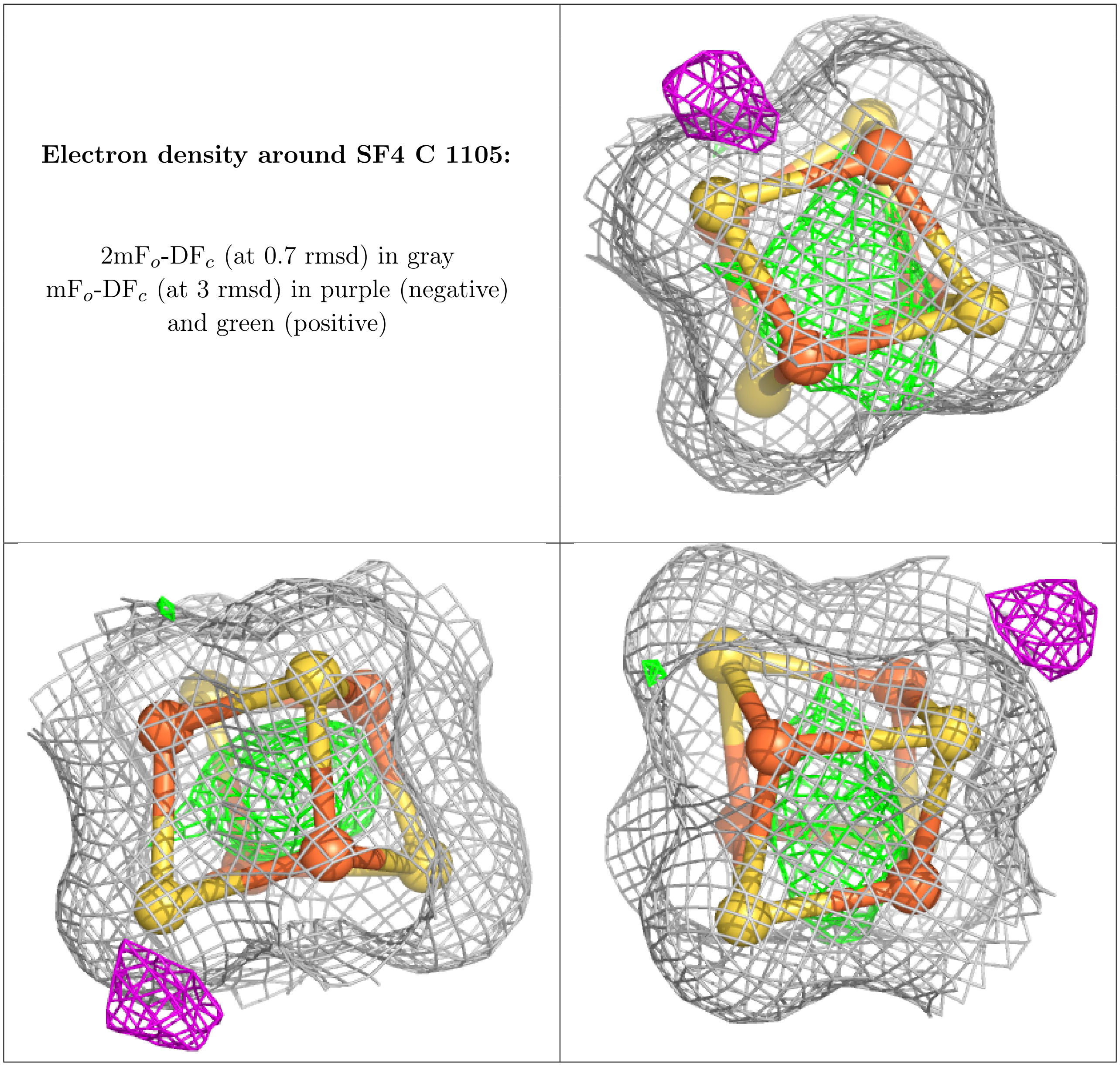




Electron density around SF4 B 1103:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



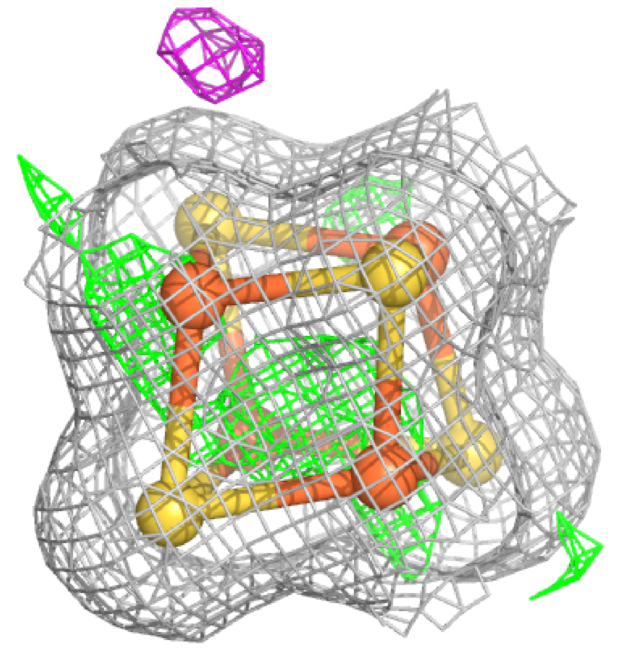


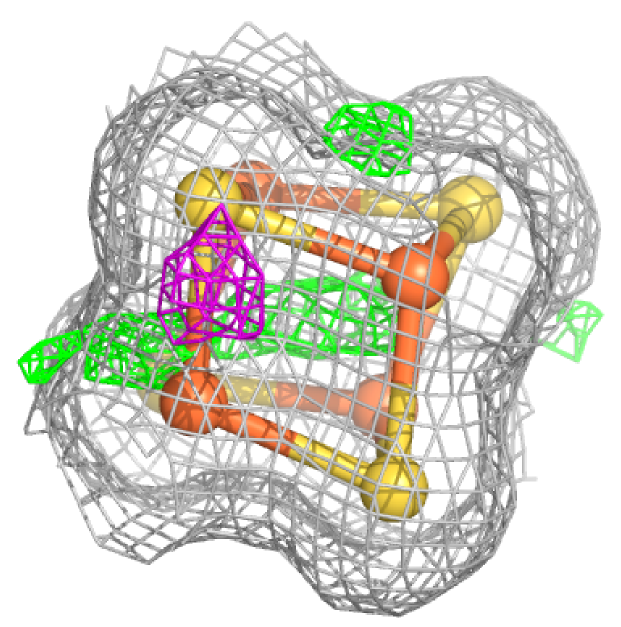
Electron density around SF4 C 1105:

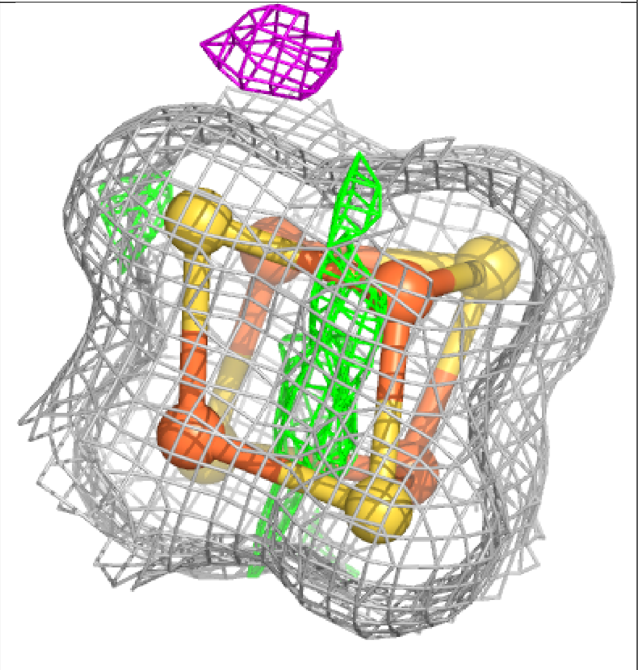
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

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)

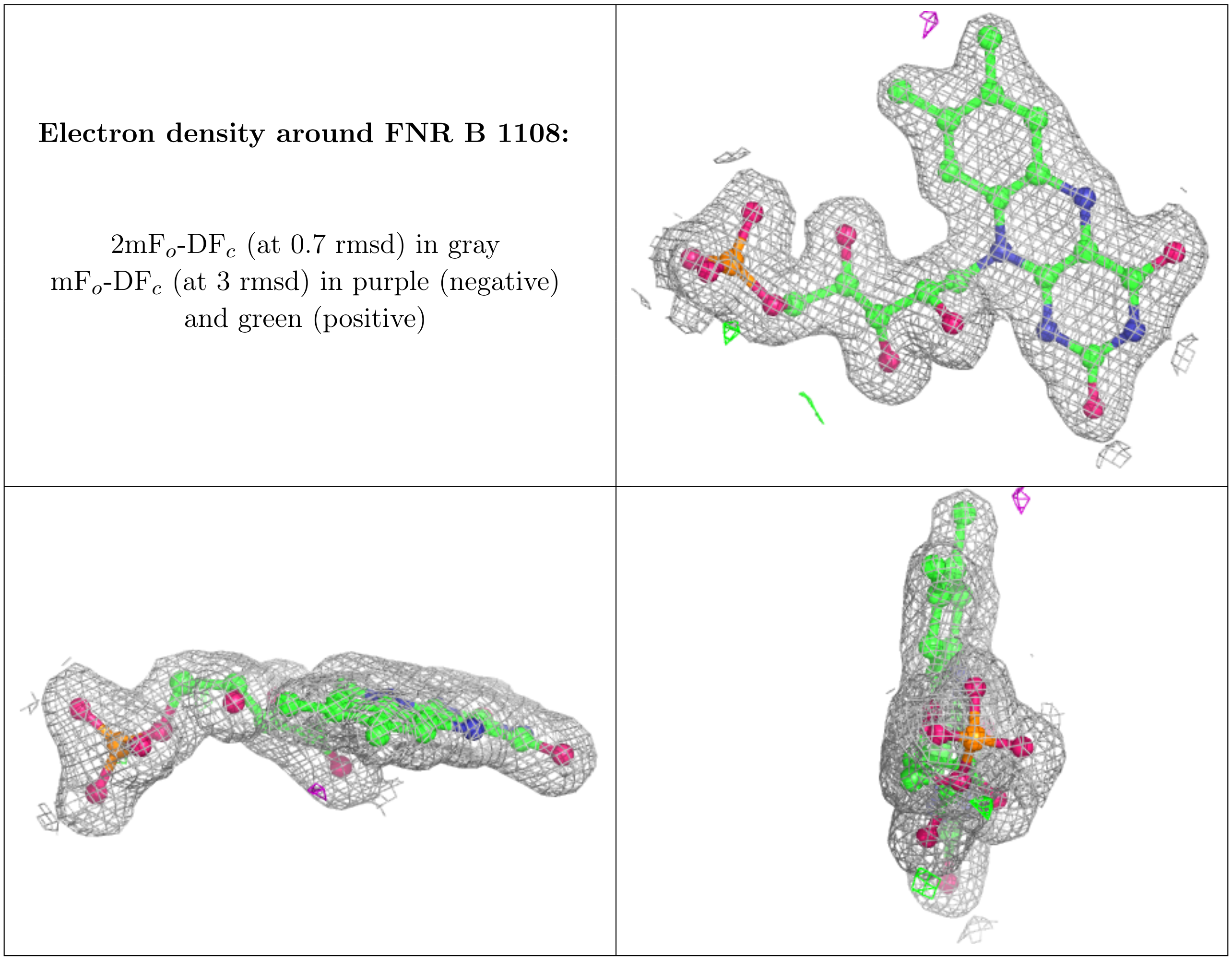






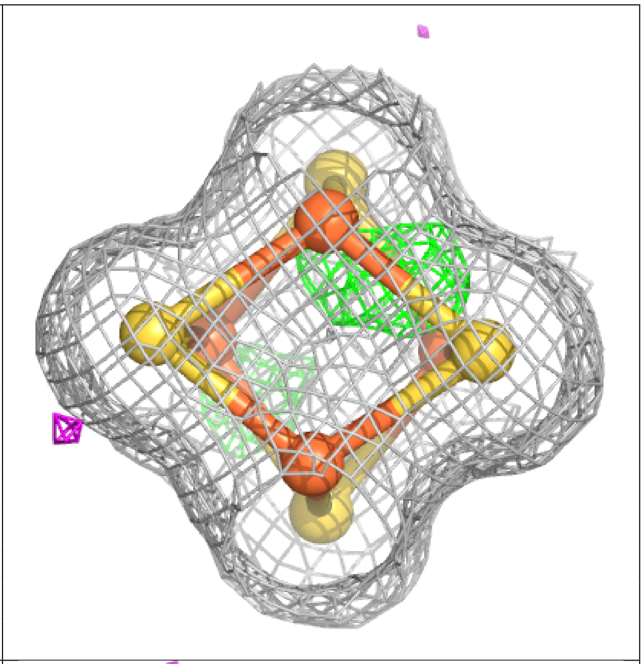
Electron density around FNR B 1108:

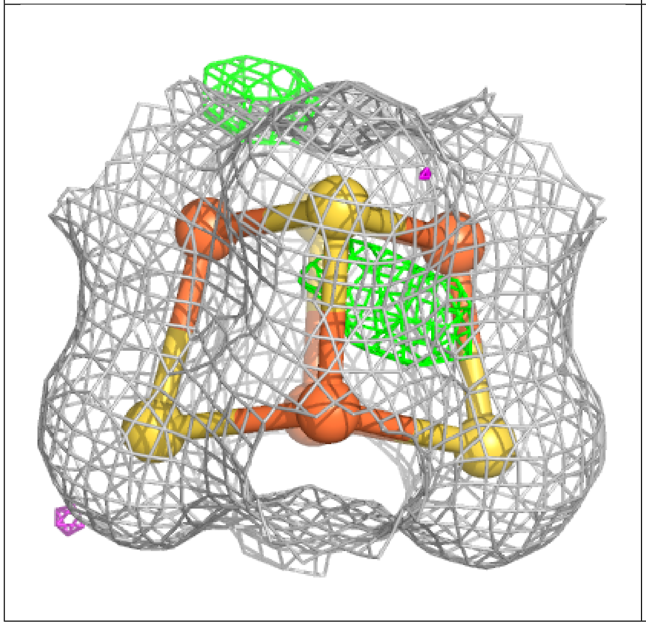
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

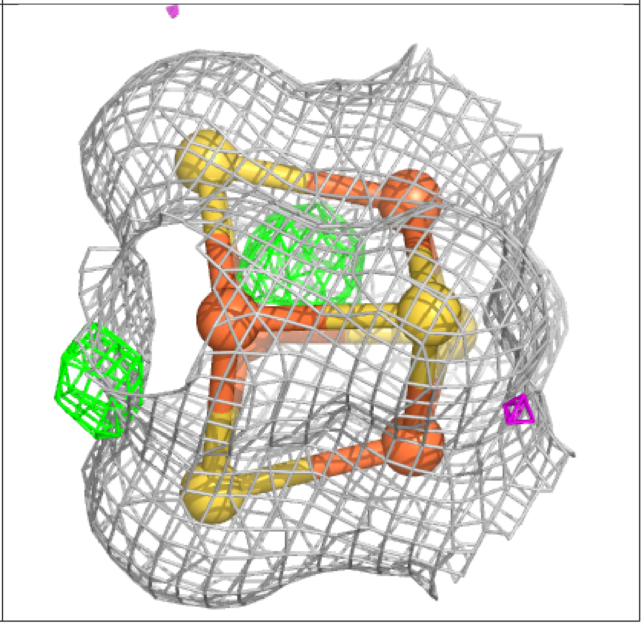


Electron density around SF4 A 1104:

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

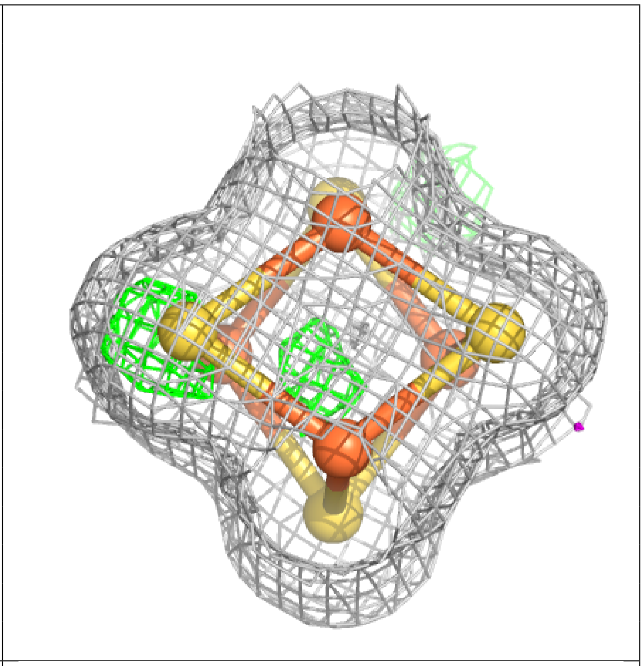


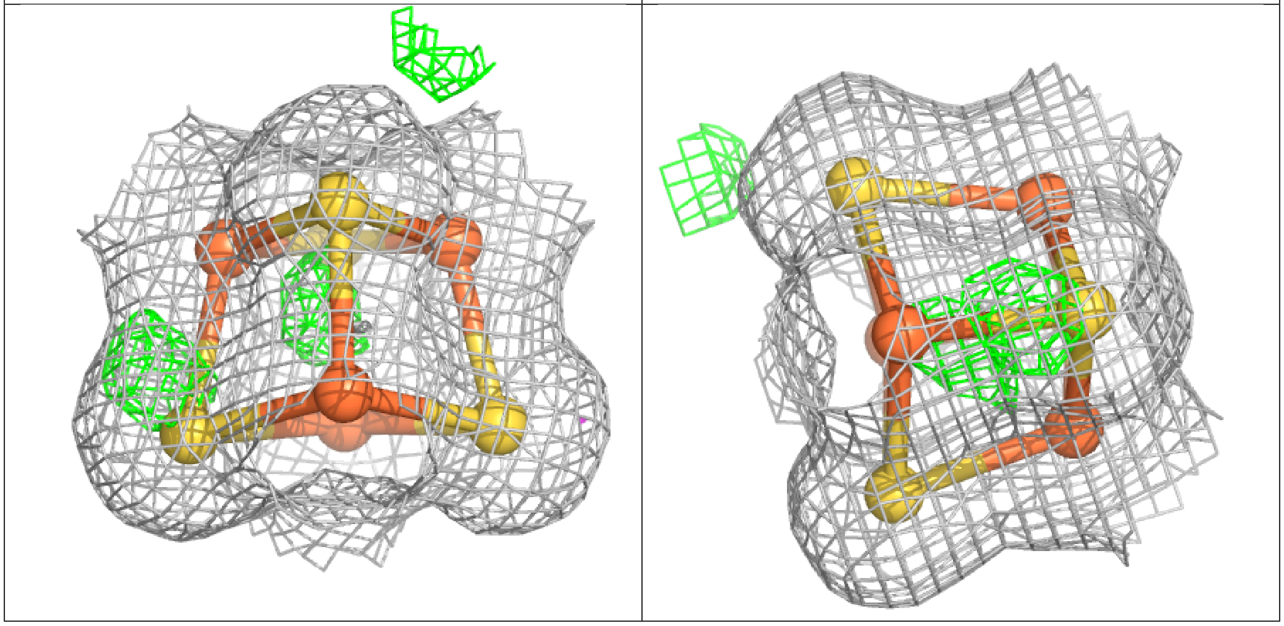




Electron density around SF4 B 1102:

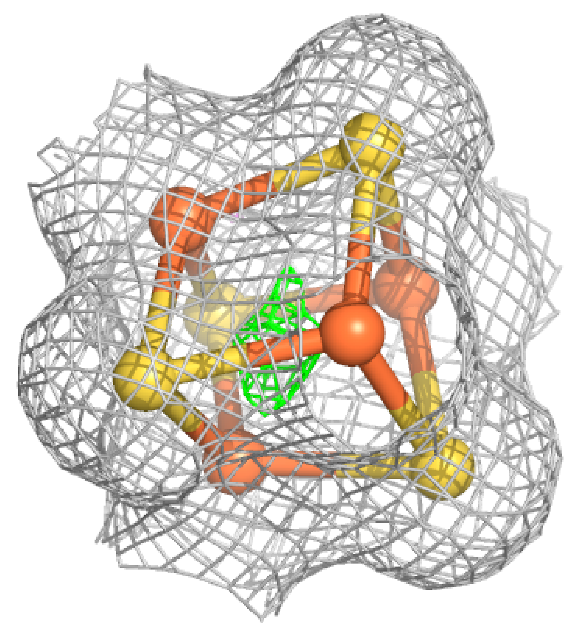
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

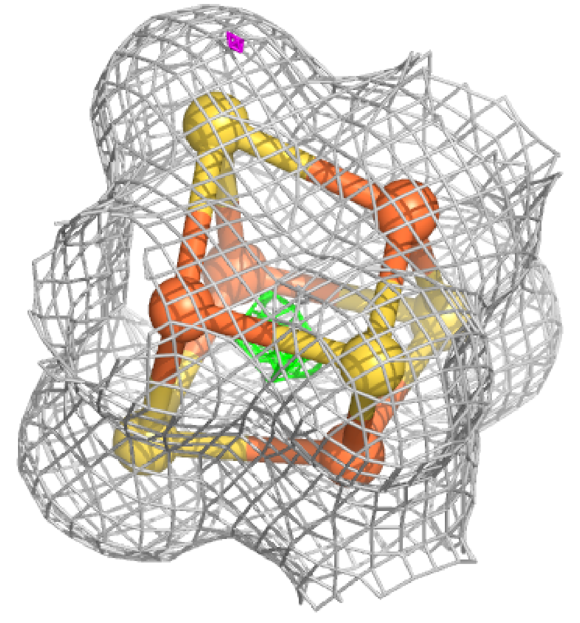


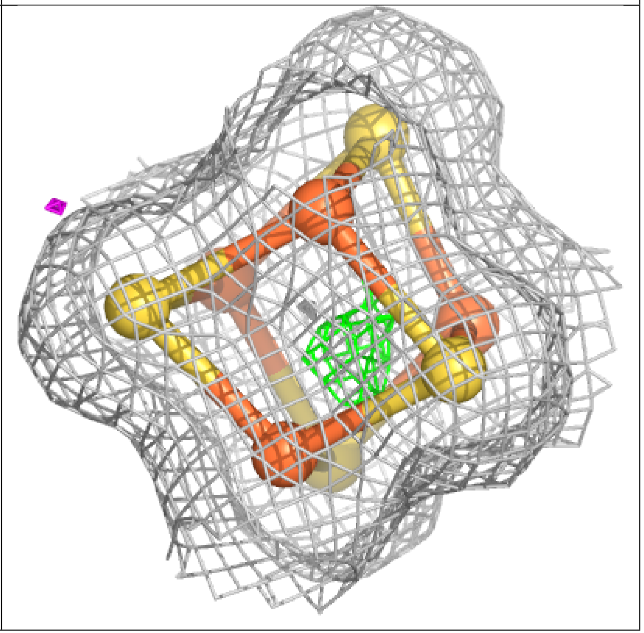


Electron density around SF4 A 1101:

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

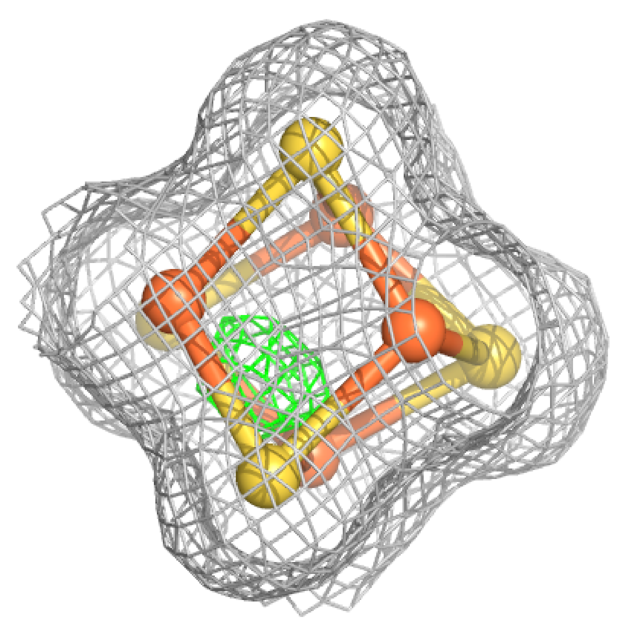


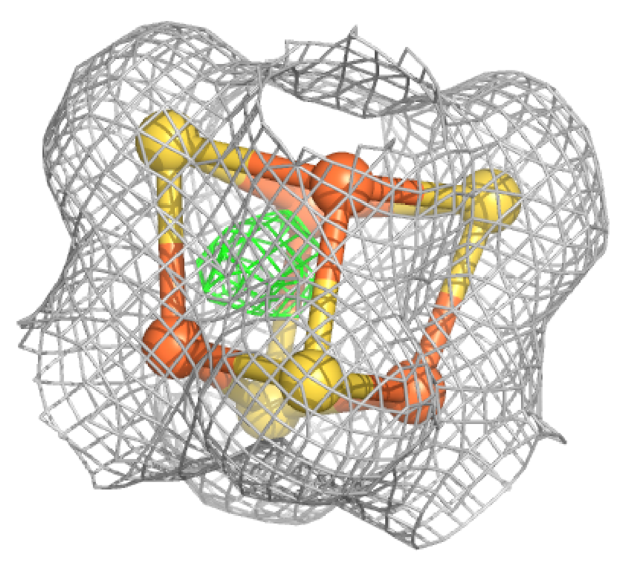


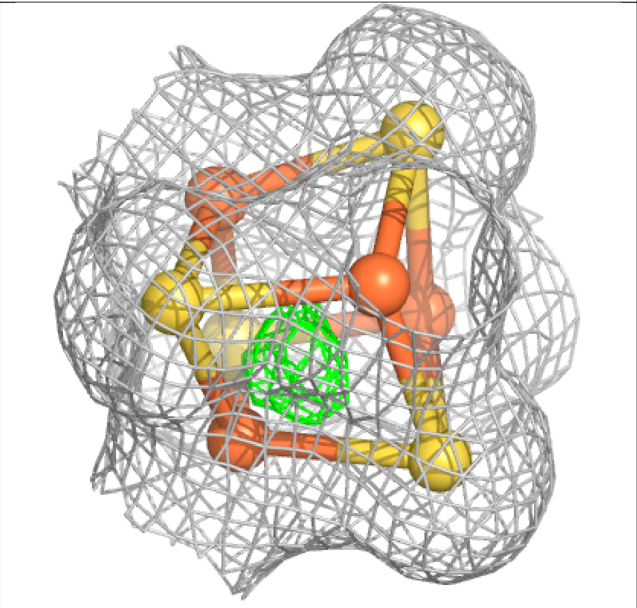


Electron density around SF4 B 1104:

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

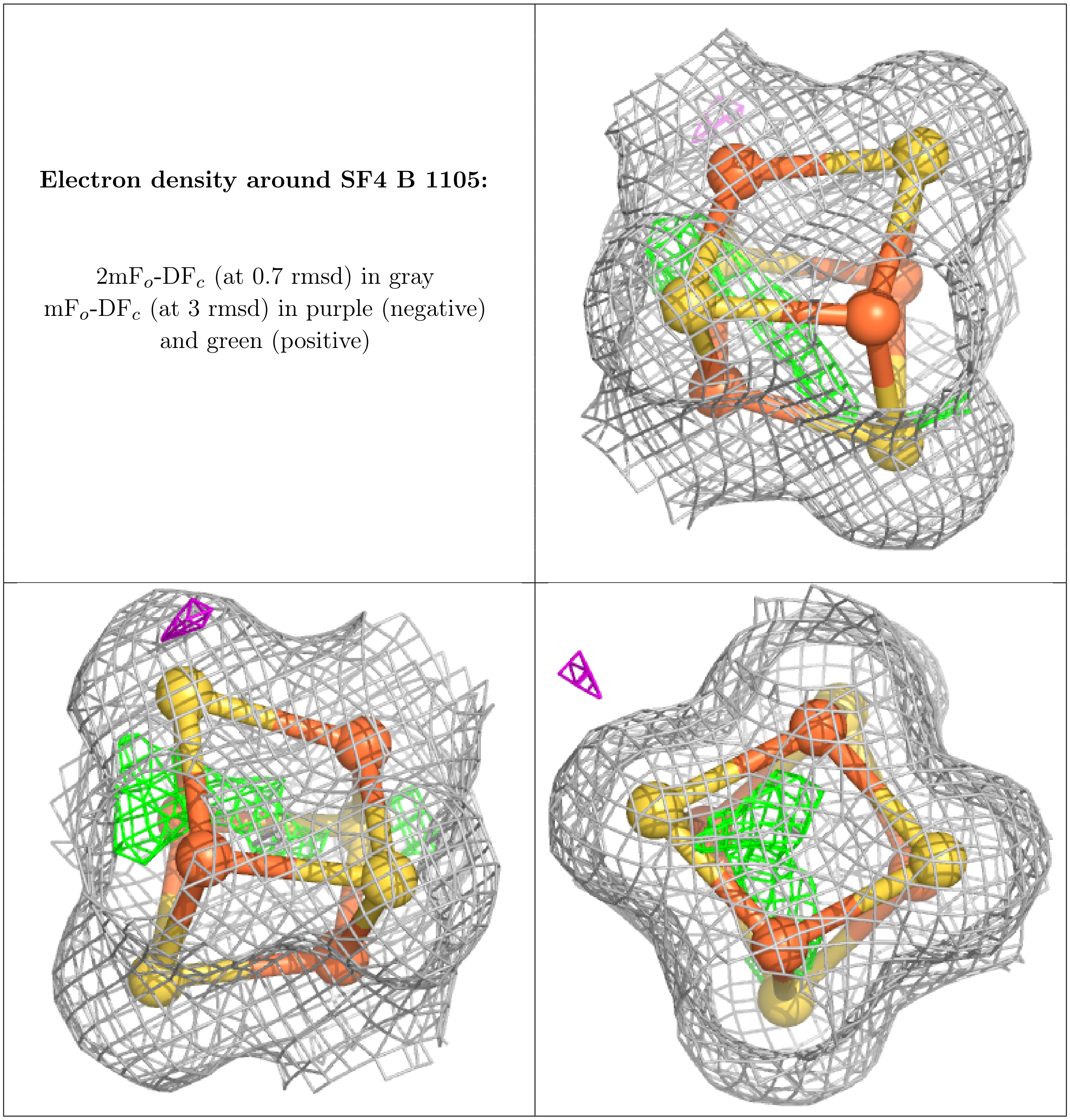






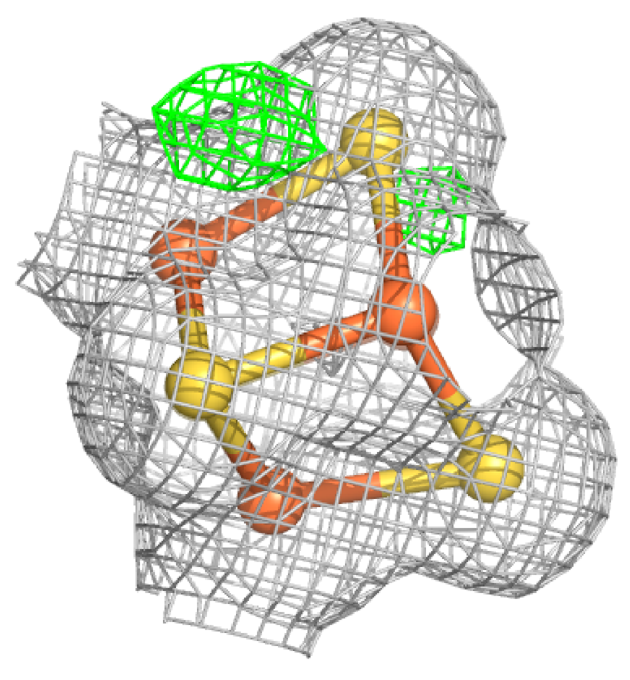
Electron density around SF4 B 1105:

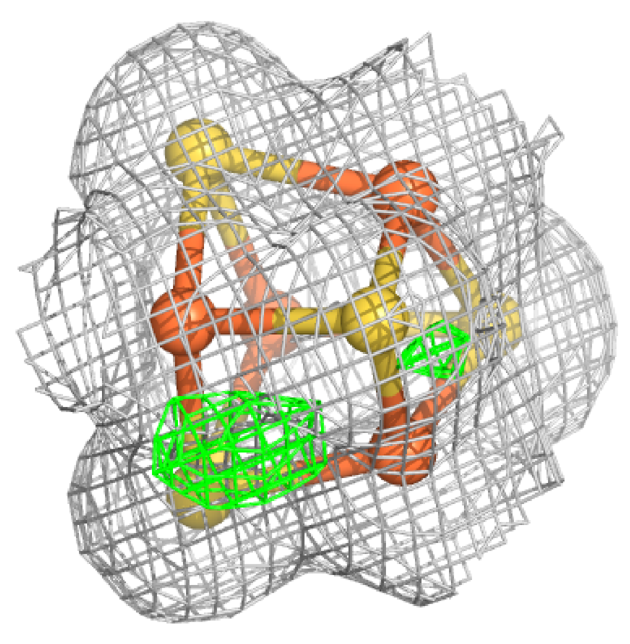
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

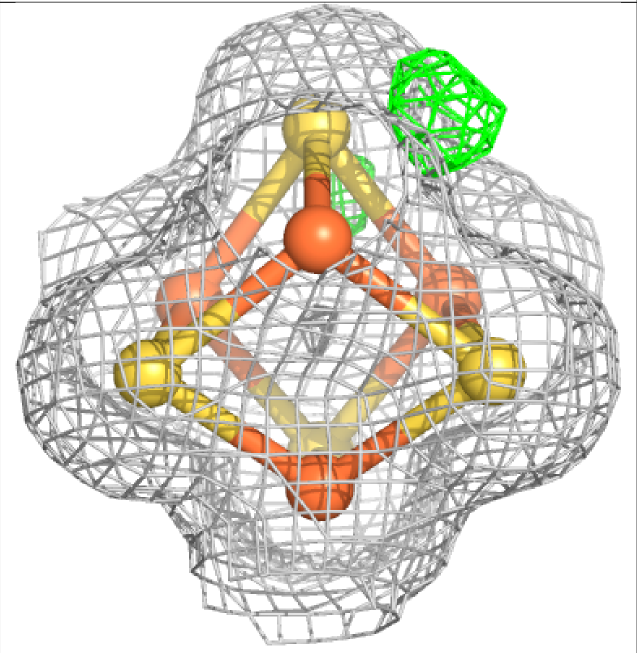


Electron density around SF4 C 1102:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

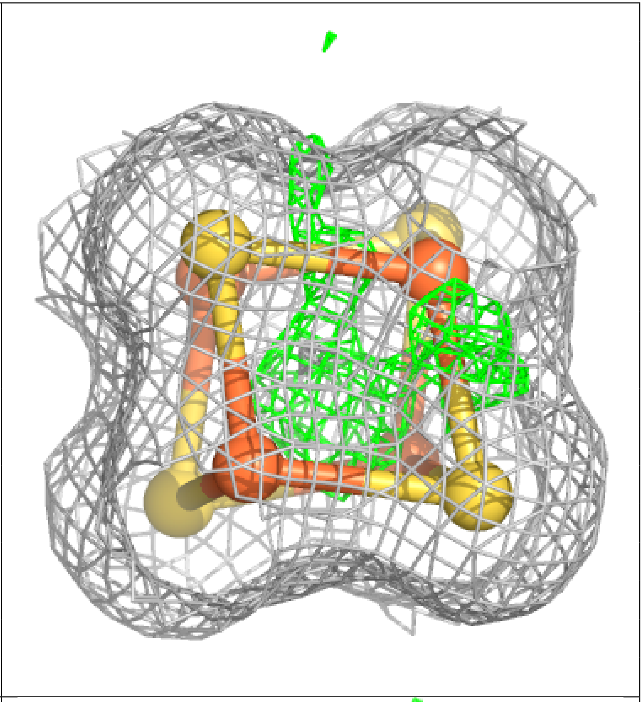


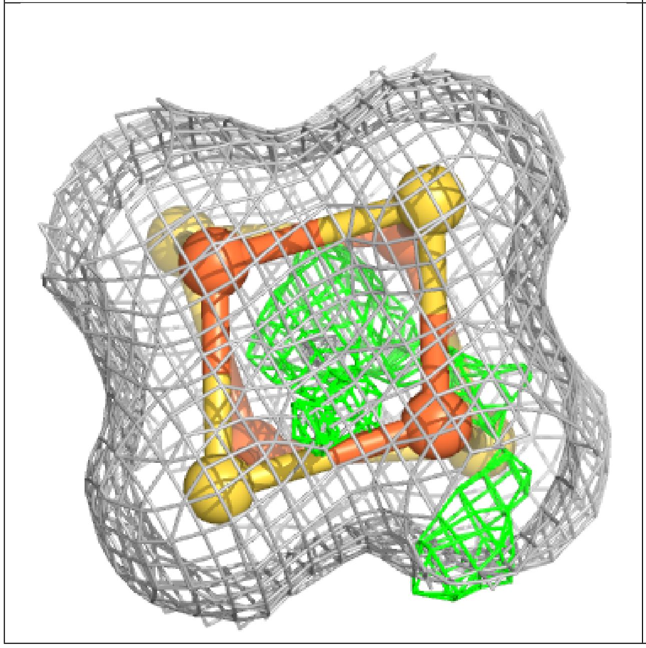


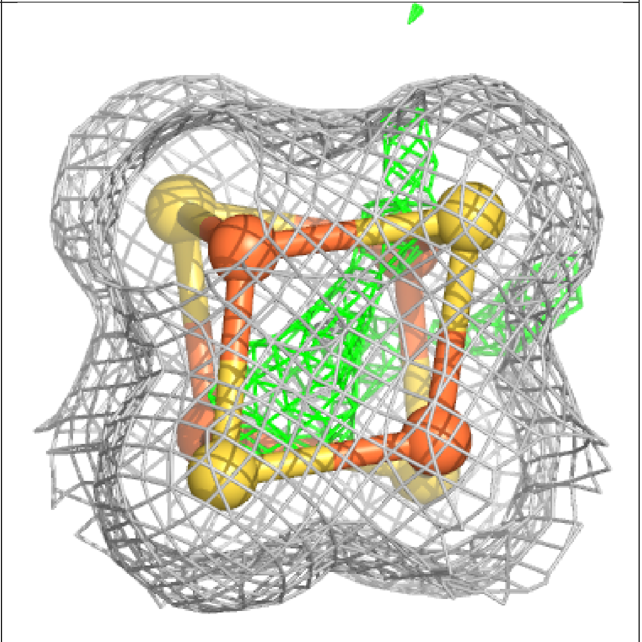


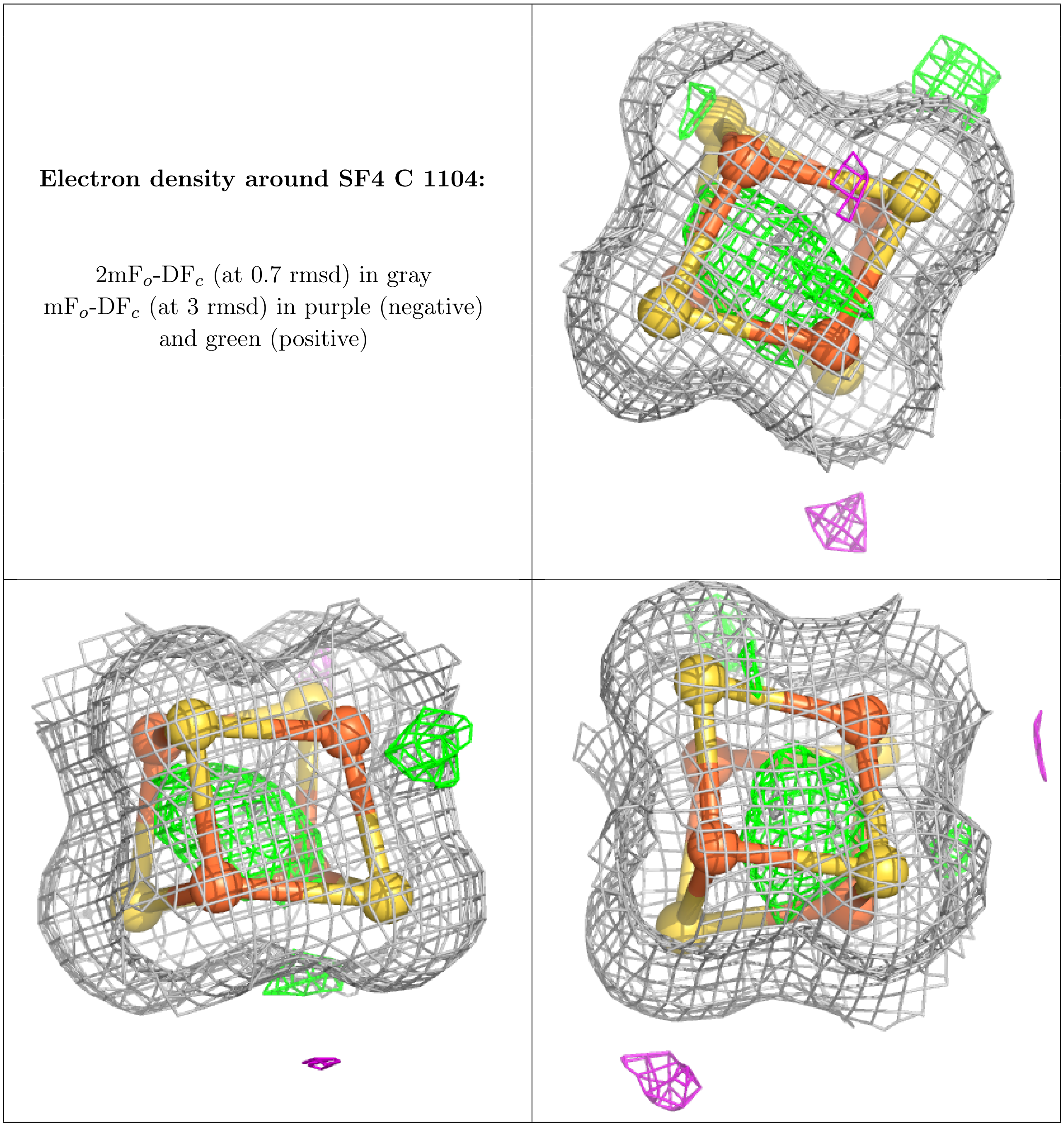
Electron density around SF4 C 1103:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







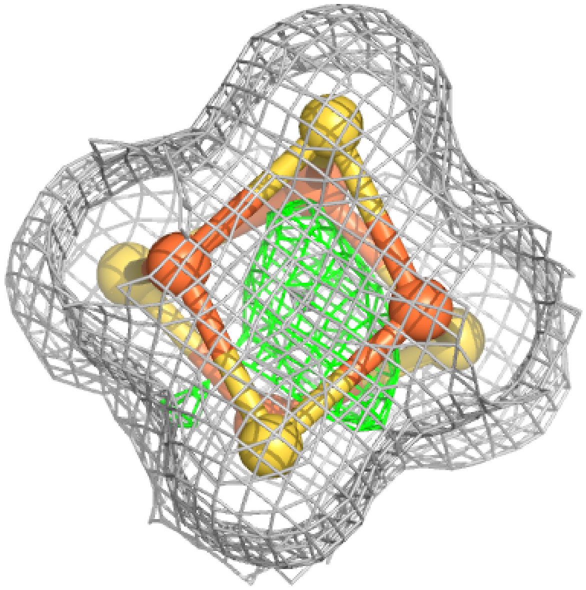


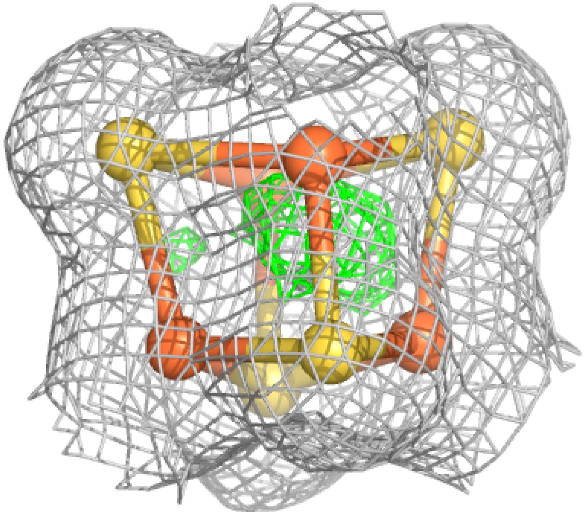
Electron density around SF4 C 1104:

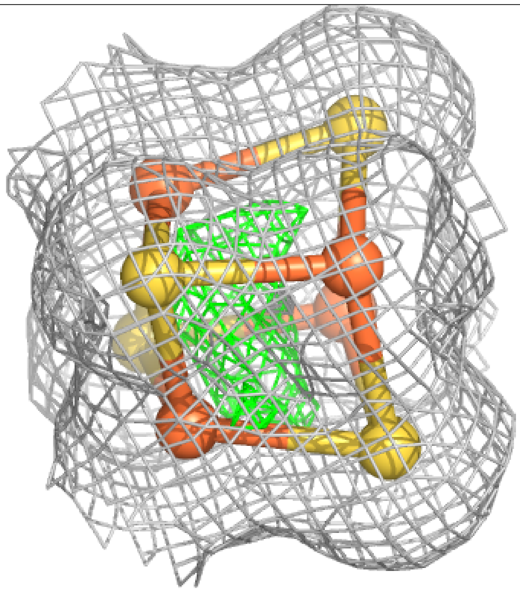
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

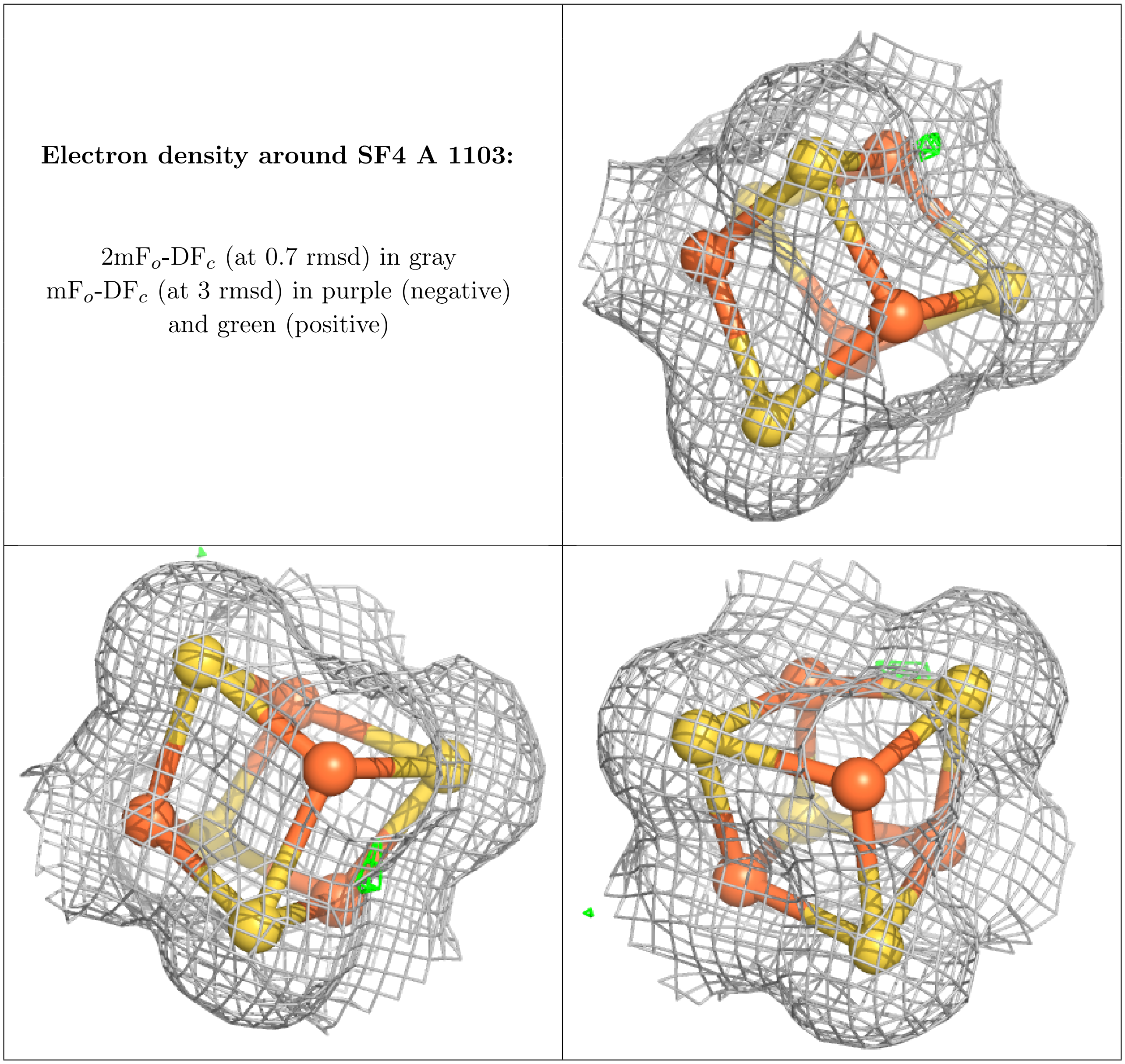
Electron density around SF4 A 1102:

$2mF_o$-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.