



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:32 PM UTC

PDB ID : 8F6N / pdb_00008f6n
Title : Dihydropyrimidine Dehydrogenase (DPD) C671S Mutant Soaked with
Thymine Quasi-Anaerobically
Authors : Kaley, N.; Smith, M.; Forouzesh, D.; Liu, D.; Moran, G.
Deposited on : 2022-11-16
Resolution : 2.12 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

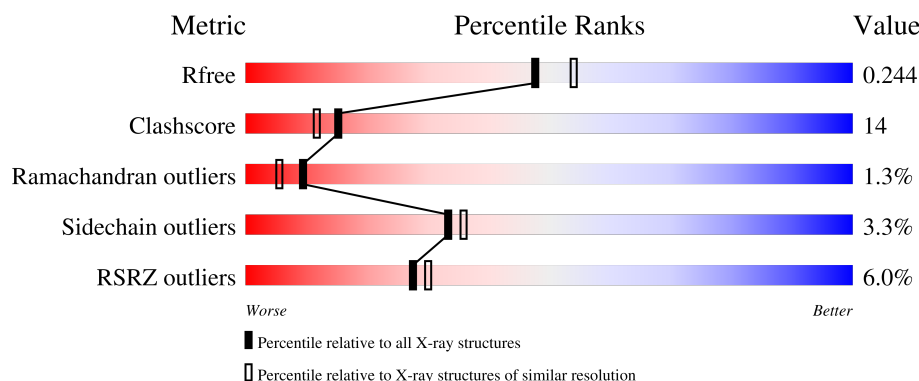
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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% 65% 29% • •
1	B	1025	6% 66% 27% • •
1	C	1025	5% 66% 28% • •
1	D	1025	7% 65% 29% • • •

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF4	A	1103	-	-	X	-
2	SF4	C	1102	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31607 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	996	Total	C	N	O	S	0	4	0
			7608	4829	1283	1443	53			
1	B	1001	Total	C	N	O	S	0	5	0
			7662	4860	1298	1450	54			
1	C	1002	Total	C	N	O	S	0	4	0
			7654	4856	1292	1453	53			
1	D	992	Total	C	N	O	S	0	5	0
			7590	4816	1282	1441	51			

There are 36 discrepancies between the modelled and reference sequences:

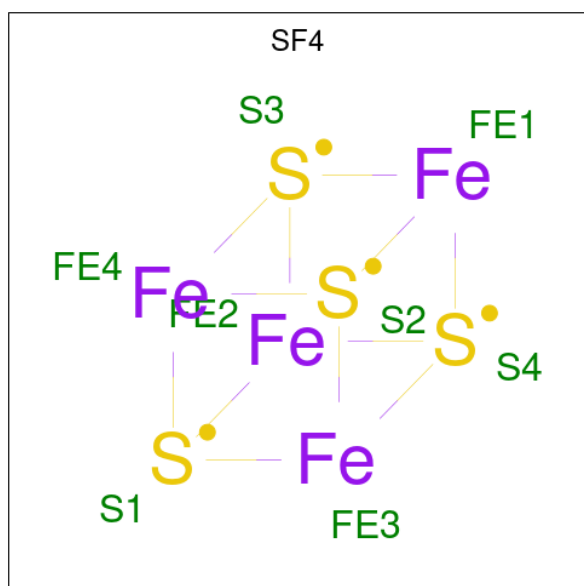
Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLY	conflict	UNP Q28943
A	671	SER	CYS	engineered mutation	UNP Q28943
A	1019	LEU	-	expression tag	UNP Q28943
A	1020	ALA	-	expression tag	UNP Q28943
A	1021	VAL	-	expression tag	UNP Q28943
A	1022	ASN	-	expression tag	UNP Q28943
A	1023	PRO	-	expression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

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

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



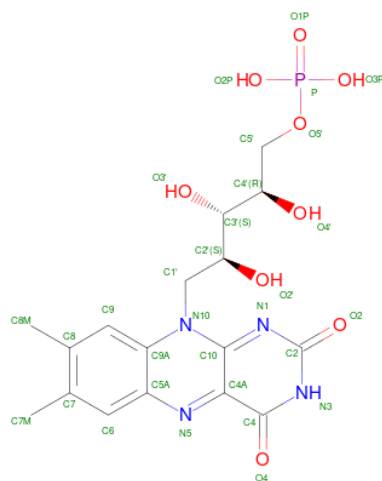
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0
2	A	1	Total Fe S 8 4 4	0	0

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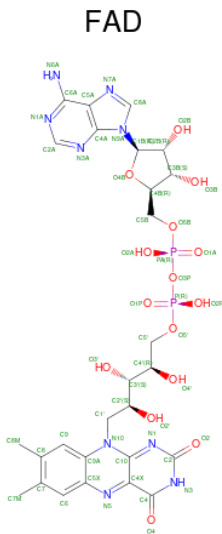
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2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

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



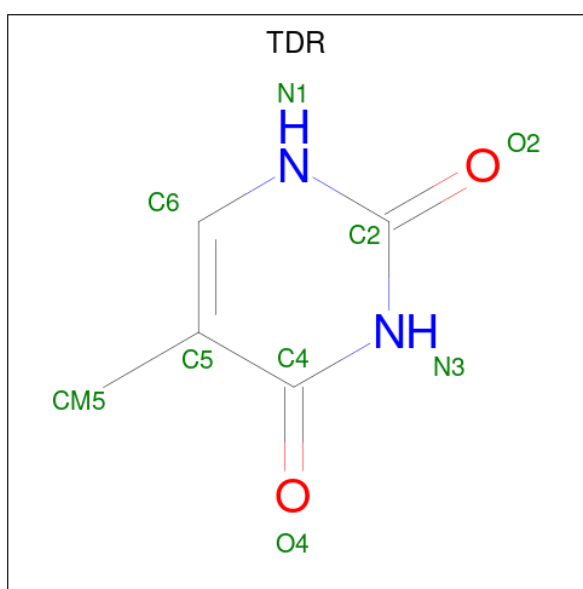
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	B	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	C	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	D	1	Total 31	C 17	N 4	O 9	P 1	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is THYMINE (CCD ID: TDR) (formula: $C_5H_6N_2O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is water.

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

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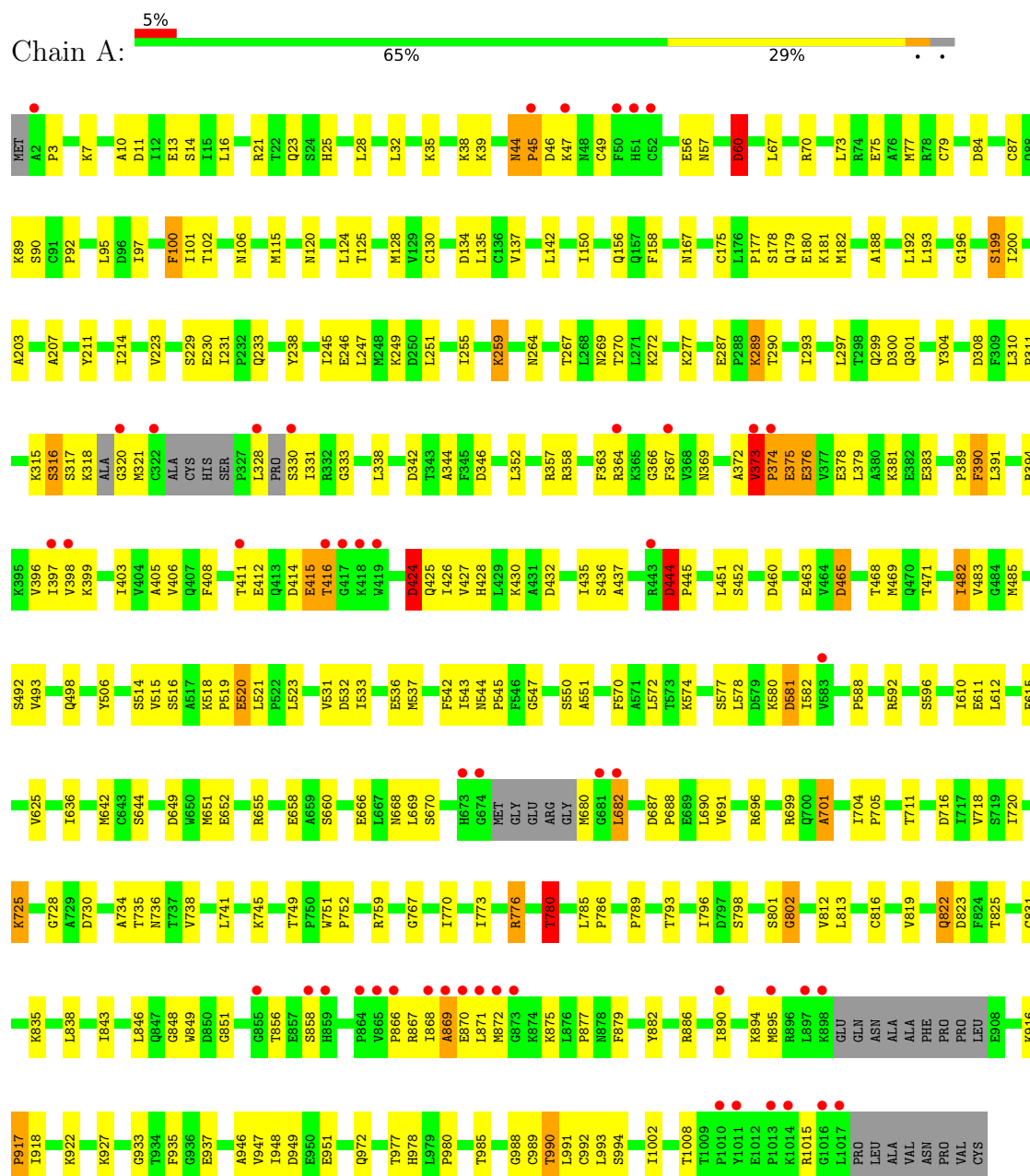
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	141	Total 141	O 141	0	0
6	C	159	Total 159	O 159	0	0
6	D	144	Total 144	O 144	0	0

3 Residue-property plots

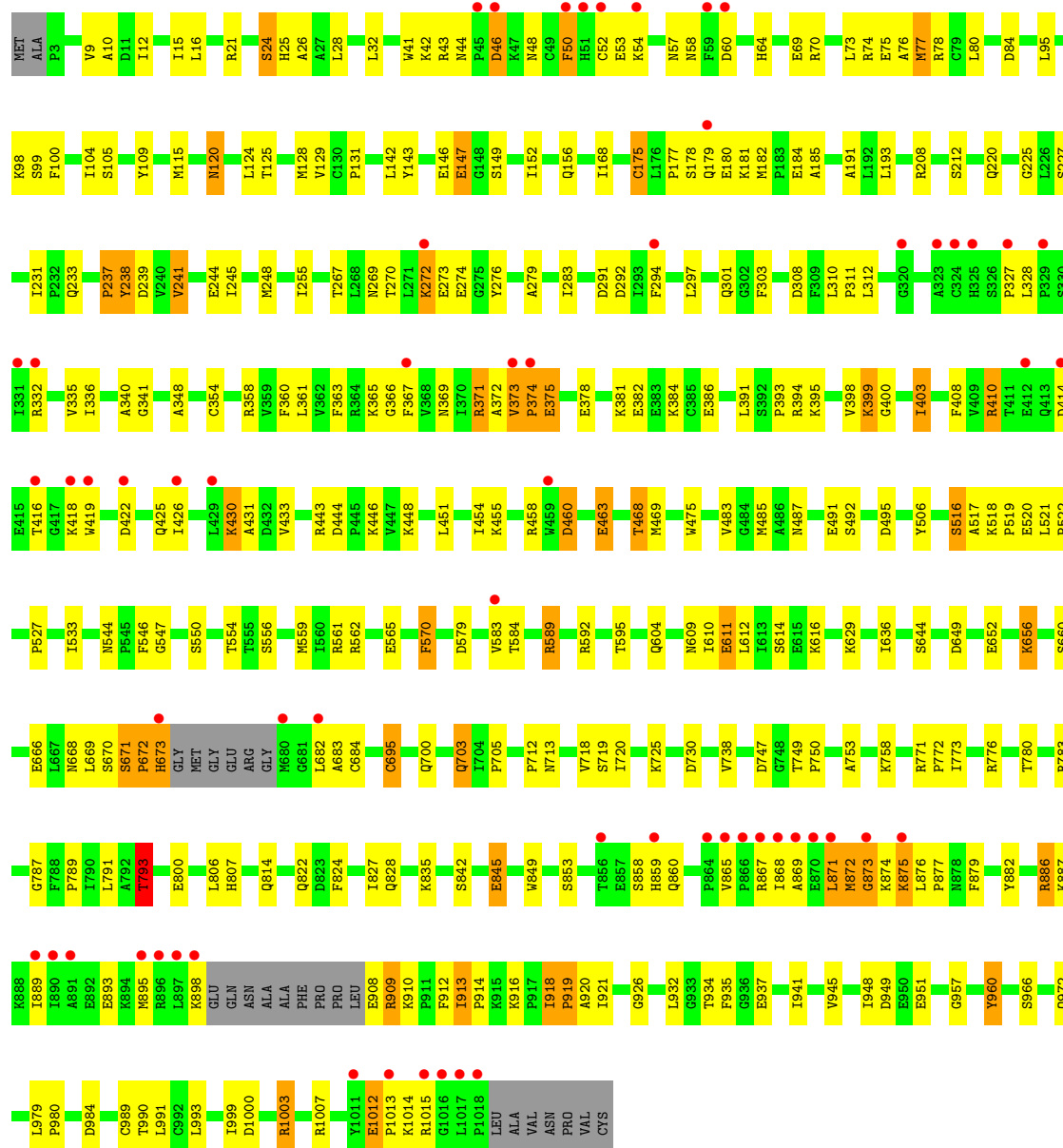
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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(+)]



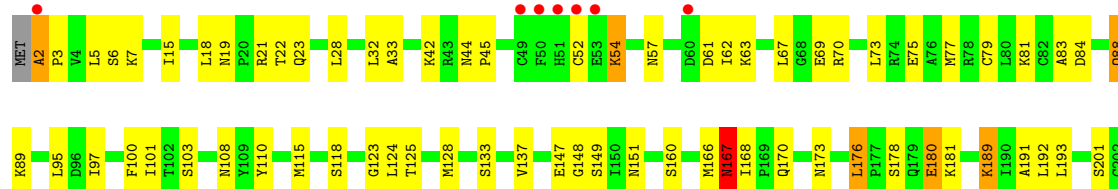
• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]

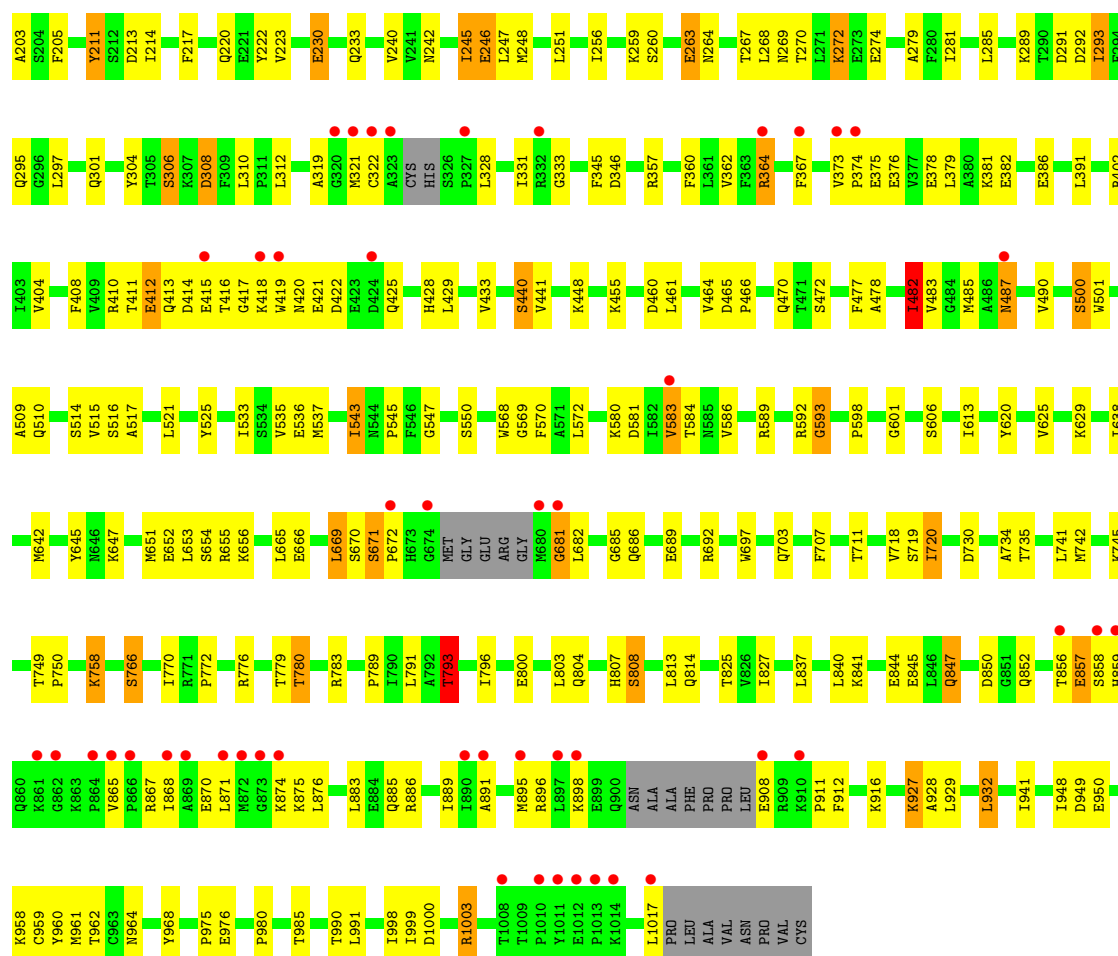
Chain B:  6% 66% 27%



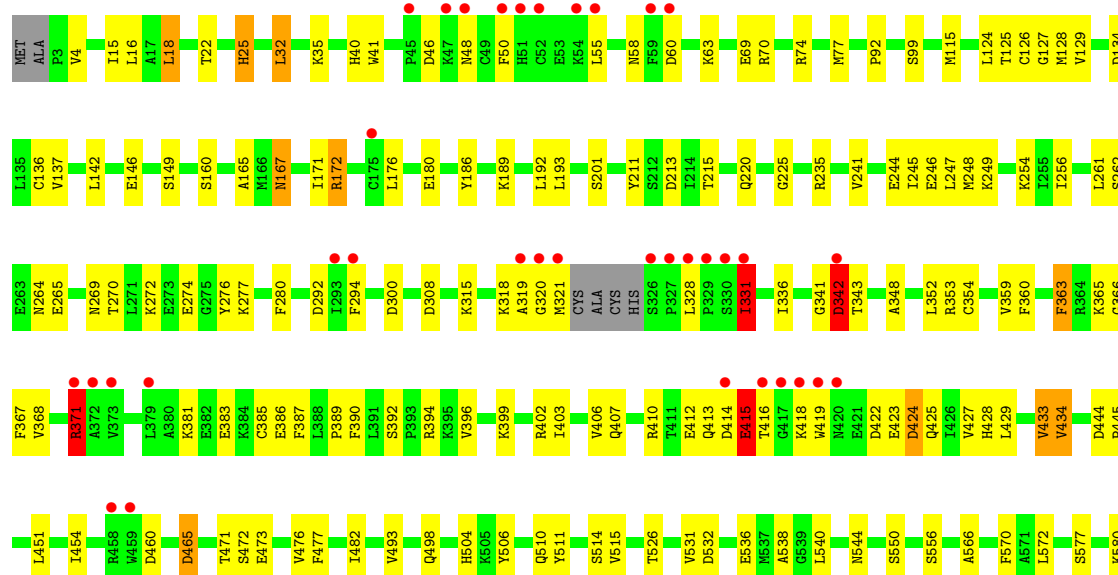
• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]

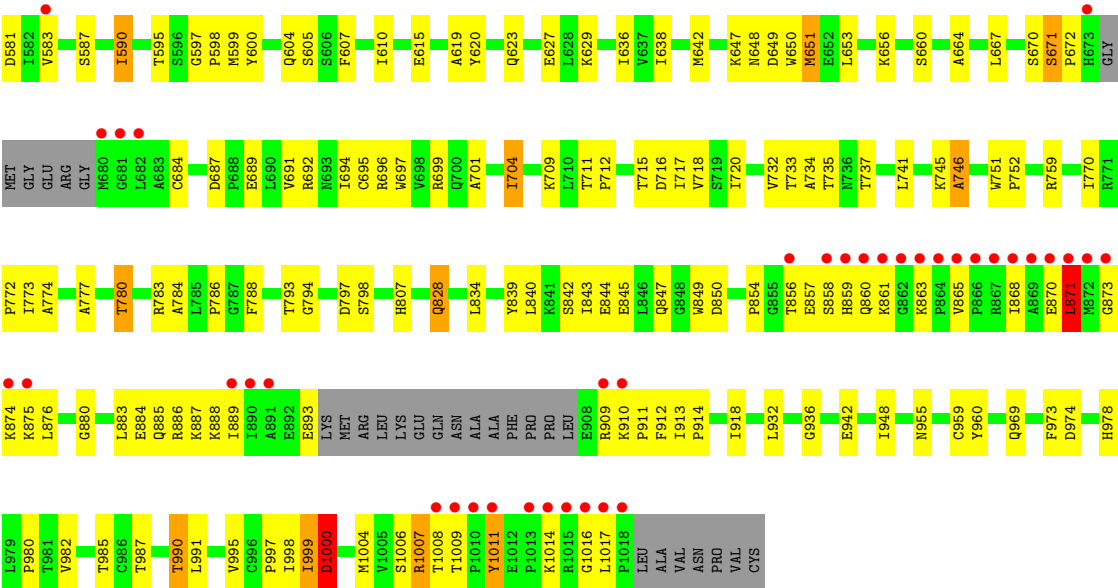
Chain C:  5% 66% 28%





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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.44Å 158.14Å 165.71Å 90.00° 96.78° 90.00°	Depositor
Resolution (Å)	26.98 – 2.12 26.98 – 2.12	Depositor EDS
% Data completeness (in resolution range)	61.4 (26.98-2.12) 61.4 (26.98-2.12)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.182 , 0.244 0.182 , 0.244	Depositor DCC
R_{free} test set	7342 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31607	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: TDR, SF4, FMN, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.50	25/7773 (0.3%)	1.52	53/10525 (0.5%)
1	B	1.51	36/7839 (0.5%)	1.53	52/10620 (0.5%)
1	C	1.51	28/7823 (0.4%)	1.54	55/10598 (0.5%)
1	D	1.43	25/7765 (0.3%)	1.53	59/10522 (0.6%)
All	All	1.49	114/31200 (0.4%)	1.53	219/42265 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	12
1	C	0	4
1	D	0	7
All	All	0	31

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	671	SER	C-N	-31.50	0.96	1.33
1	B	671	SER	C-N	-9.55	1.11	1.33
1	A	652	GLU	CG-CD	8.38	1.73	1.52
1	D	828	GLN	CG-CD	7.96	1.72	1.52
1	B	175	CYS	CB-SG	7.67	2.06	1.81

The worst 5 of 219 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	670	SER	O-C-N	-23.24	93.76	122.35
1	D	167[A]	ASN	CA-C-N	11.34	132.72	122.85
1	D	167[A]	ASN	C-N-CA	11.34	132.72	122.85
1	D	167[B]	ASN	CA-C-N	11.34	132.72	122.85
1	D	167[B]	ASN	C-N-CA	11.34	132.72	122.85

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ARG	Sidechain
1	A	364	ARG	Sidechain
1	A	415	GLU	Peptide
1	A	44	ASN	Peptide
1	A	70	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7608	0	7645	227	0
1	B	7662	0	7694	233	0
1	C	7654	0	7686	231	0
1	D	7590	0	7612	203	0
2	A	32	0	0	3	0
2	B	32	0	0	2	0
2	C	32	0	0	3	0
2	D	32	0	0	1	0
3	A	31	0	19	1	0
3	B	31	0	19	1	0
3	C	31	0	19	1	0
3	D	31	0	19	1	0
4	A	53	0	31	1	0
4	B	53	0	31	2	0
4	C	53	0	31	1	0
4	D	53	0	31	2	0
5	A	9	0	6	1	0
5	B	9	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	9	0	6	0	0
5	D	9	0	6	0	0
6	A	149	0	0	24	0
6	B	141	0	0	23	0
6	C	159	0	0	18	0
6	D	144	0	0	10	0
All	All	31607	0	30861	841	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 841 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LYS:NZ	1:A:259:LYS:CE	1.70	1.53
1:B:695:CYS:CB	1:B:695:CYS:SG	2.04	1.46
1:B:175:CYS:SG	1:B:175:CYS:CB	2.06	1.42
1:B:414:ASP:HB3	1:B:416:THR:HG22	1.32	1.09
1:B:115:MET:SD	6:B:1334:HOH:O	2.08	1.08

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	988/1025 (96%)	895 (91%)	80 (8%)	13 (1%)	9 5
1	B	1000/1025 (98%)	904 (90%)	83 (8%)	13 (1%)	9 5
1	C	998/1025 (97%)	913 (92%)	70 (7%)	15 (2%)	8 4
1	D	989/1025 (96%)	892 (90%)	85 (9%)	12 (1%)	10 6
All	All	3975/4100 (97%)	3604 (91%)	318 (8%)	53 (1%)	9 5

5 of 53 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	834/854 (98%)	803 (96%)	31 (4%)	30	31
1	B	842/854 (99%)	822 (98%)	20 (2%)	43	48
1	C	839/854 (98%)	811 (97%)	28 (3%)	33	36
1	D	834/854 (98%)	800 (96%)	34 (4%)	27	27
All	All	3349/3416 (98%)	3236 (97%)	113 (3%)	33	35

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	181	LYS
1	D	1000	ASP
1	C	780	THR
1	D	999	ILE
1	D	526	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	804	GLN
1	D	264	ASN
1	C	859	HIS
1	D	88	GLN
1	D	498	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	SF4	C	1101	1	0,12,12	-	-	-		
3	FMN	C	1105	-	33,33,33	1.74	6 (18%)	48,50,50	2.32	16 (33%)
5	TDR	A	1107	-	9,9,9	1.06	1 (11%)	12,12,12	1.73	2 (16%)
2	SF4	B	1104	1	0,12,12	-	-	-		
2	SF4	A	1103	1	0,12,12	-	-	-		
2	SF4	C	1103	1	0,12,12	-	-	-		
4	FAD	B	1106	-	58,58,58	1.05	3 (5%)	85,89,89	1.18	6 (7%)
5	TDR	D	1107	-	9,9,9	2.64	5 (55%)	12,12,12	1.74	2 (16%)
2	SF4	D	1103	1	0,12,12	-	-	-		
2	SF4	A	1102	1	0,12,12	-	-	-		
2	SF4	A	1104	1	0,12,12	-	-	-		
2	SF4	C	1104	1	0,12,12	-	-	-		
2	SF4	B	1101	1	0,12,12	-	-	-		
4	FAD	D	1106	-	58,58,58	0.95	2 (3%)	85,89,89	0.84	4 (4%)
2	SF4	D	1104	1	0,12,12	-	-	-		
4	FAD	A	1106	-	58,58,58	0.86	3 (5%)	85,89,89	1.12	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SF4	B	1102	1	0,12,12	-	-	-		
2	SF4	A	1101	1	0,12,12	-	-	-		
3	FMN	A	1105	-	33,33,33	1.87	7 (21%)	48,50,50	2.41	20 (41%)
4	FAD	C	1106	-	58,58,58	1.29	2 (3%)	85,89,89	0.66	0
5	TDR	B	1107	-	9,9,9	1.54	2 (22%)	12,12,12	1.53	2 (16%)
2	SF4	B	1103	1	0,12,12	-	-	-		
2	SF4	C	1102	1	0,12,12	-	-	-		
2	SF4	D	1102	1	0,12,12	-	-	-		
2	SF4	D	1101	1	0,12,12	-	-	-		
3	FMN	D	1105	-	33,33,33	1.99	11 (33%)	48,50,50	2.29	17 (35%)
3	FMN	B	1105	-	33,33,33	1.48	5 (15%)	48,50,50	2.40	22 (45%)
5	TDR	C	1107	-	9,9,9	1.40	1 (11%)	12,12,12	2.74	5 (41%)

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
2	SF4	C	1101	1	-	-	0/6/5/5
3	FMN	C	1105	-	-	2/18/18/18	0/3/3/3
5	TDR	A	1107	-	-	-	0/1/1/1
2	SF4	B	1104	1	-	-	0/6/5/5
2	SF4	A	1103	1	-	-	0/6/5/5
2	SF4	C	1103	1	-	-	0/6/5/5
4	FAD	B	1106	-	-	1/34/50/50	0/6/6/6
5	TDR	D	1107	-	-	-	0/1/1/1
2	SF4	D	1103	1	-	-	0/6/5/5
2	SF4	A	1102	1	-	-	0/6/5/5
2	SF4	A	1104	1	-	-	0/6/5/5
2	SF4	B	1101	1	-	-	0/6/5/5
2	SF4	C	1104	1	-	-	0/6/5/5
4	FAD	D	1106	-	-	2/34/50/50	0/6/6/6
4	FAD	A	1106	-	-	5/34/50/50	0/6/6/6
2	SF4	D	1104	1	-	-	0/6/5/5
2	SF4	B	1102	1	-	-	0/6/5/5
2	SF4	A	1101	1	-	-	0/6/5/5
3	FMN	A	1105	-	-	1/18/18/18	0/3/3/3
4	FAD	C	1106	-	-	2/34/50/50	0/6/6/6
5	TDR	B	1107	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	B	1103	1	-	-	0/6/5/5
2	SF4	C	1102	1	-	-	0/6/5/5
2	SF4	D	1102	1	-	-	0/6/5/5
2	SF4	D	1101	1	-	-	0/6/5/5
3	FMN	D	1105	-	-	5/18/18/18	0/3/3/3
3	FMN	B	1105	-	-	2/18/18/18	0/3/3/3
5	TDR	C	1107	-	-	-	0/1/1/1

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1106	FAD	C10-N1	-5.86	1.21	1.33
4	C	1106	FAD	P-O3P	-5.73	1.53	1.59
3	A	1105	FMN	C4A-N5	5.39	1.42	1.30
5	D	1107	TDR	C2-N1	4.83	1.43	1.36
3	C	1105	FMN	C4A-N5	4.73	1.41	1.30

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1107	TDR	CM5-C5-C4	-6.70	111.63	118.78
3	C	1105	FMN	C4A-C10-N10	5.85	124.85	116.48
3	C	1105	FMN	C4'-C3'-C2'	-5.84	103.86	113.57
3	D	1105	FMN	C4A-C10-N10	5.69	124.62	116.48
3	A	1105	FMN	C4-N3-C2	-5.40	116.05	125.64

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

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

There are no ring outliers.

15 monomers are involved in 20 short contacts:

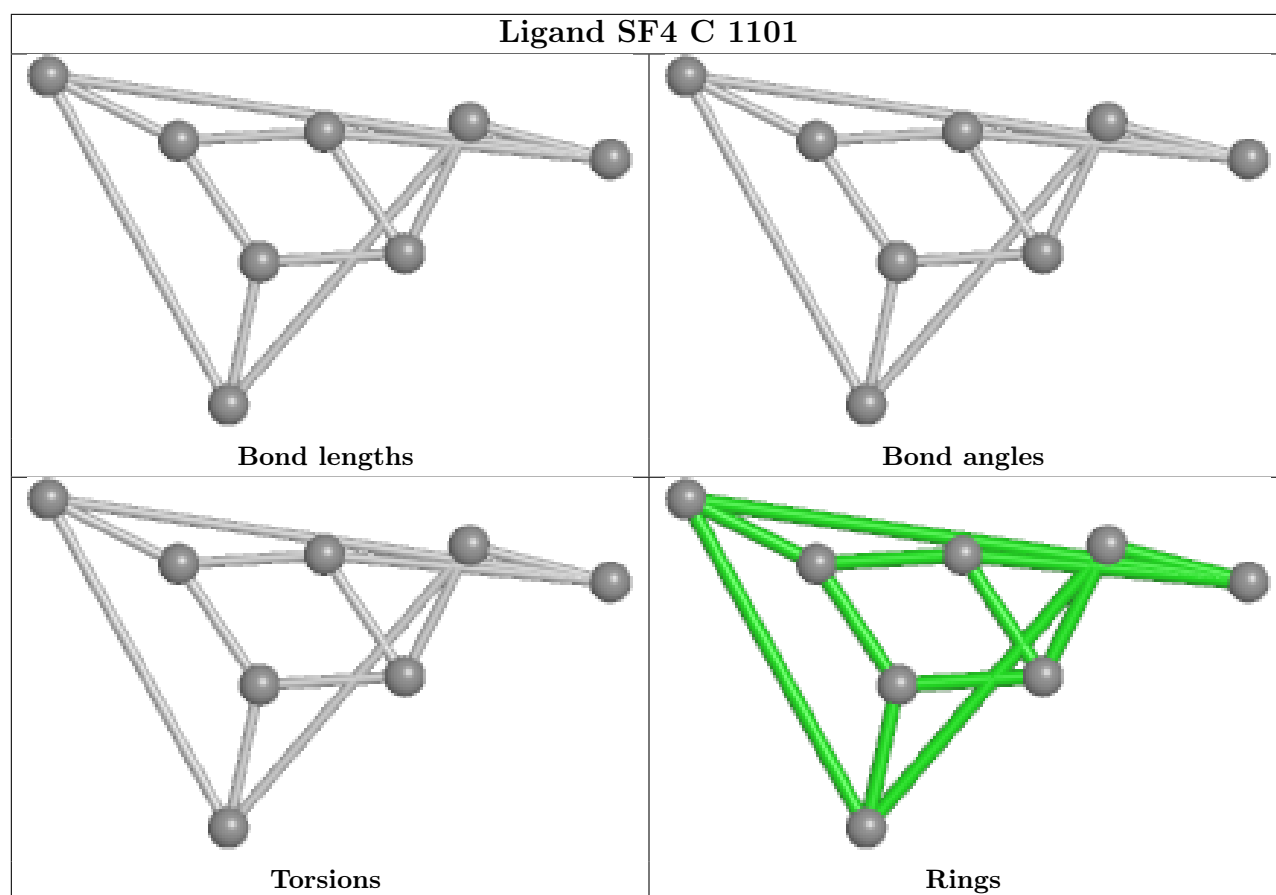
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1105	FMN	1	0

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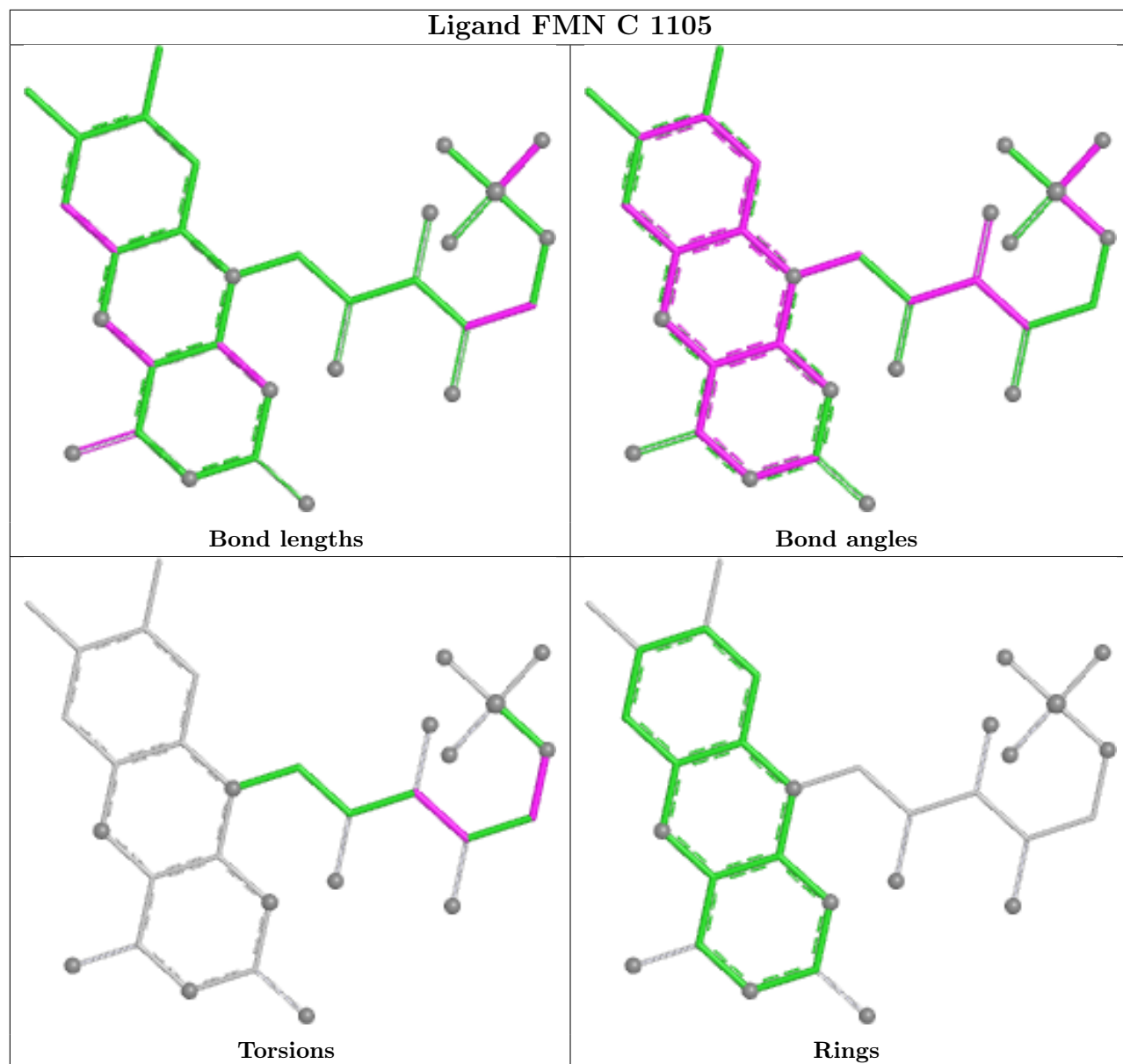
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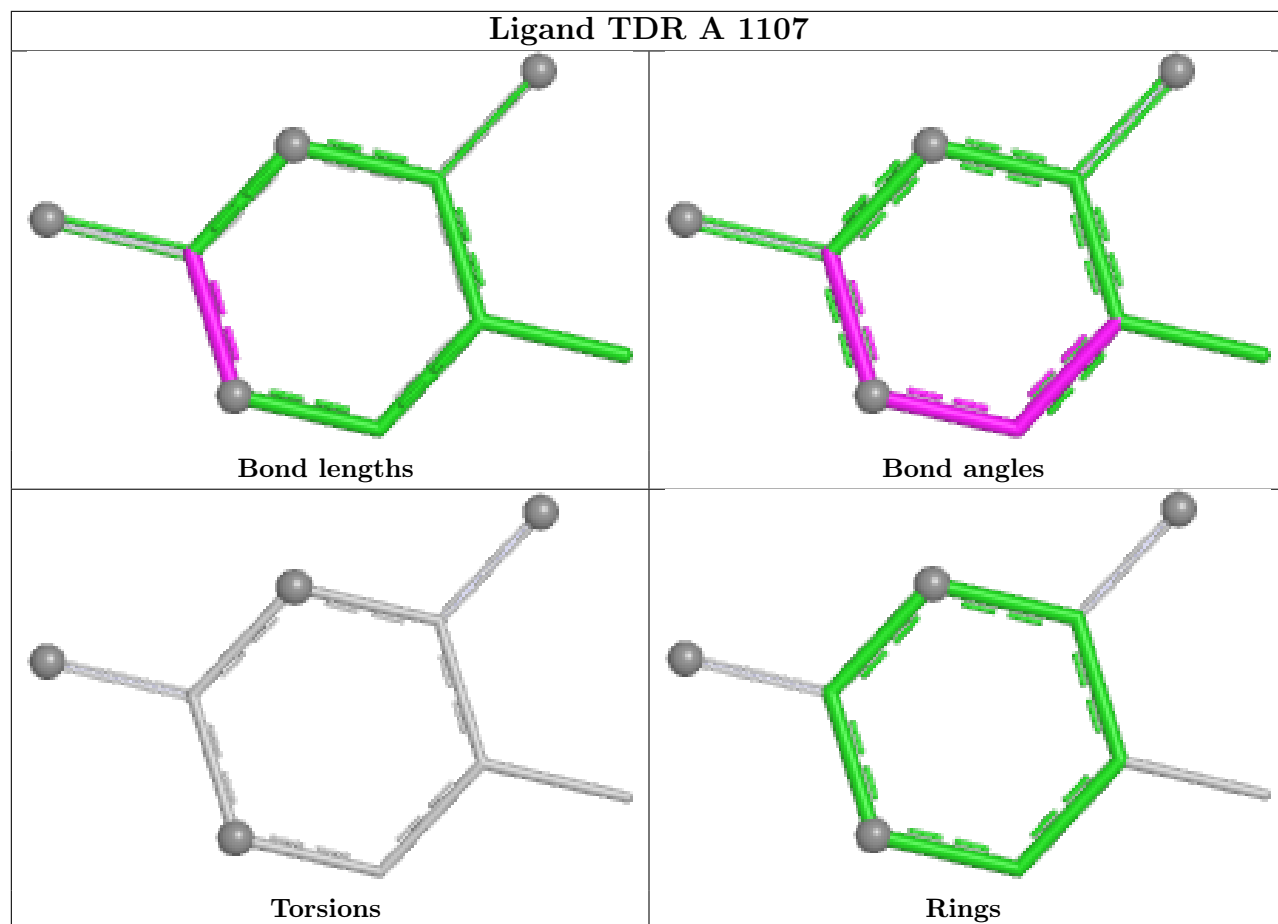
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1107	TDR	1	0
2	A	1103	SF4	2	0
4	B	1106	FAD	2	0
2	A	1102	SF4	1	0
2	B	1101	SF4	1	0
4	D	1106	FAD	2	0
4	A	1106	FAD	1	0
3	A	1105	FMN	1	0
4	C	1106	FAD	1	0
2	B	1103	SF4	1	0
2	C	1102	SF4	3	0
2	D	1101	SF4	1	0
3	D	1105	FMN	1	0
3	B	1105	FMN	1	0

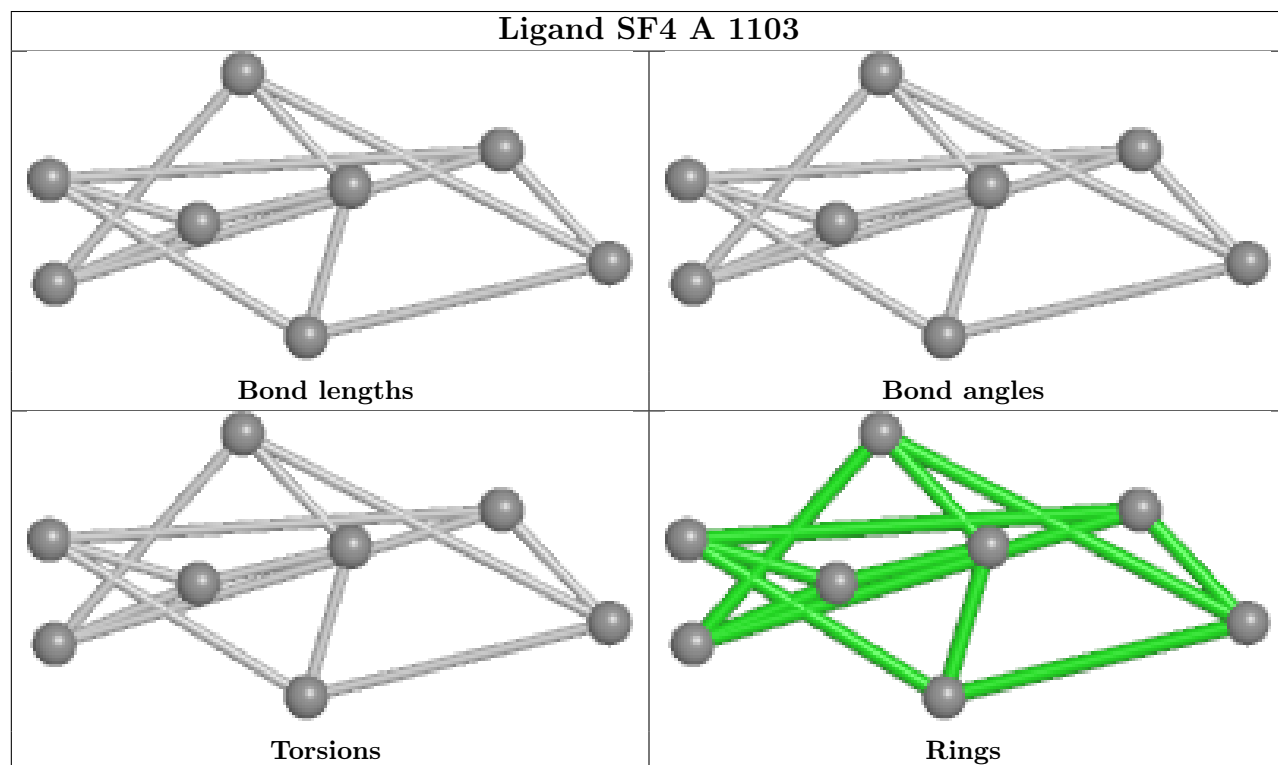
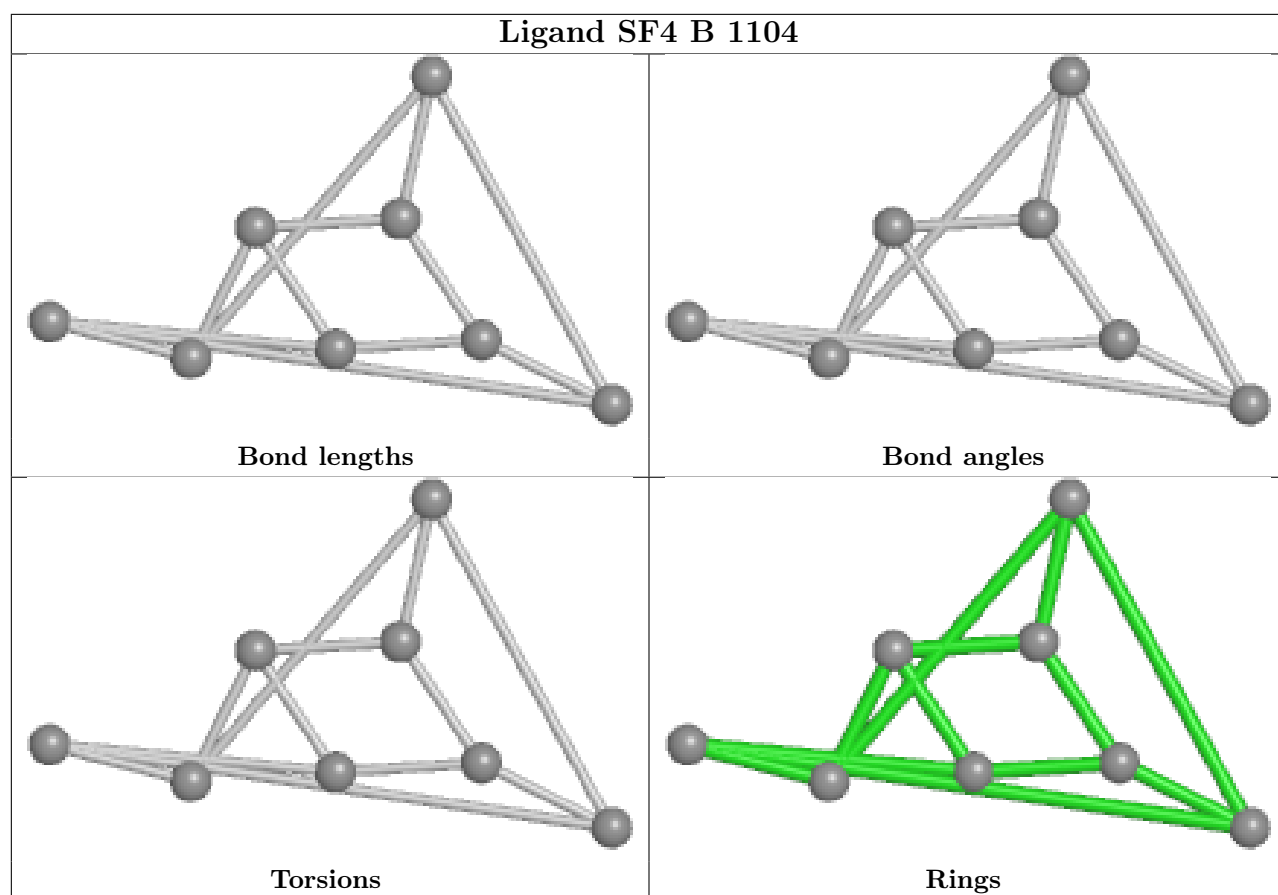
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

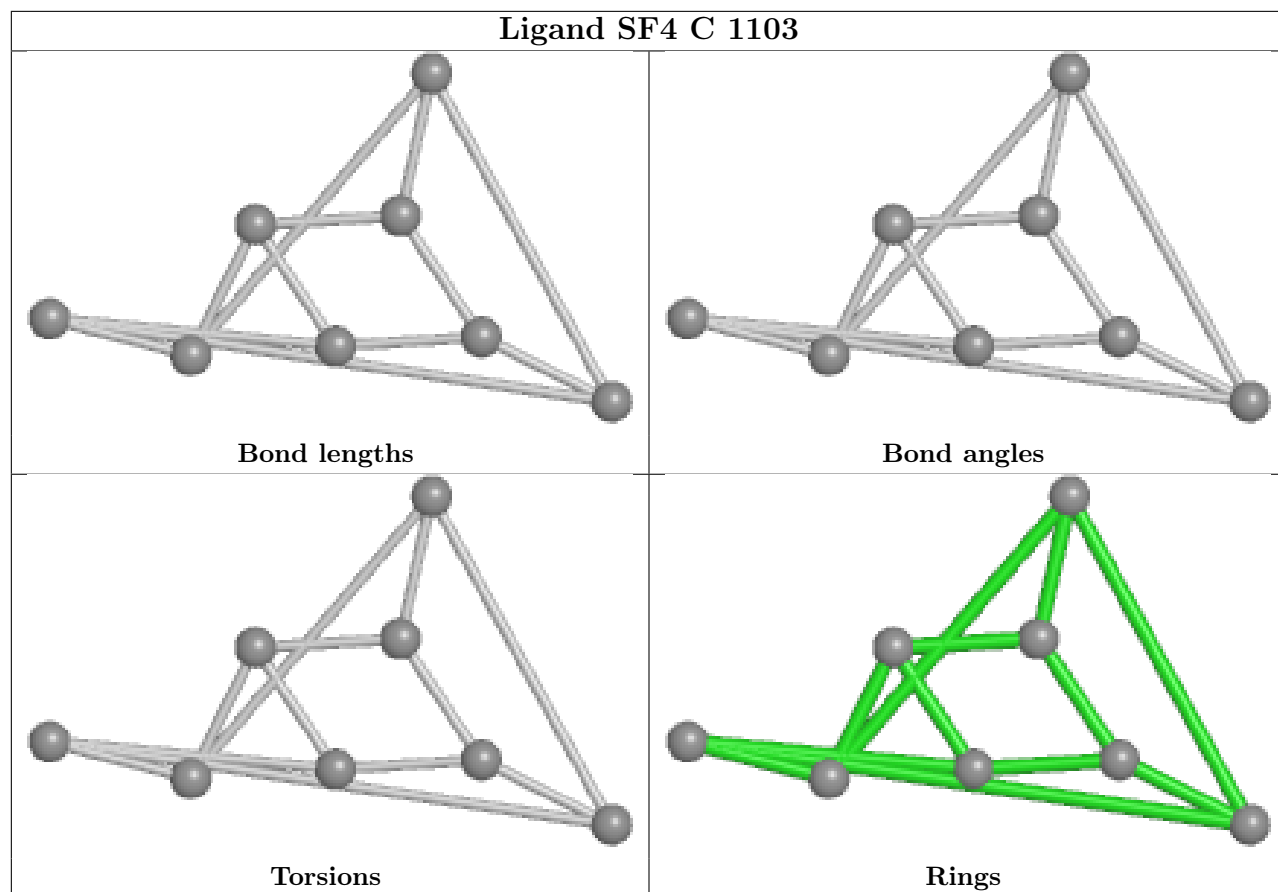


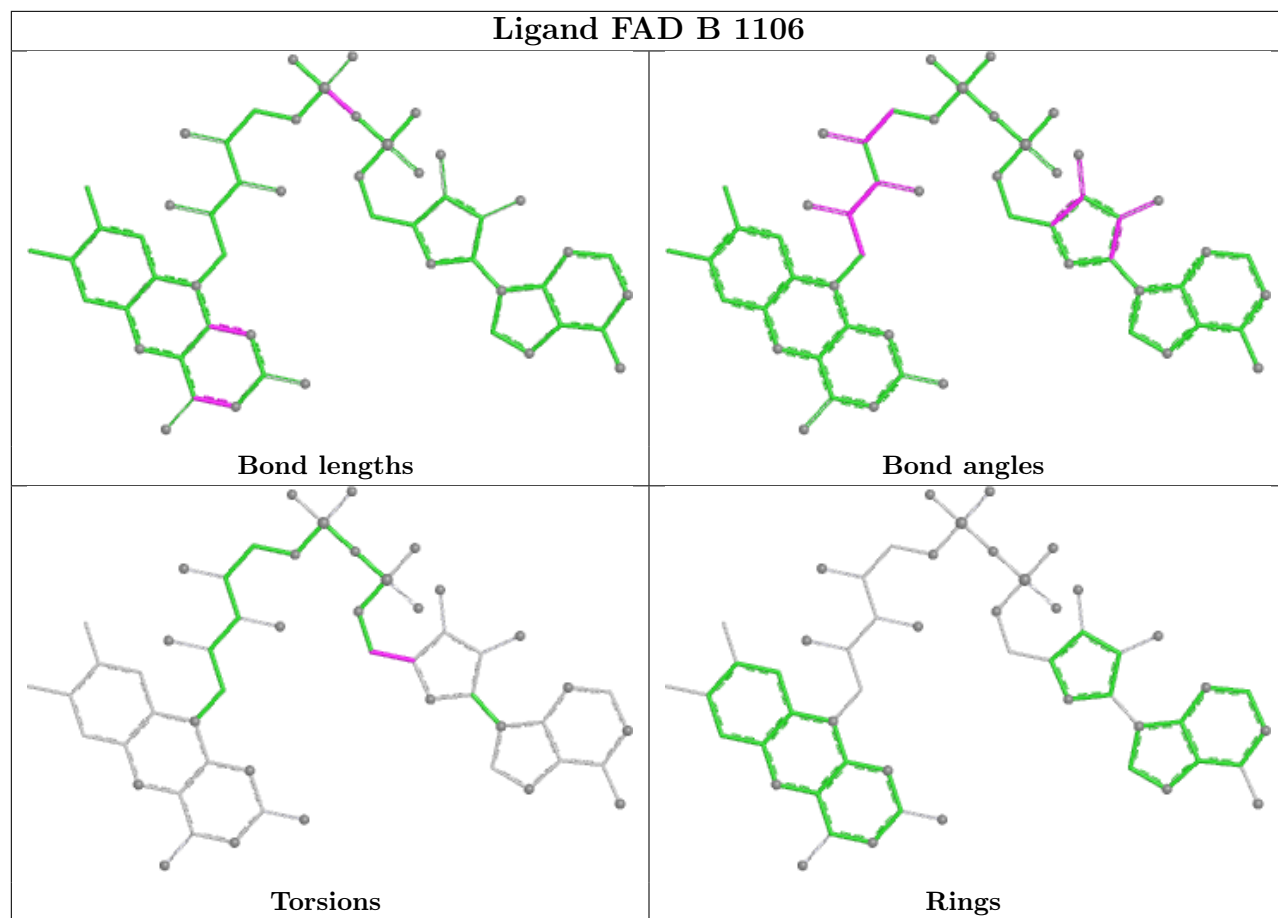
Ligand FMN C 1105

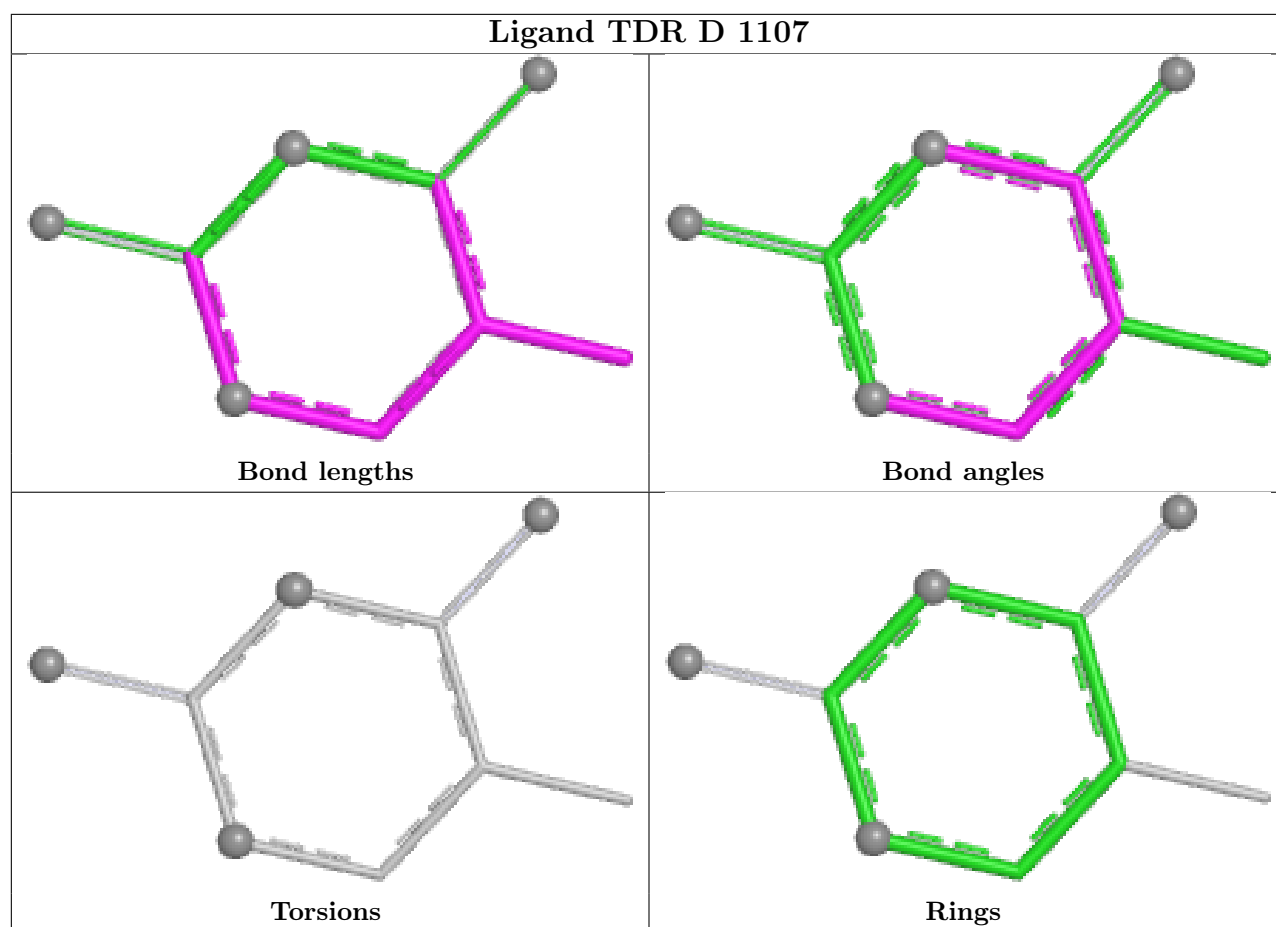


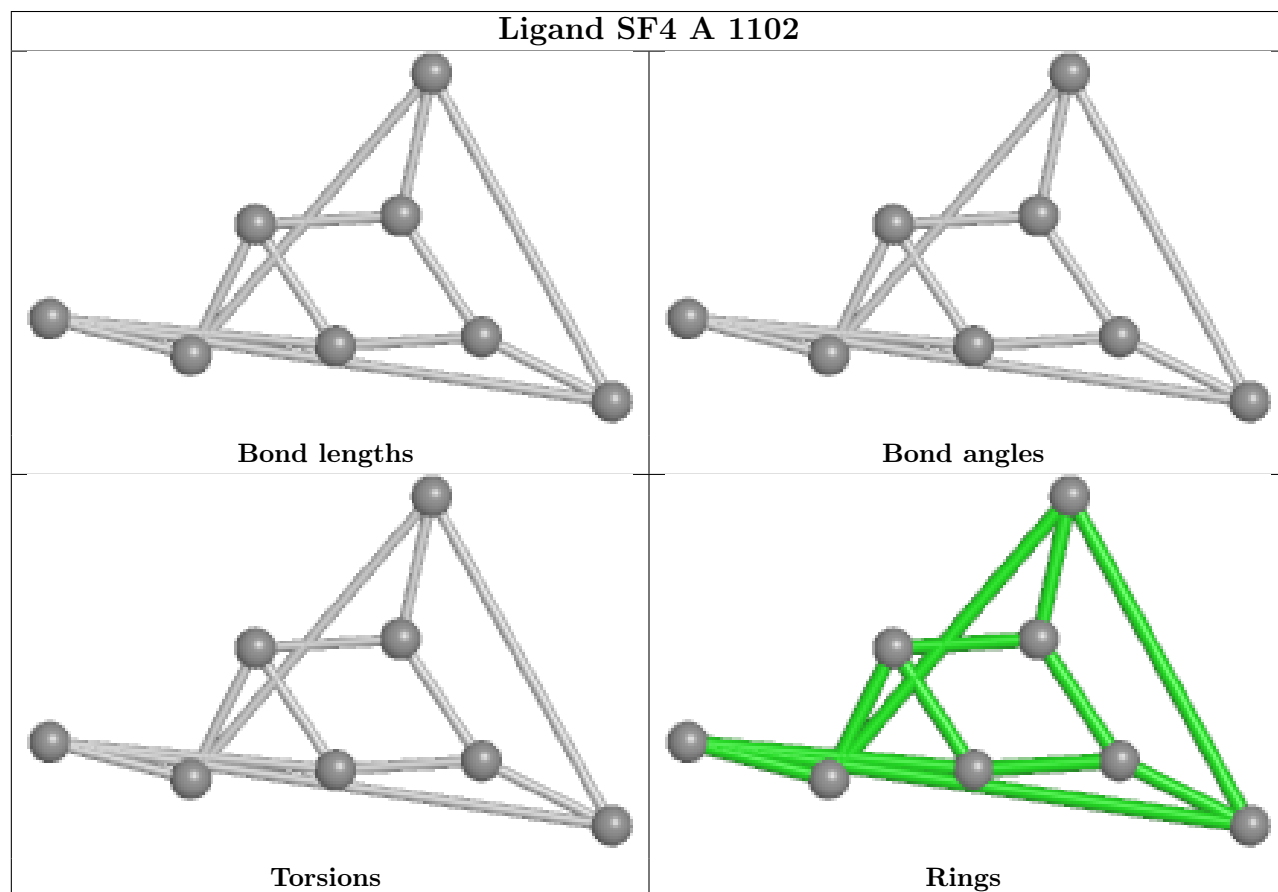
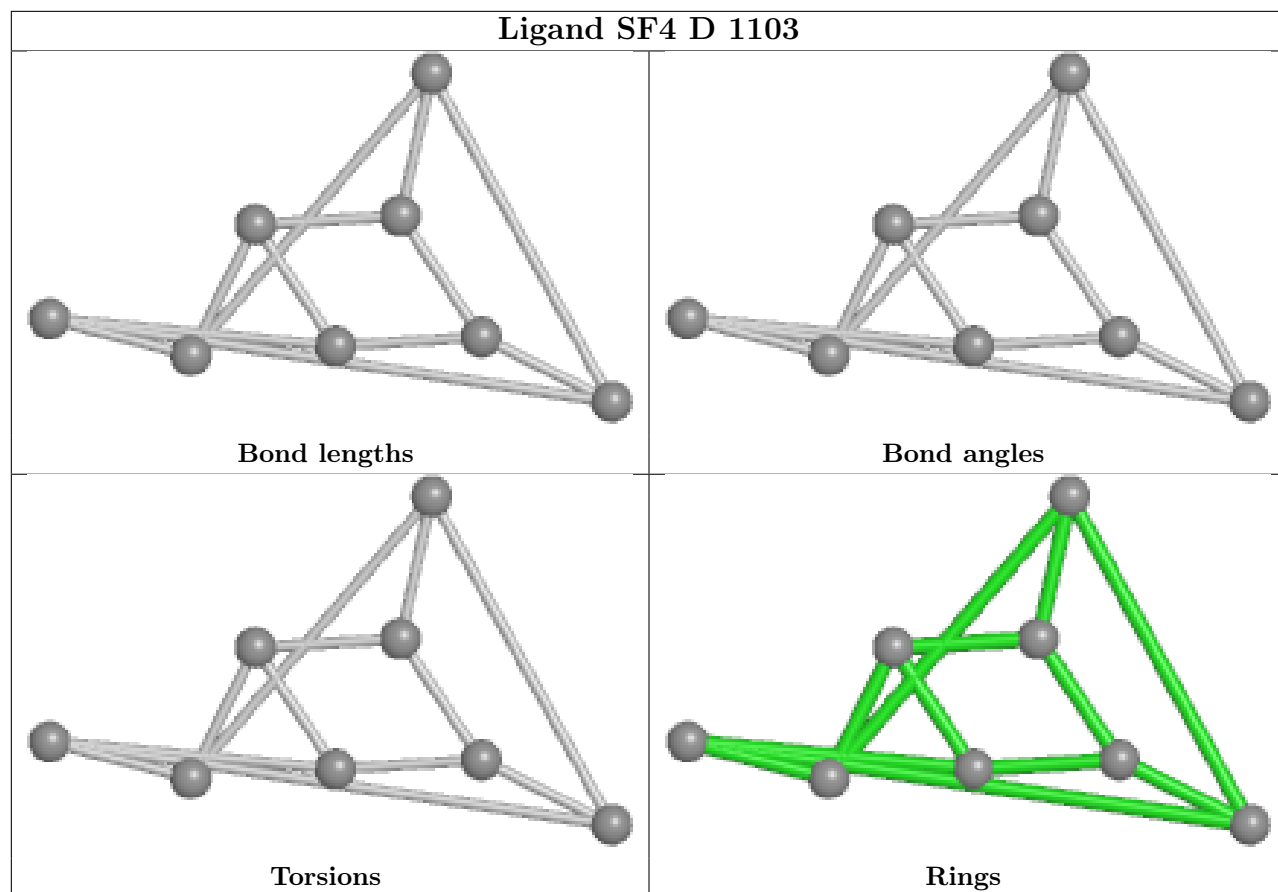


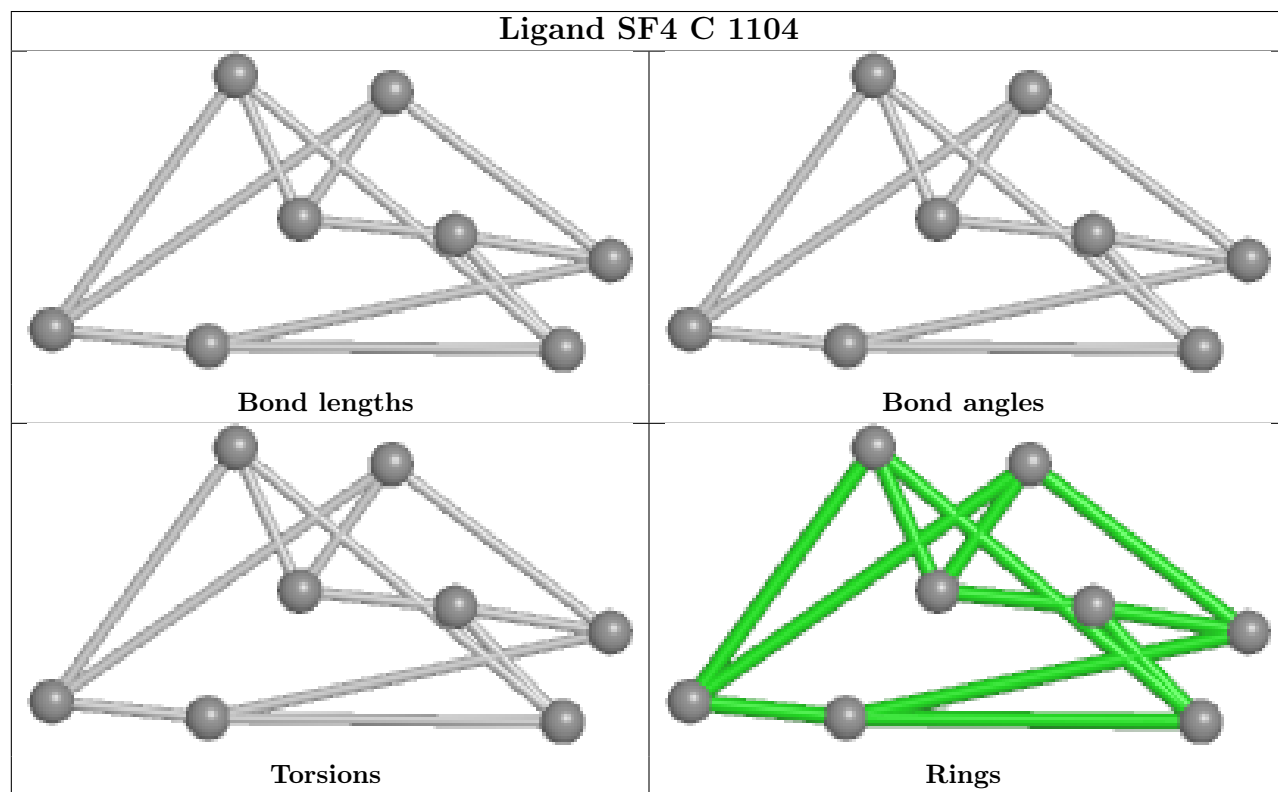
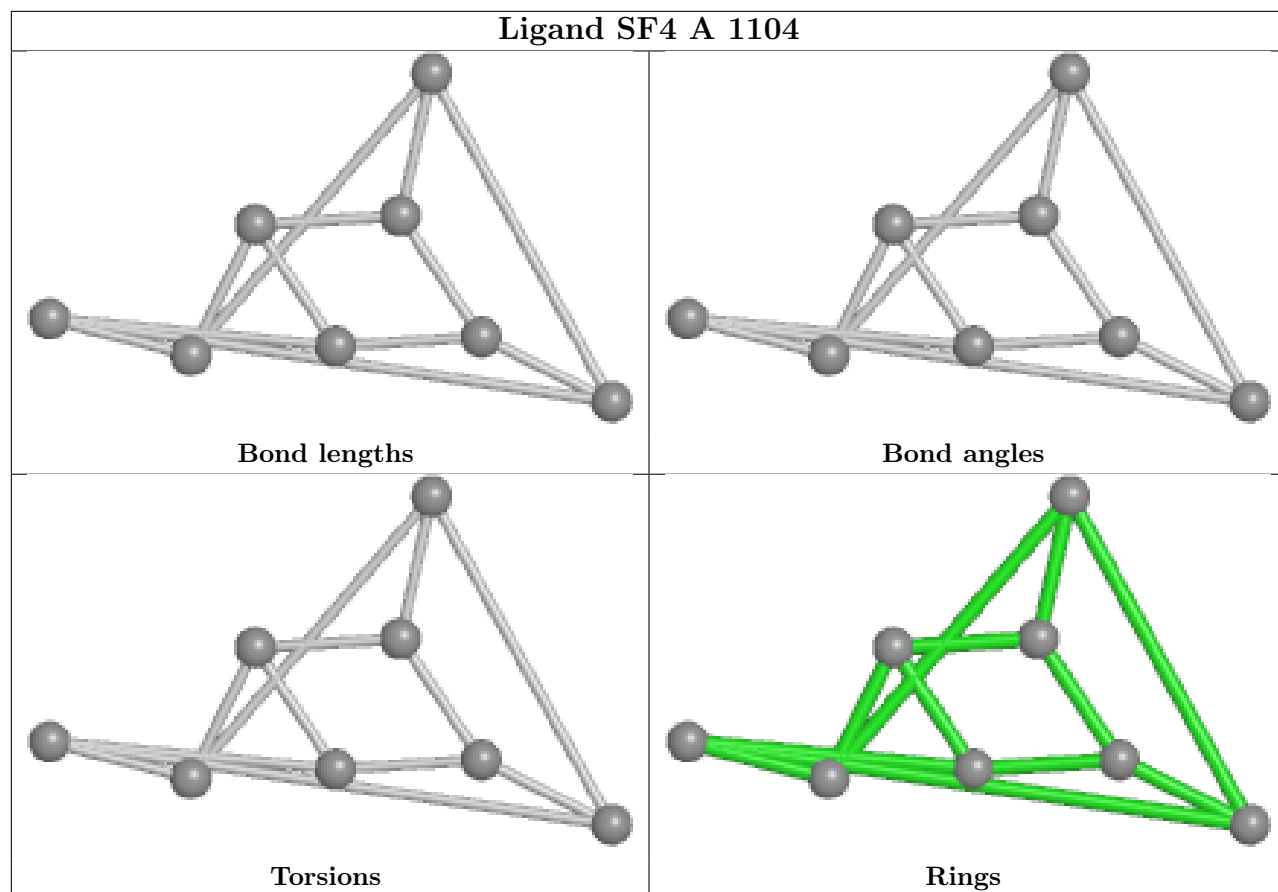


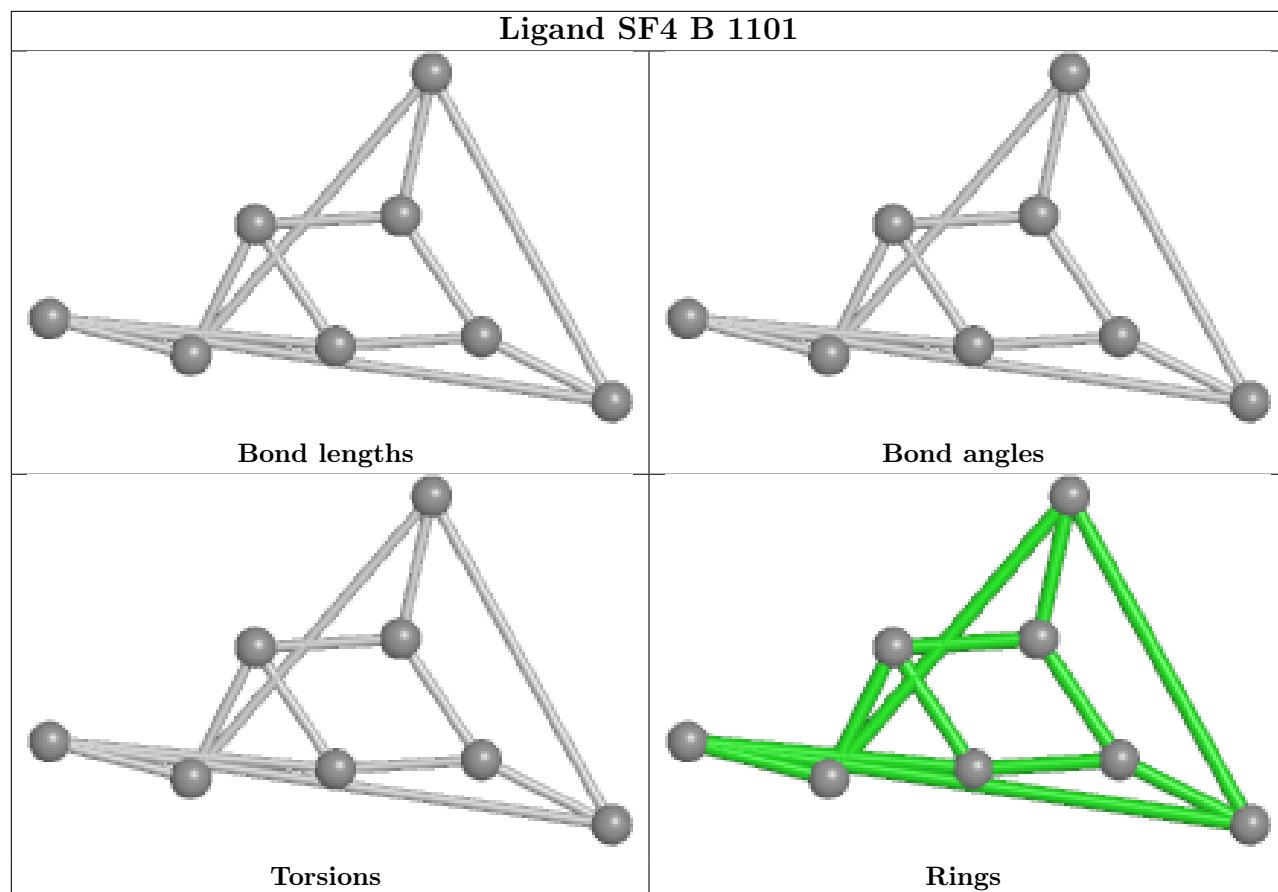


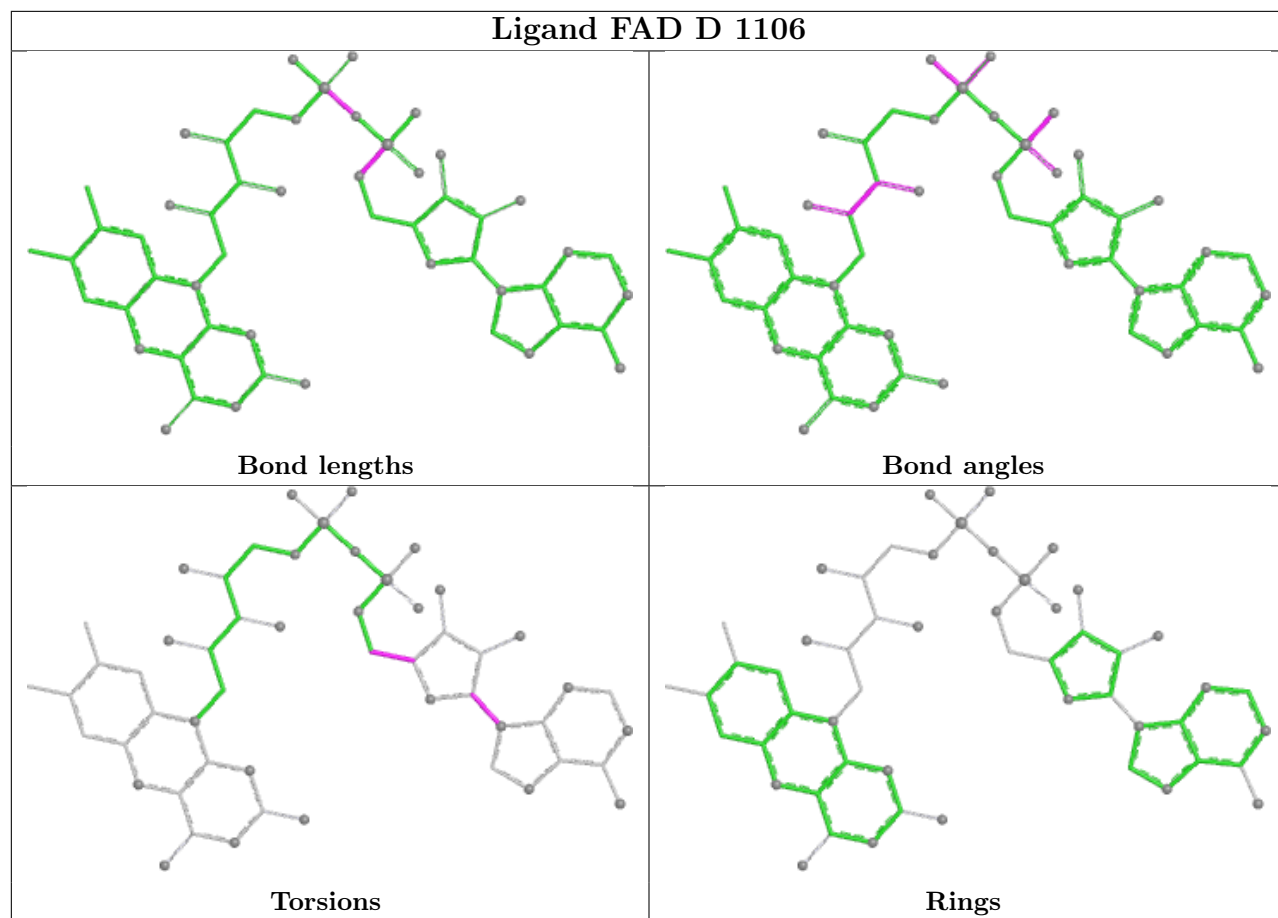


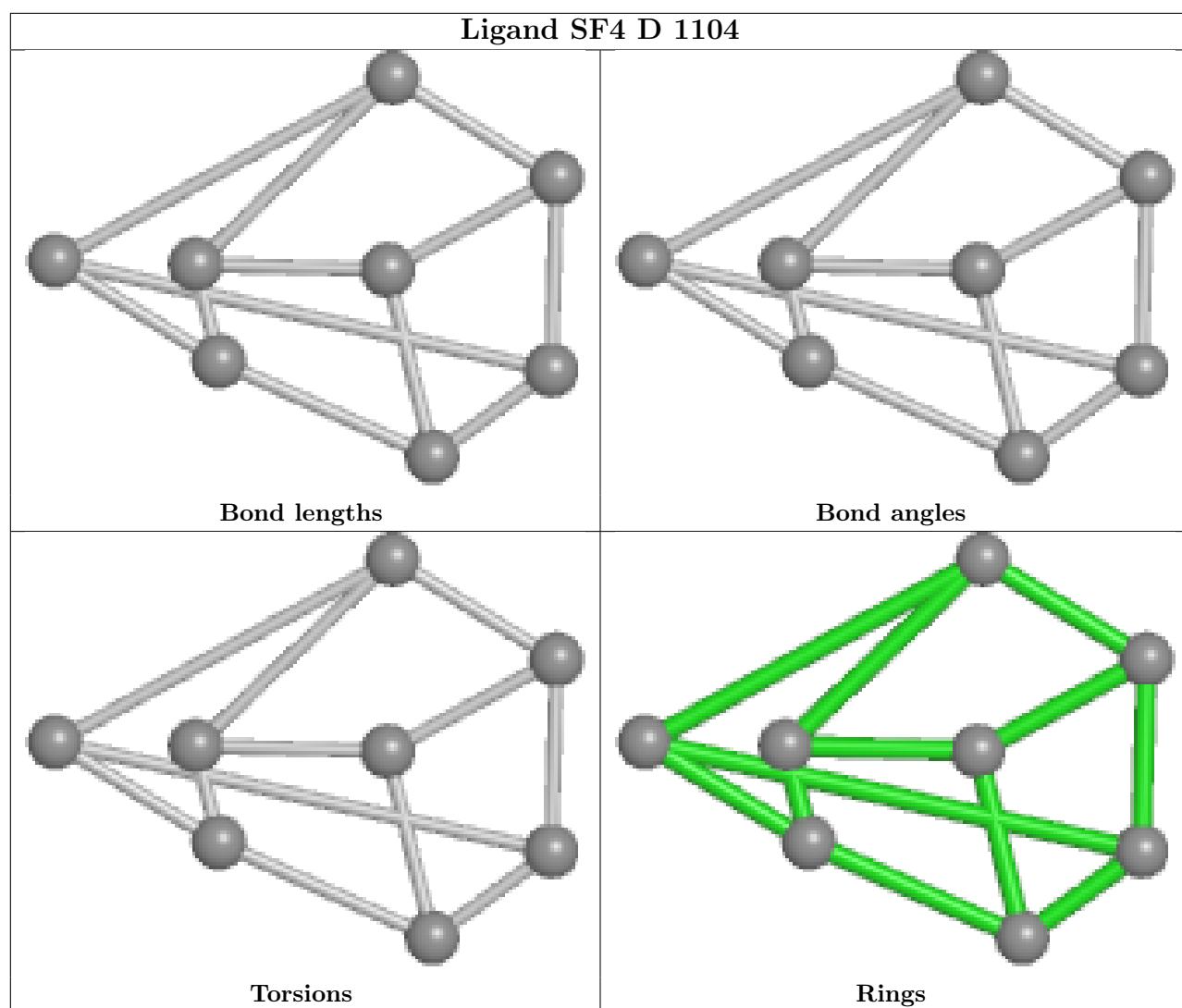


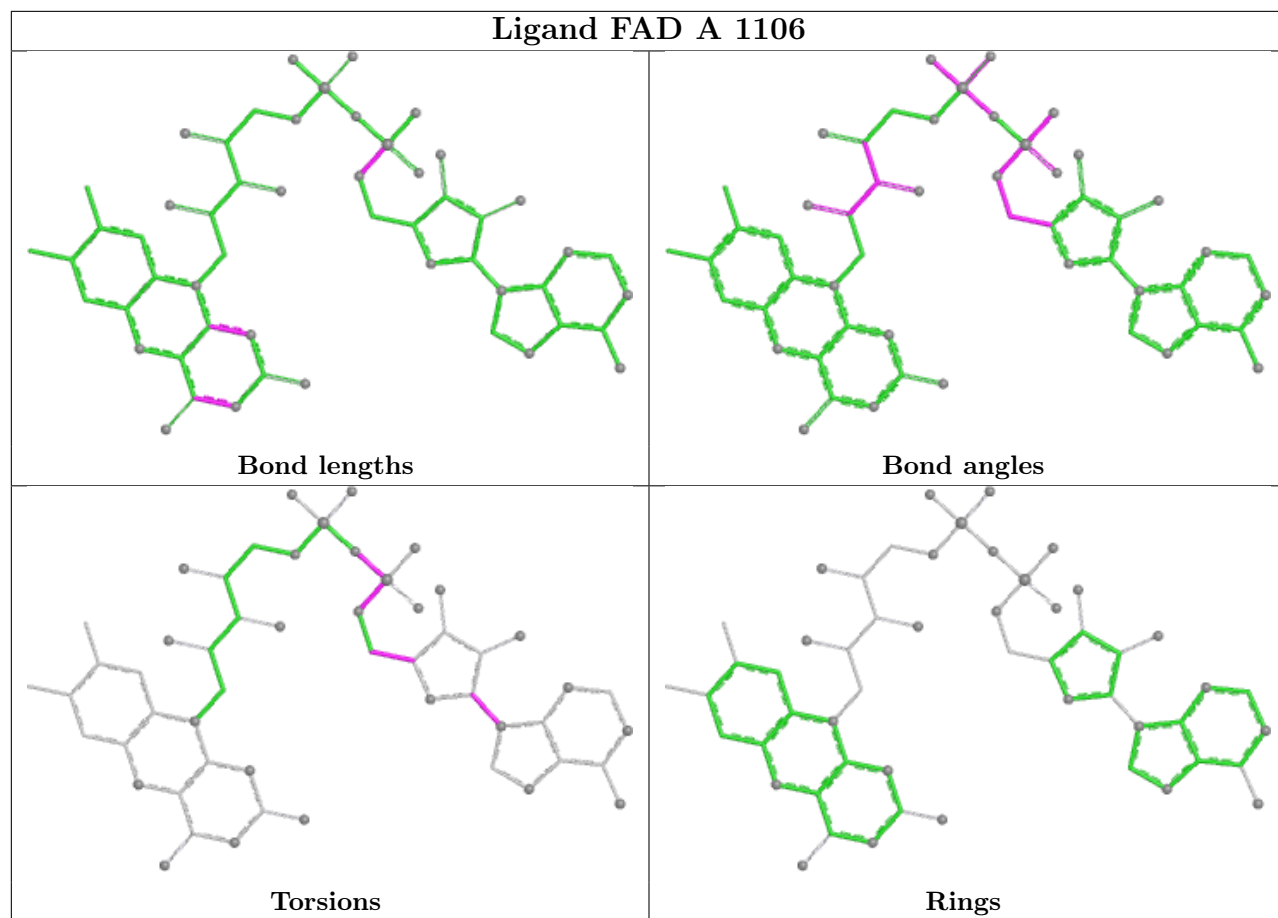




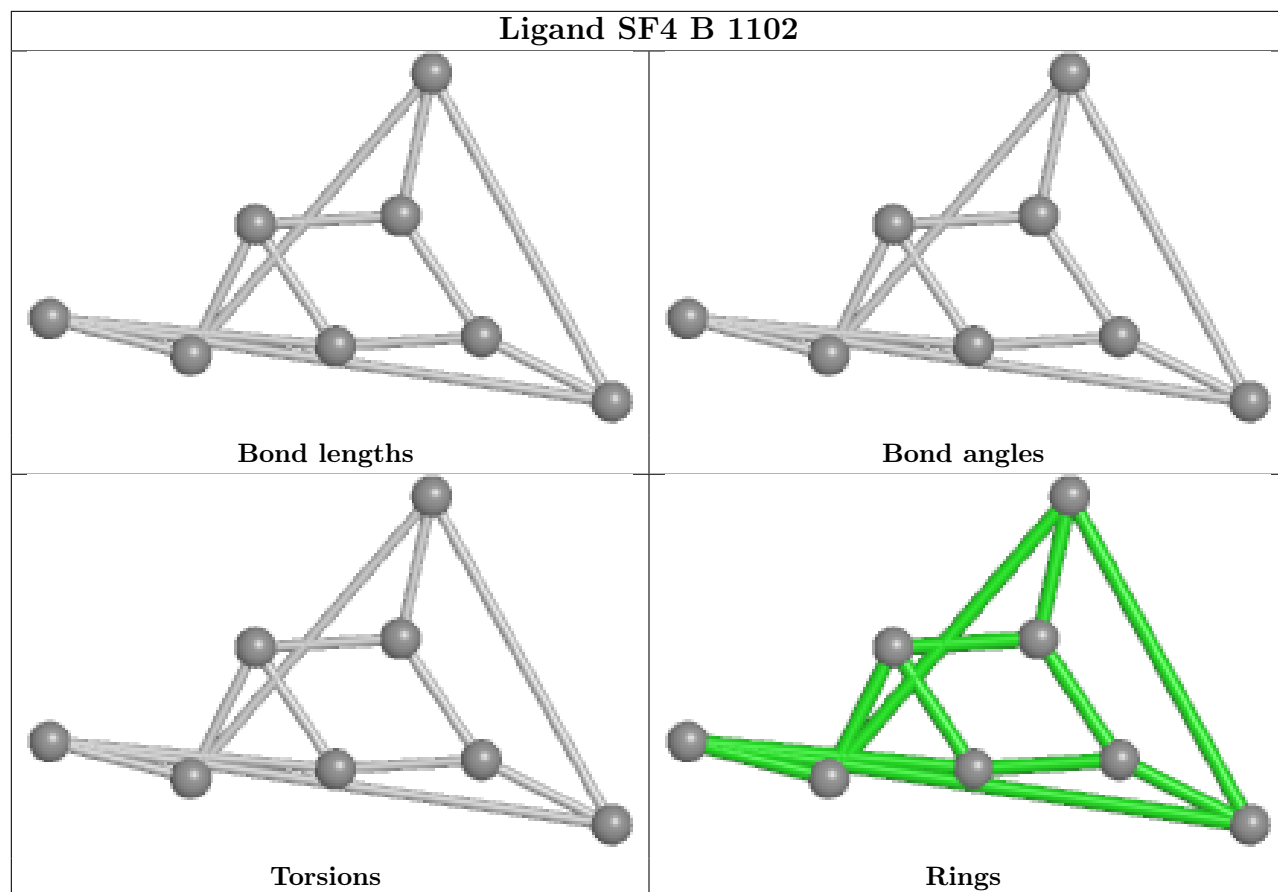




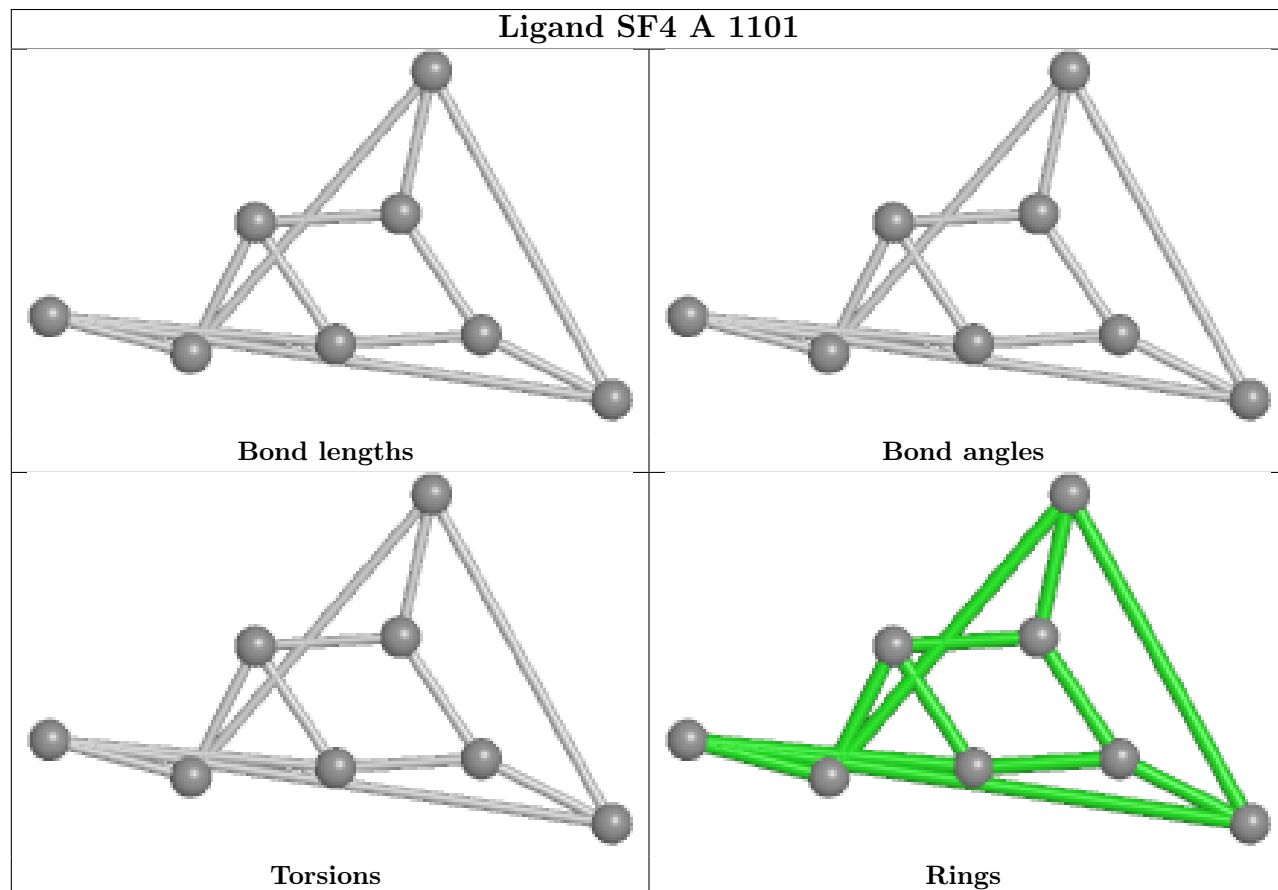




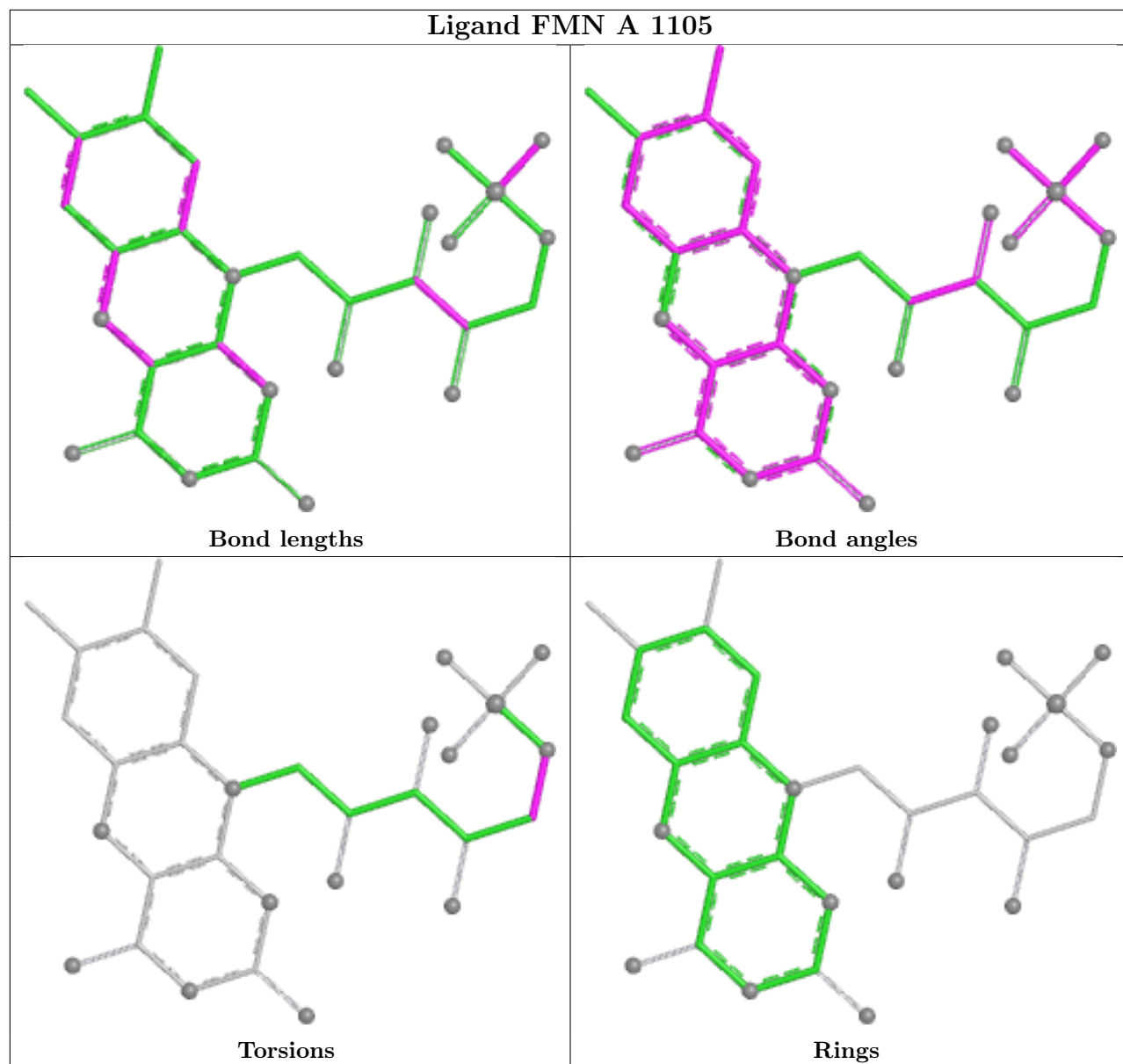
Ligand SF4 B 1102

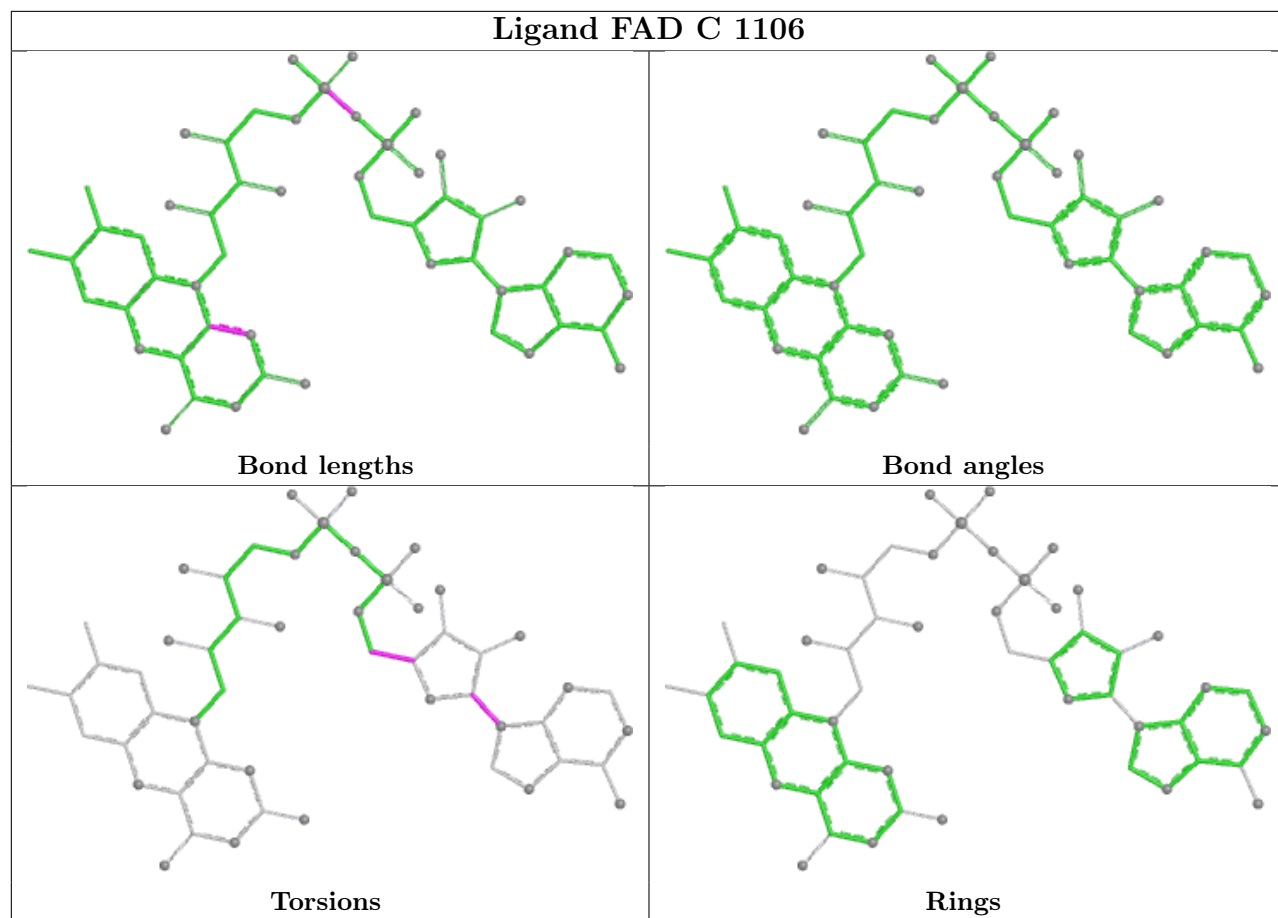


Ligand SF4 A 1101

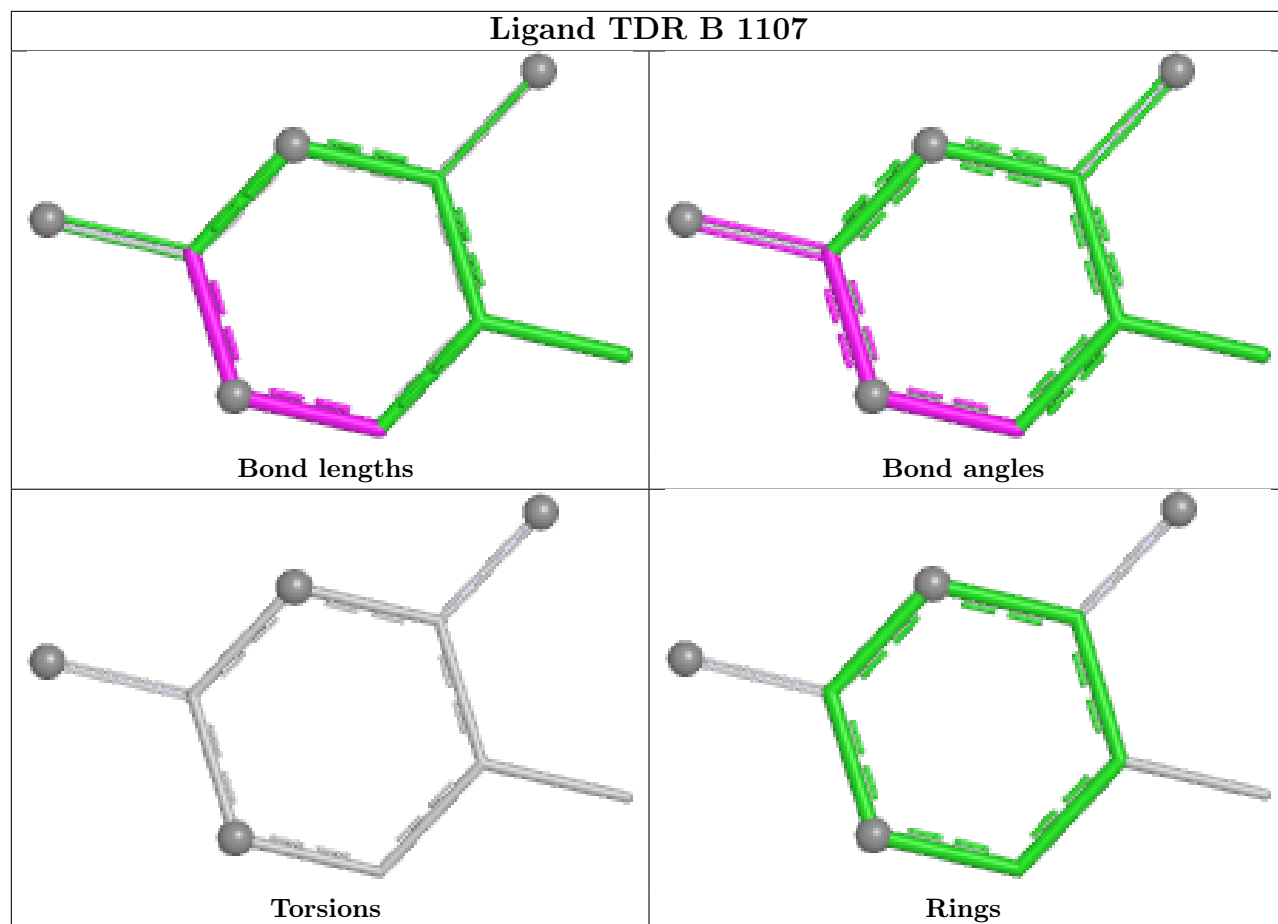


Ligand FMN A 1105

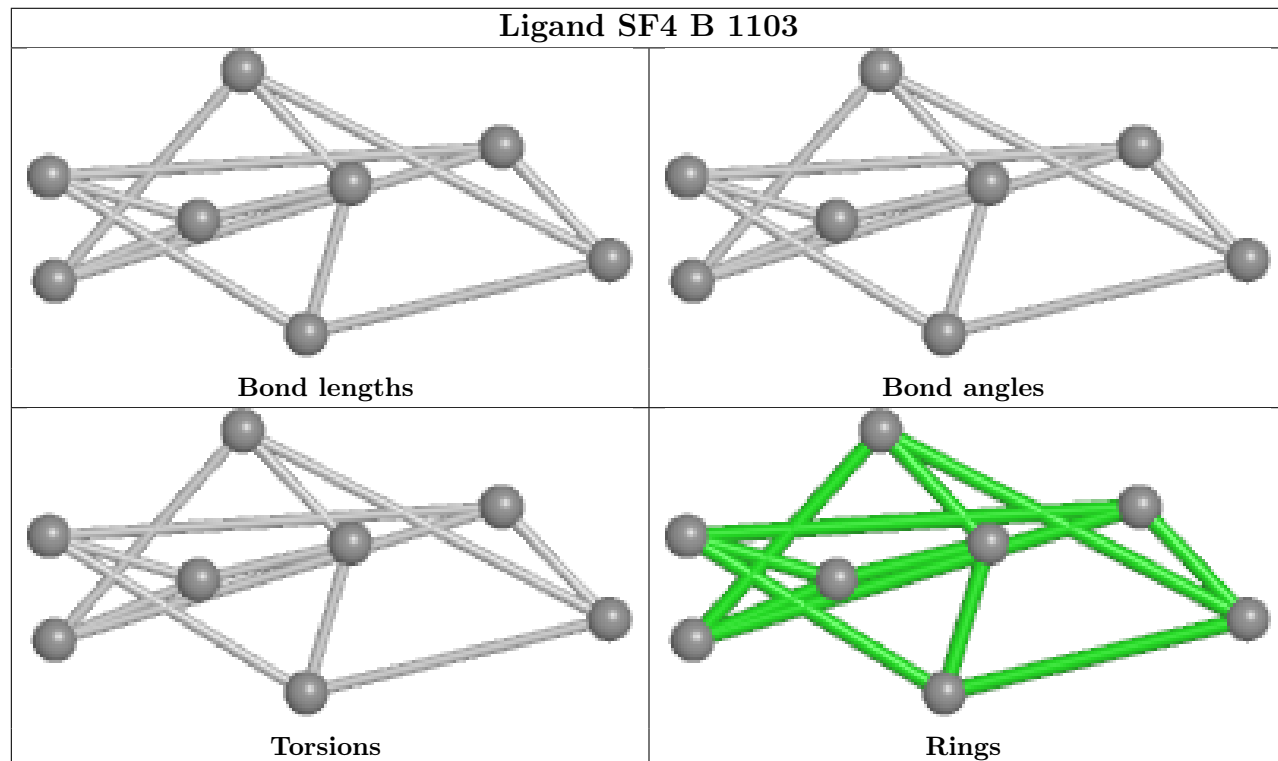


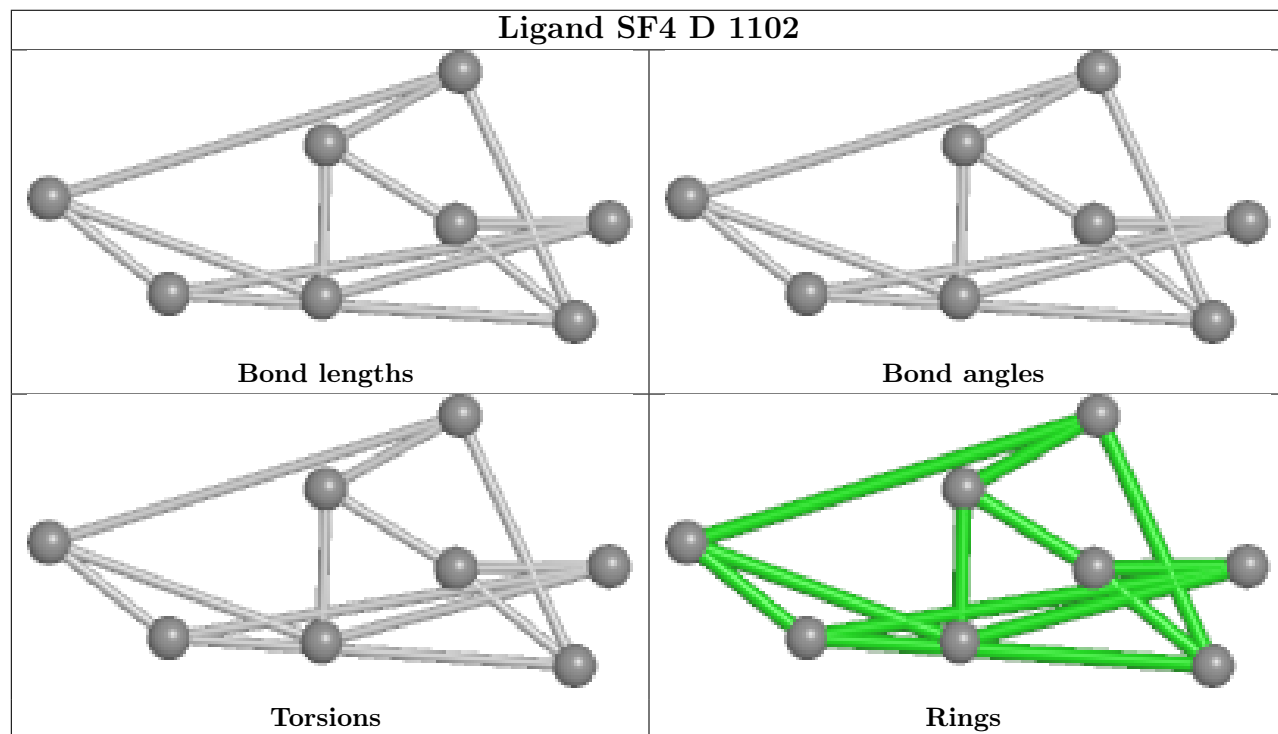
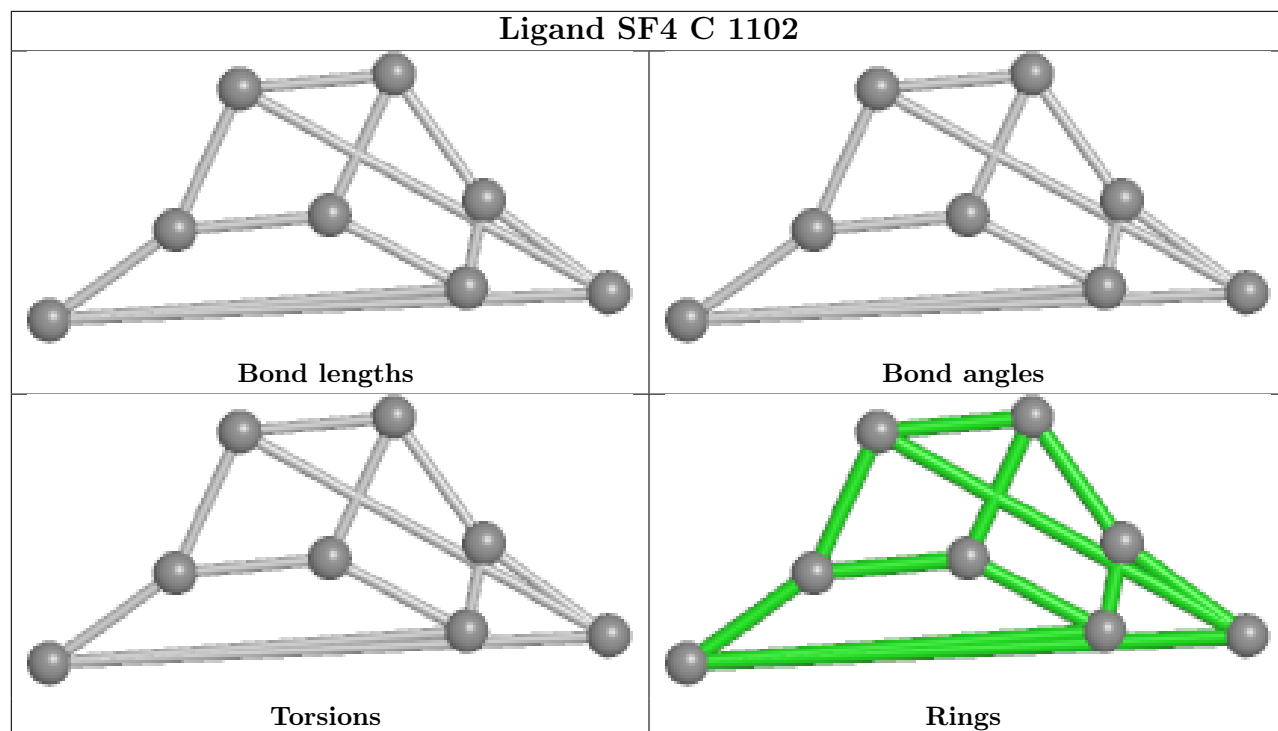


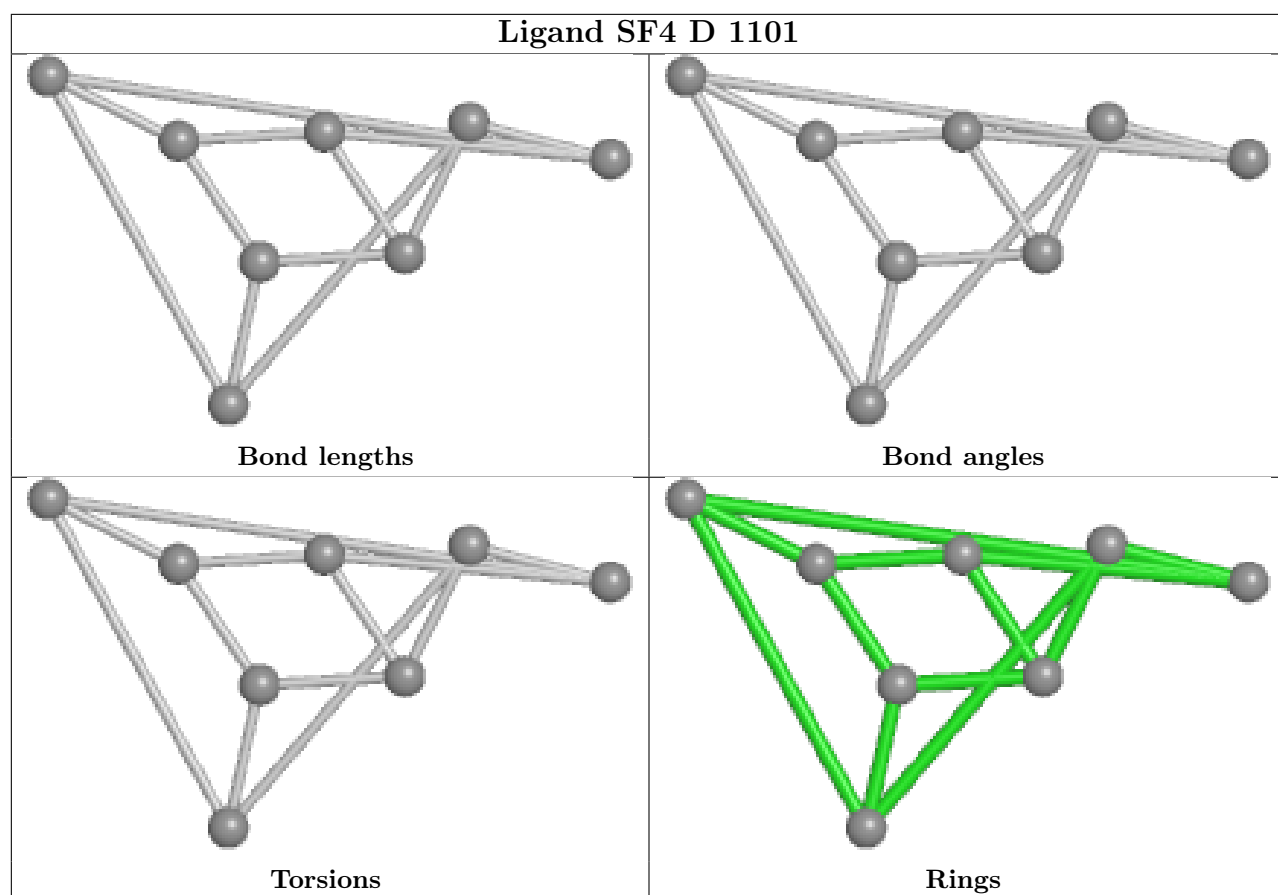
Ligand TDR B 1107



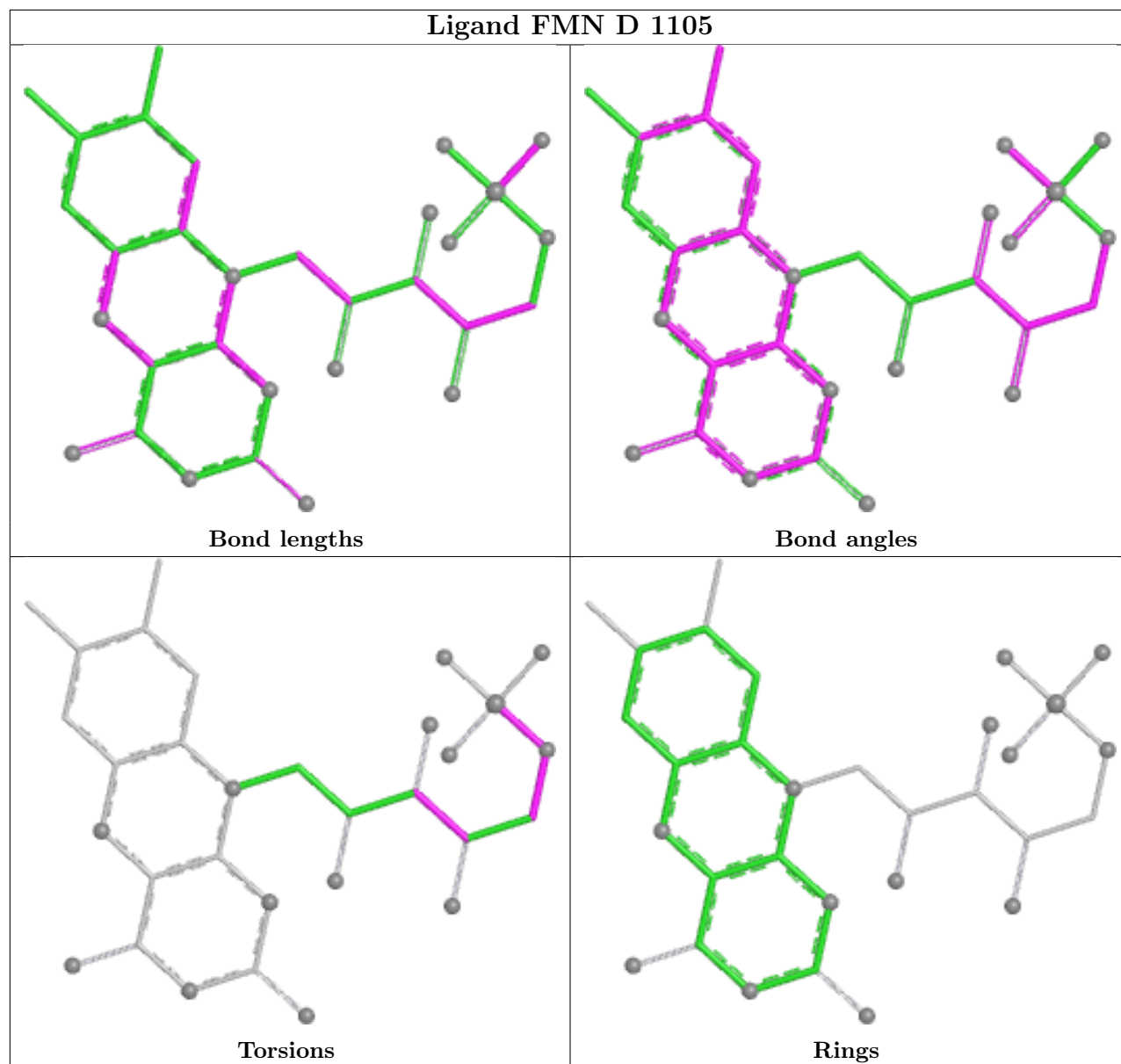
Ligand SF4 B 1103



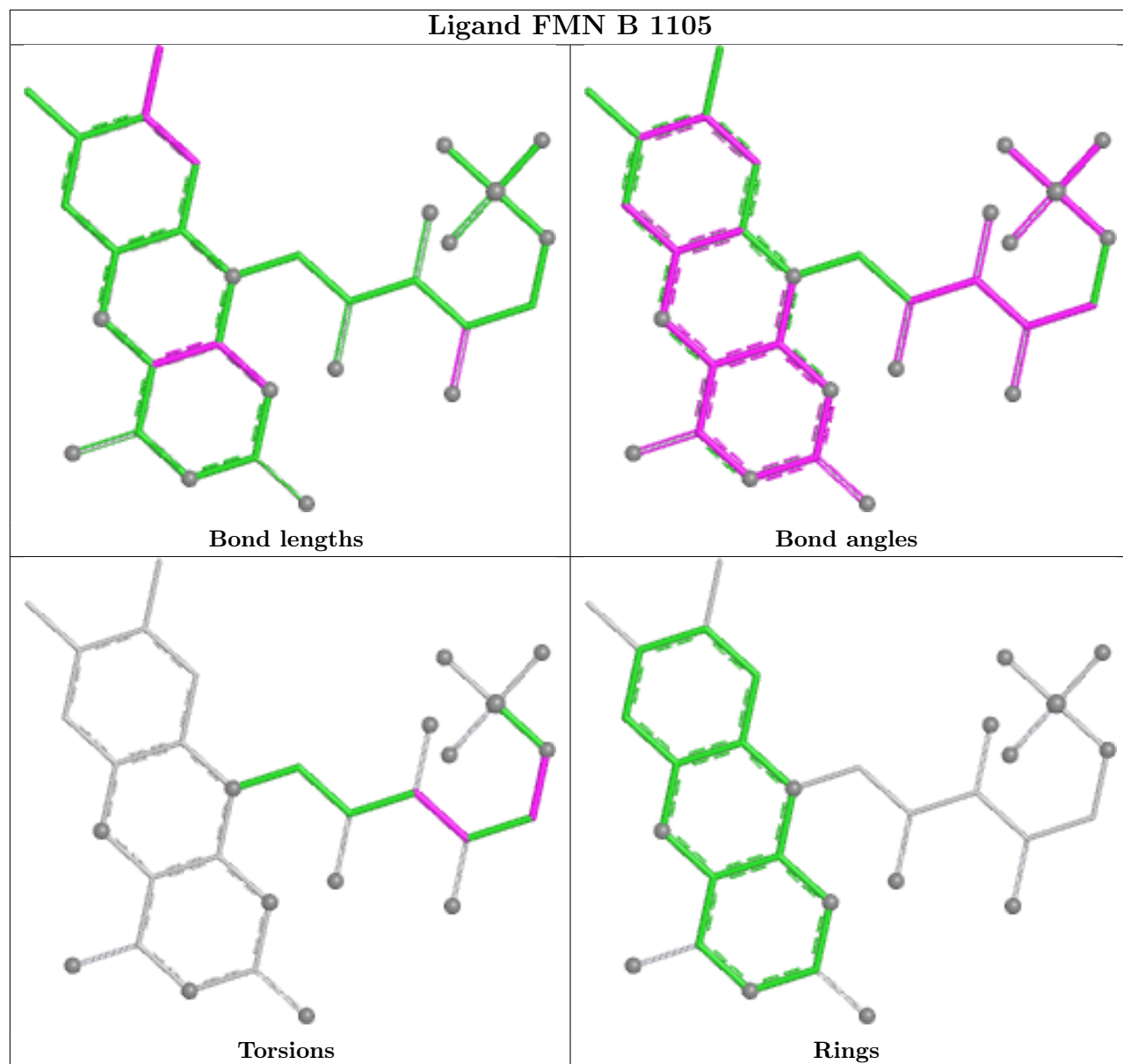


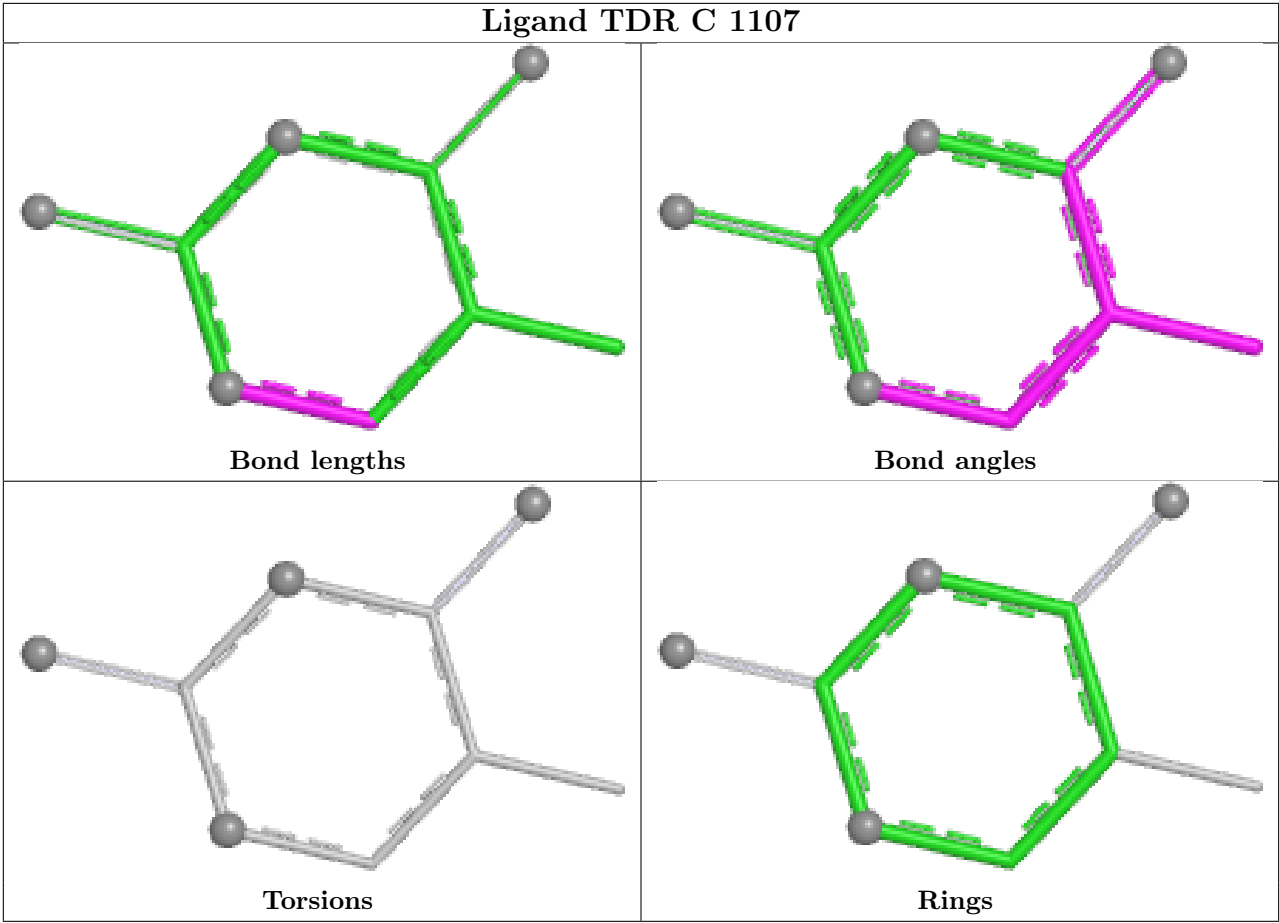


Ligand FMN D 1105



Ligand FMN B 1105





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

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

All chain breaks are listed below:

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

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

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	996/1025 (97%)	-0.03	49 (4%)	35	37	11, 30, 88, 160	4 (0%)
1	B	1001/1025 (97%)	0.03	60 (5%)	27	30	13, 31, 89, 187	5 (0%)
1	C	1002/1025 (97%)	0.00	55 (5%)	30	33	11, 32, 89, 164	4 (0%)
1	D	992/1025 (96%)	0.17	74 (7%)	20	22	15, 34, 100, 192	5 (0%)
All	All	3991/4100 (97%)	0.04	238 (5%)	27	30	11, 32, 91, 192	18 (0%)

The worst 5 of 238 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	868	ILE	7.7
1	A	2	ALA	7.2
1	A	868	ILE	6.6
1	A	1017	LEU	6.2
1	D	868	ILE	6.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

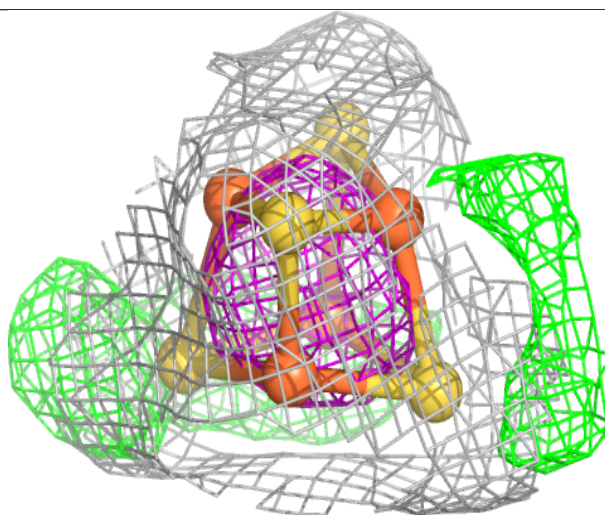
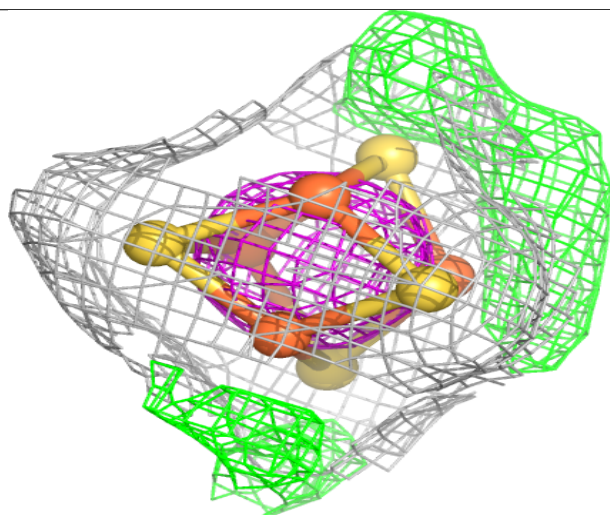
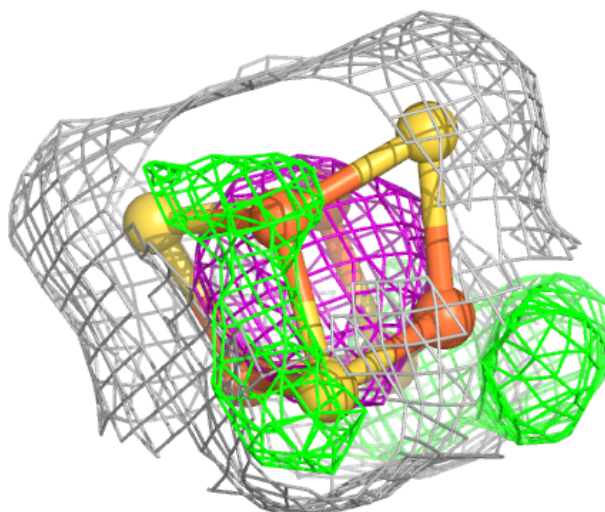
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SF4	C	1104	8/8	0.95	0.06	21,22,23,23	0
2	SF4	D	1103	8/8	0.95	0.06	17,22,24,25	0
2	SF4	B	1102	8/8	0.96	0.06	20,21,23,23	0
2	SF4	B	1103	8/8	0.96	0.05	18,19,21,21	0
2	SF4	B	1104	8/8	0.96	0.06	19,21,23,23	0
2	SF4	C	1101	8/8	0.96	0.06	19,21,22,23	0
2	SF4	C	1103	8/8	0.96	0.05	17,20,21,21	0
2	SF4	A	1101	8/8	0.96	0.05	18,21,22,23	0
2	SF4	D	1101	8/8	0.96	0.06	22,24,27,27	0
2	SF4	A	1104	8/8	0.96	0.06	20,23,24,24	0
5	TDR	D	1107	9/9	0.96	0.06	22,25,27,27	0
2	SF4	B	1101	8/8	0.97	0.05	19,21,21,22	0
2	SF4	A	1103	8/8	0.97	0.05	19,22,24,24	0
2	SF4	D	1102	8/8	0.97	0.05	19,20,21,21	0
2	SF4	C	1102	8/8	0.97	0.05	21,22,23,24	0
2	SF4	D	1104	8/8	0.97	0.06	21,23,25,25	0
3	FMN	C	1105	31/31	0.97	0.05	17,23,26,33	0
3	FMN	D	1105	31/31	0.97	0.05	19,23,28,31	0
4	FAD	A	1106	53/53	0.97	0.06	20,27,31,38	0
4	FAD	B	1106	53/53	0.97	0.06	23,31,37,43	0
4	FAD	C	1106	53/53	0.97	0.06	20,32,37,39	0
4	FAD	D	1106	53/53	0.97	0.06	25,34,41,41	0
5	TDR	A	1107	9/9	0.97	0.05	21,21,25,27	0
5	TDR	B	1107	9/9	0.97	0.06	22,25,27,28	0
2	SF4	A	1102	8/8	0.97	0.05	15,16,19,20	0
3	FMN	B	1105	31/31	0.98	0.06	16,24,29,33	0
5	TDR	C	1107	9/9	0.98	0.05	18,20,23,25	0
3	FMN	A	1105	31/31	0.98	0.06	19,28,36,37	0

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

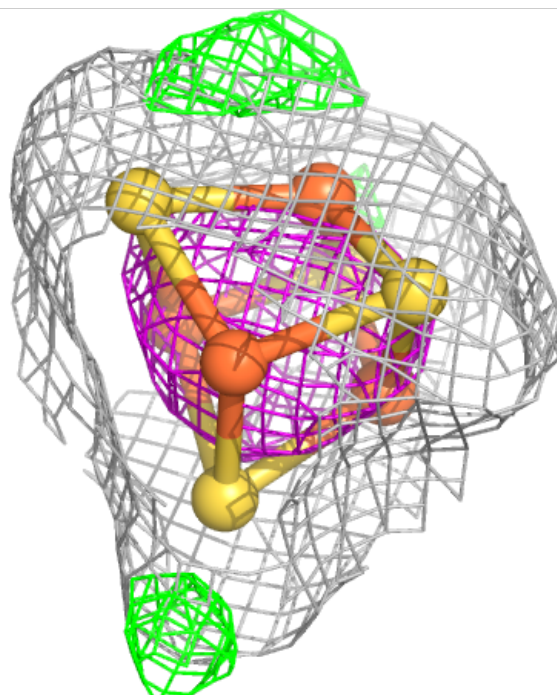
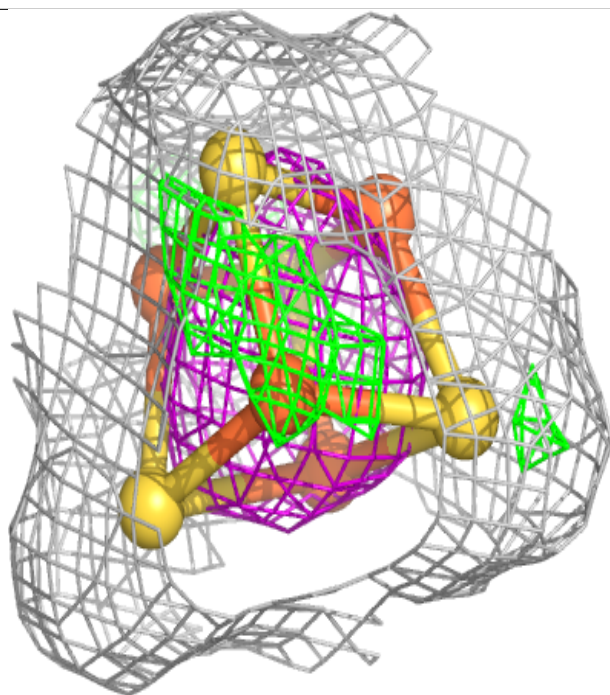
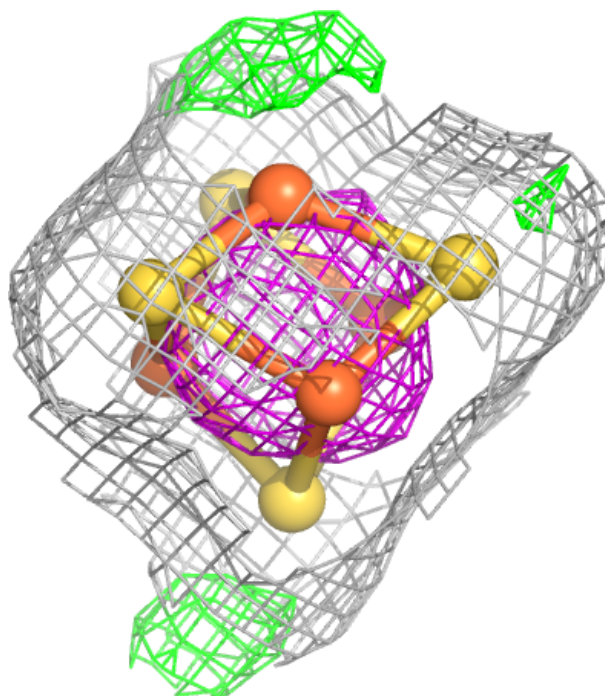
Electron density around SF4 C 1104:

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



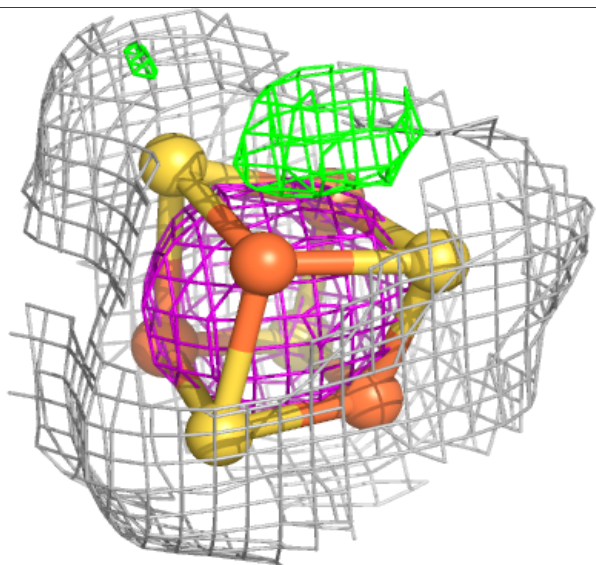
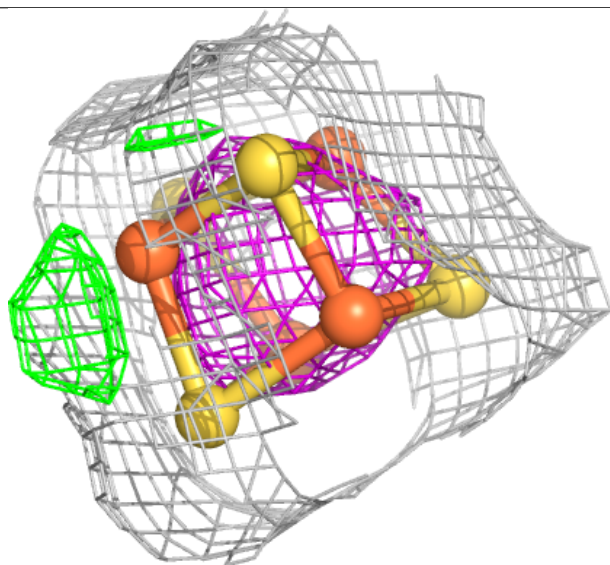
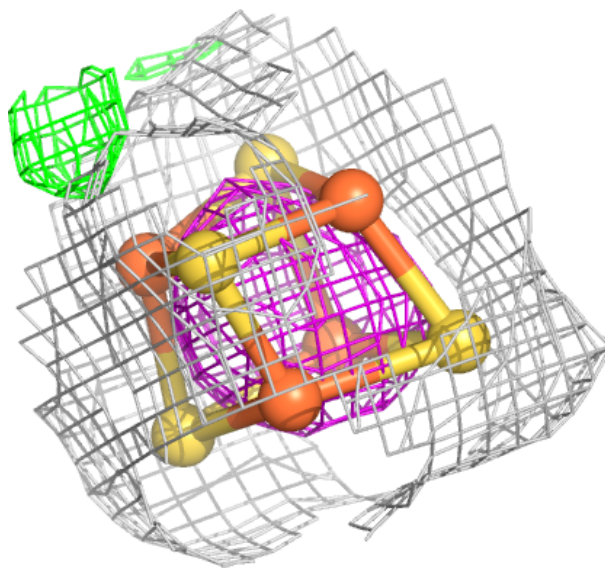
Electron density around SF4 D 1103:

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



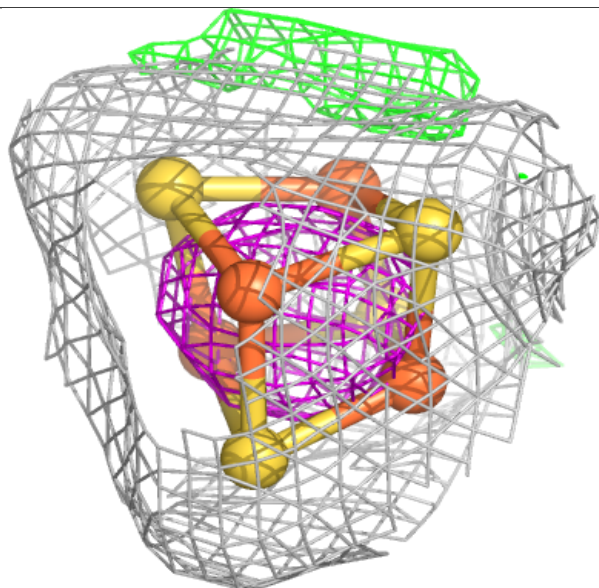
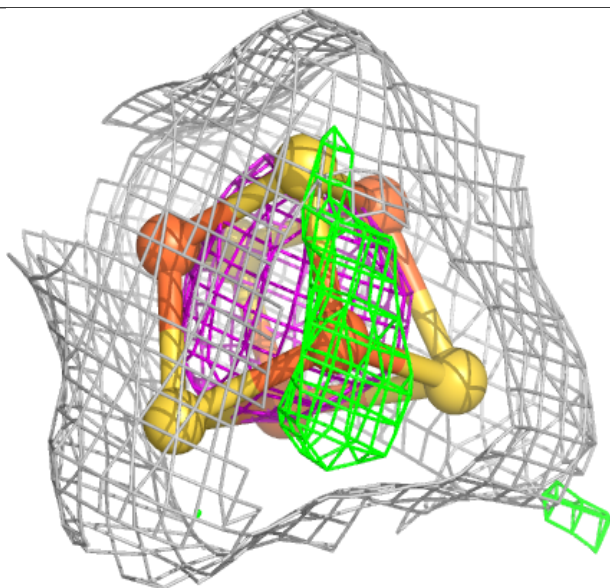
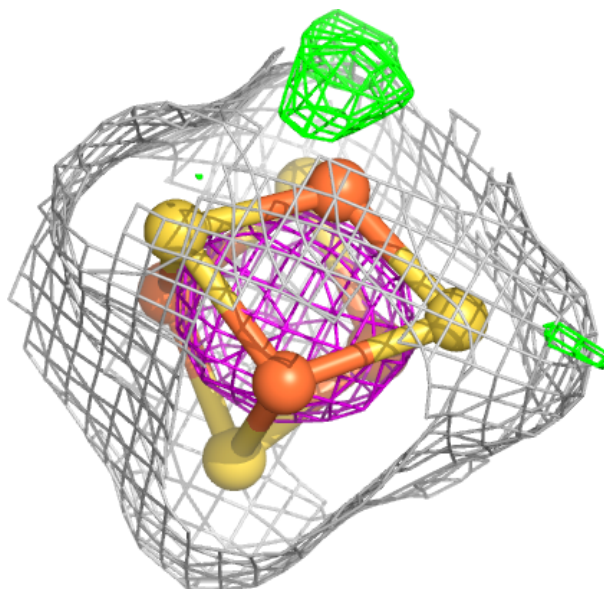
Electron density around SF4 B 1102:

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



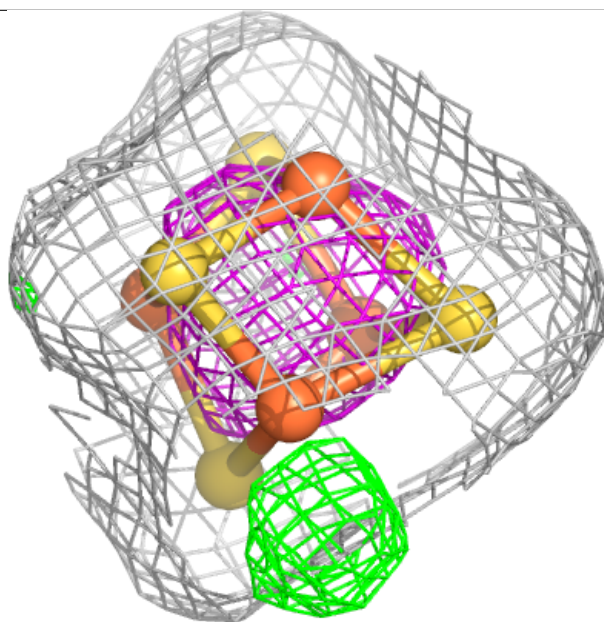
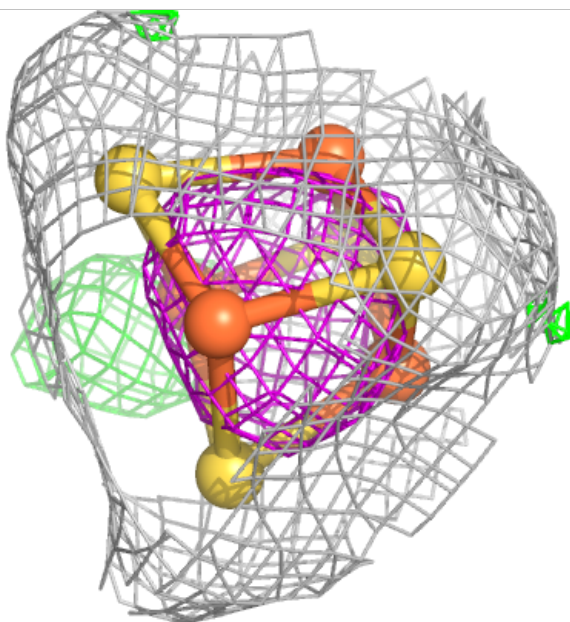
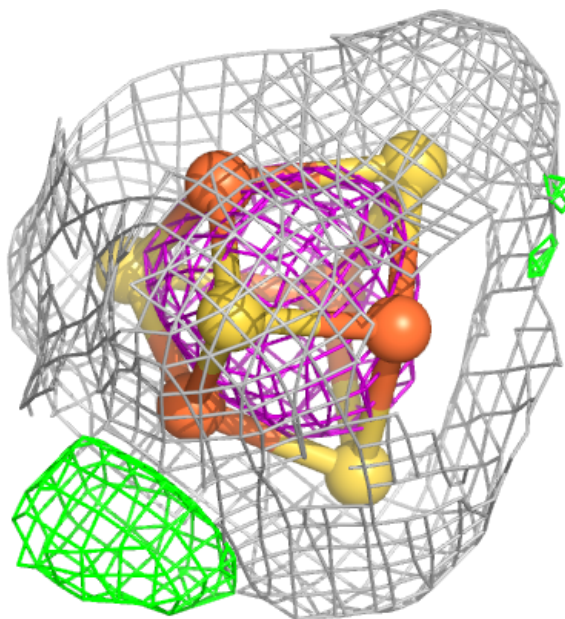
Electron density around SF4 B 1103:

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



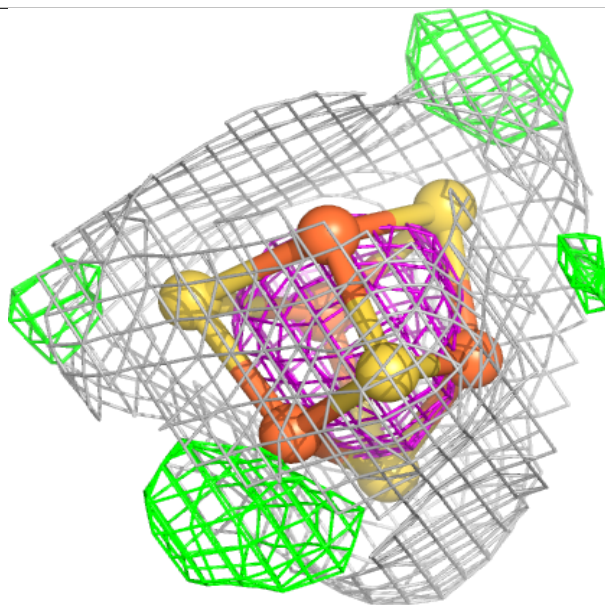
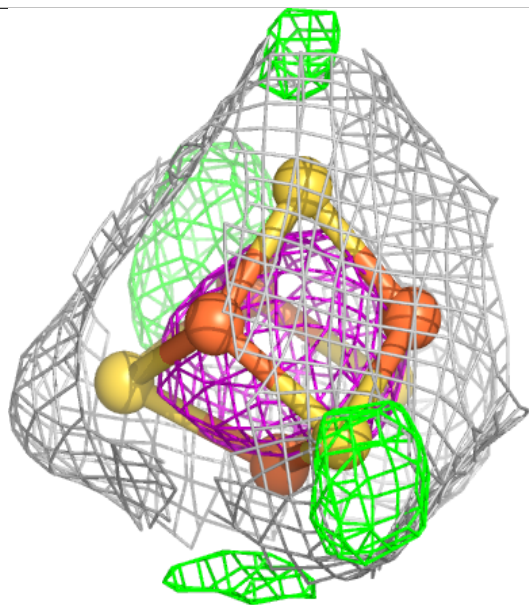
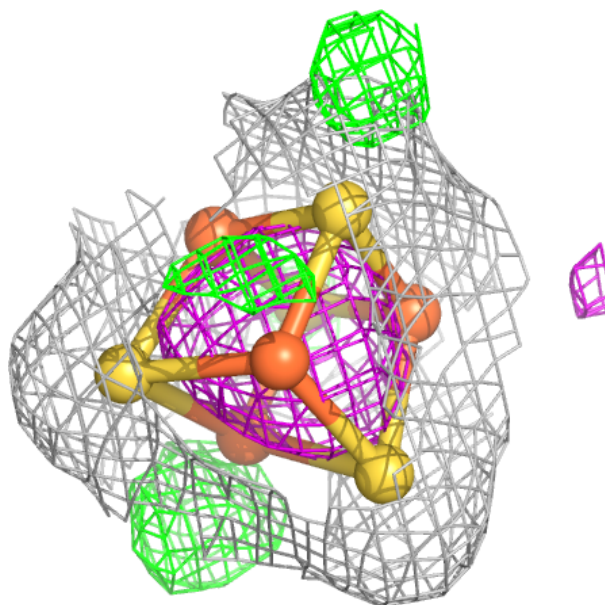
Electron density around SF4 B 1104:

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



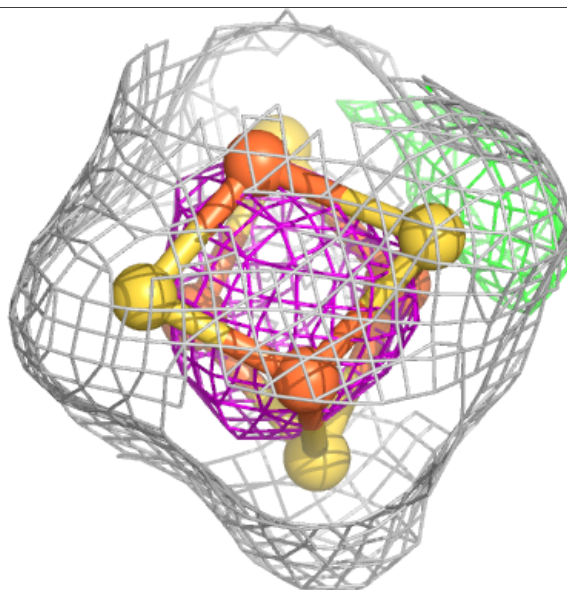
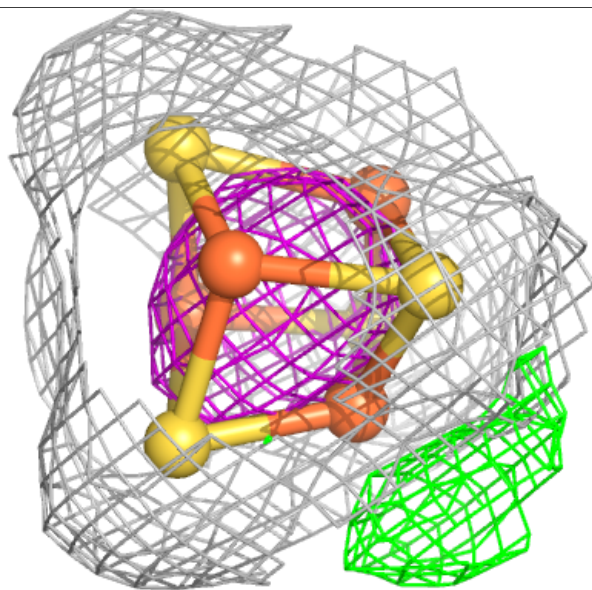
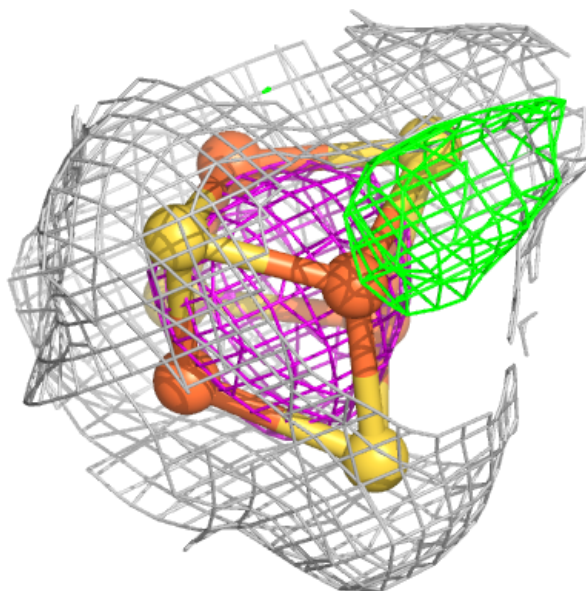
Electron density around SF4 C 1101:

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



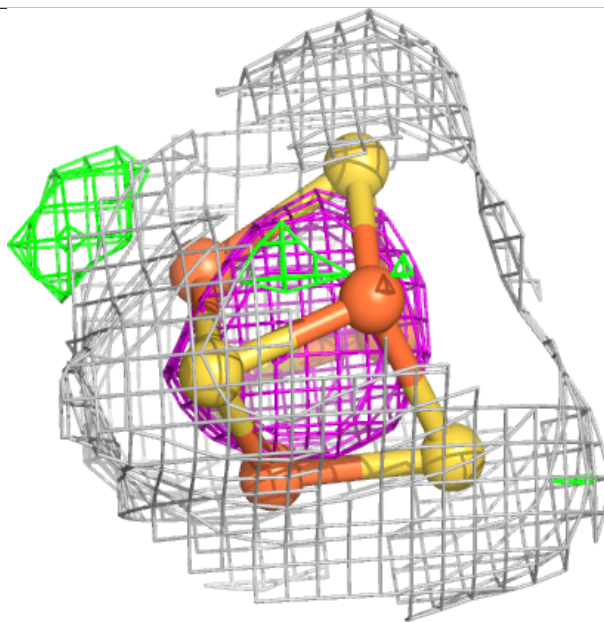
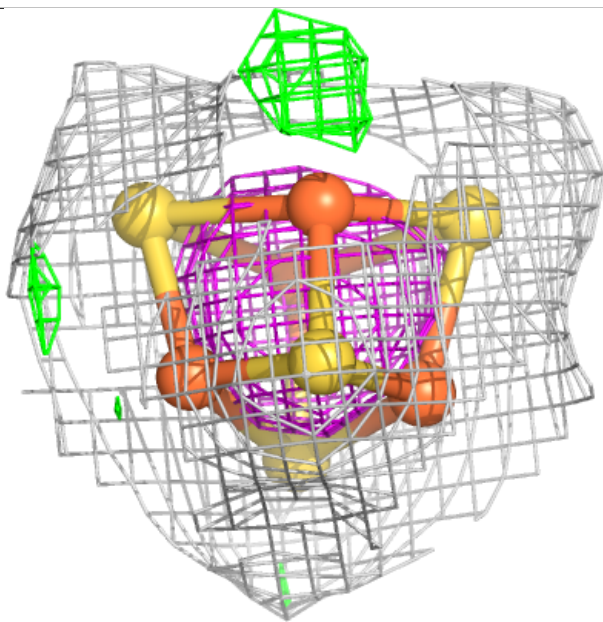
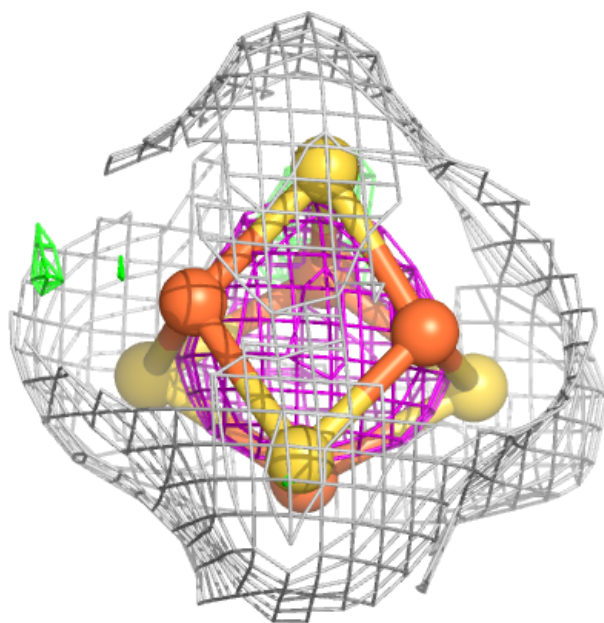
Electron density around SF4 C 1103:

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



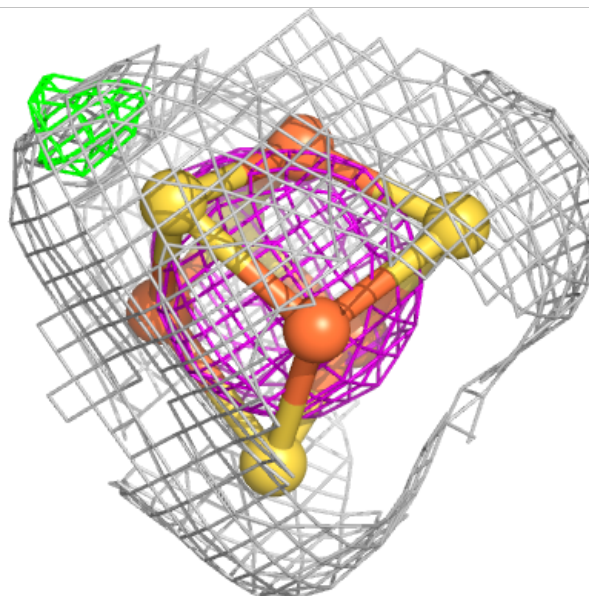
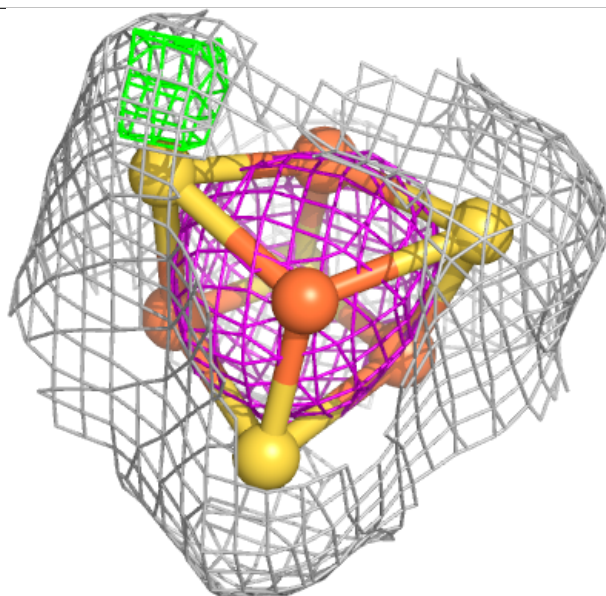
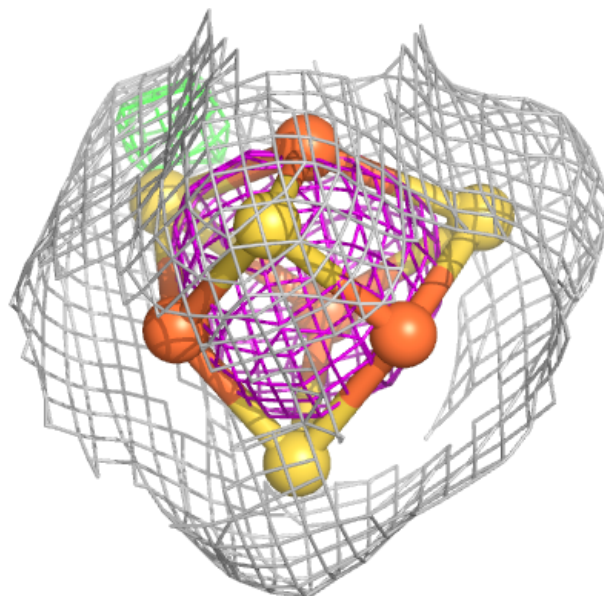
Electron density around SF4 A 1101:

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



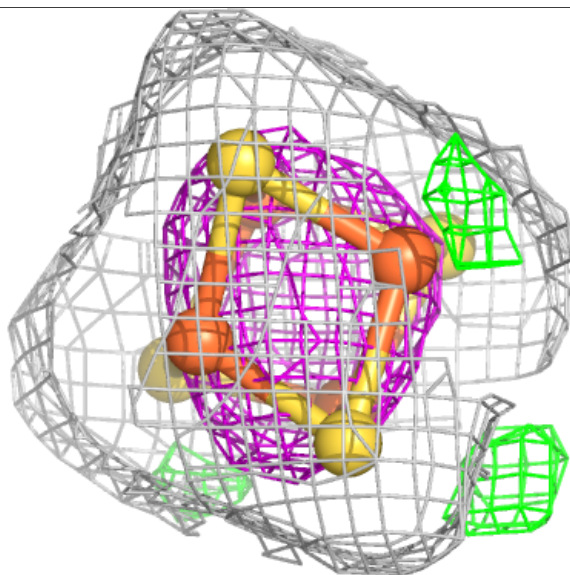
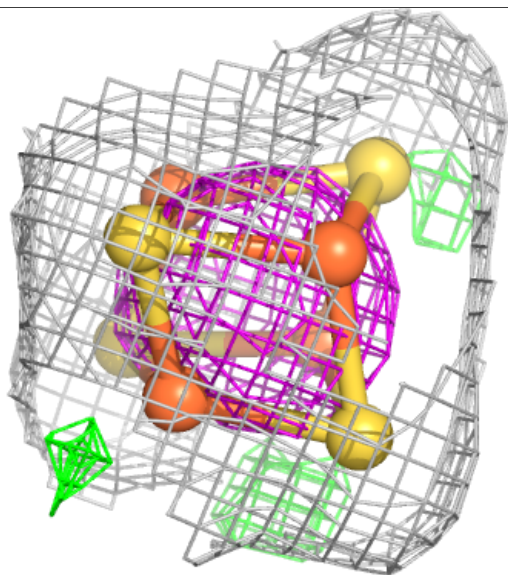
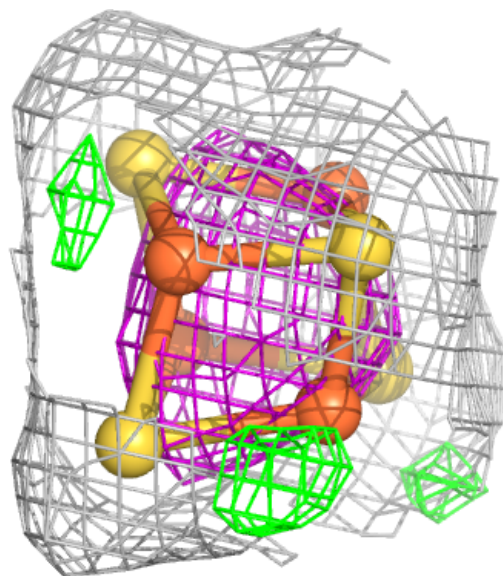
Electron density around SF4 D 1101:

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



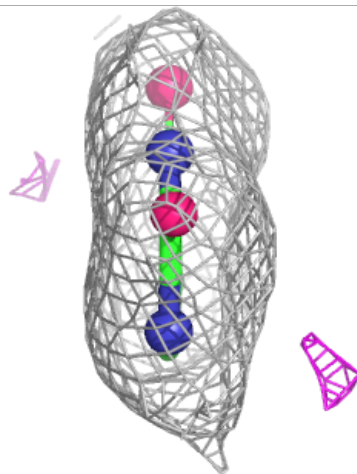
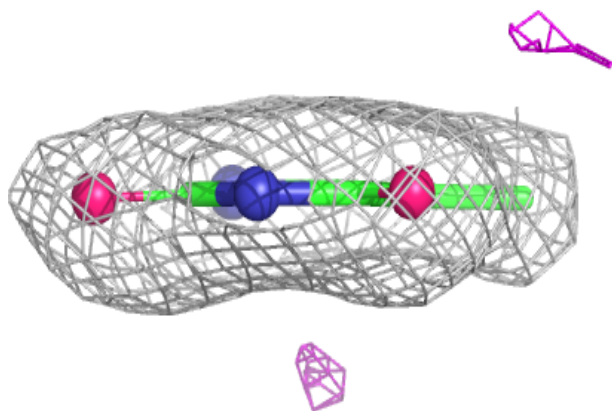
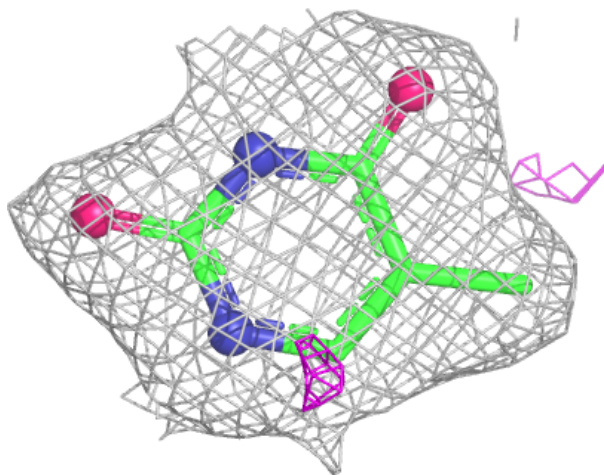
Electron density around SF4 A 1104:

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



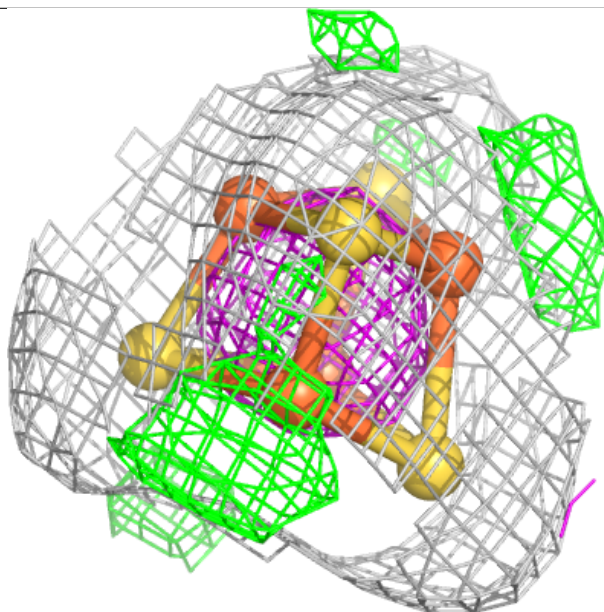
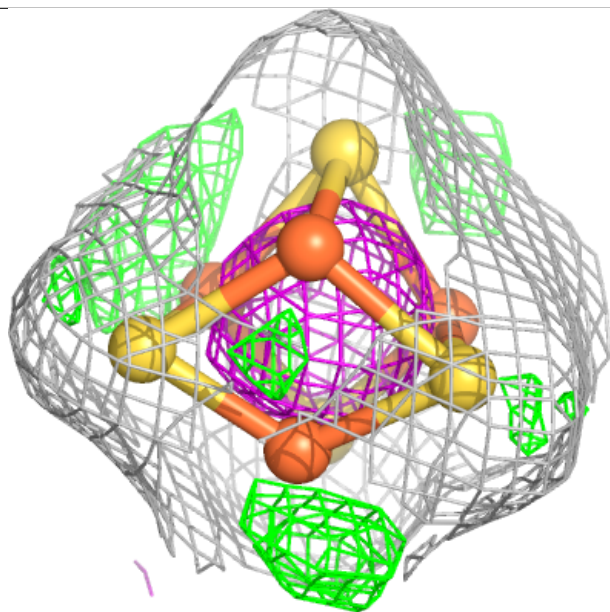
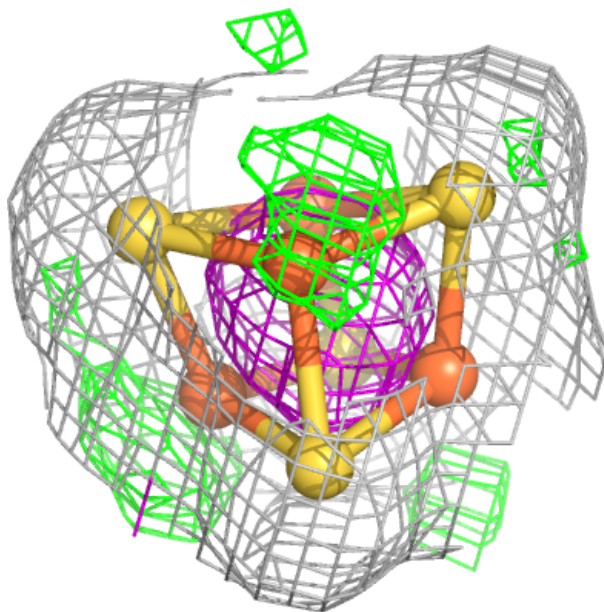
Electron density around TDR D 1107:

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



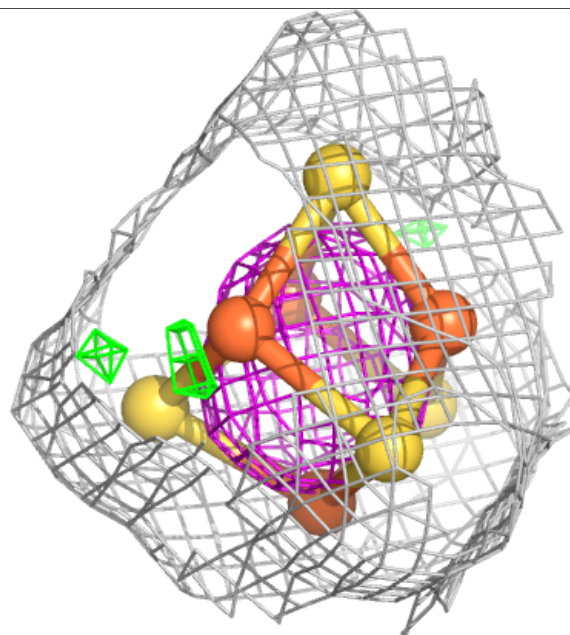
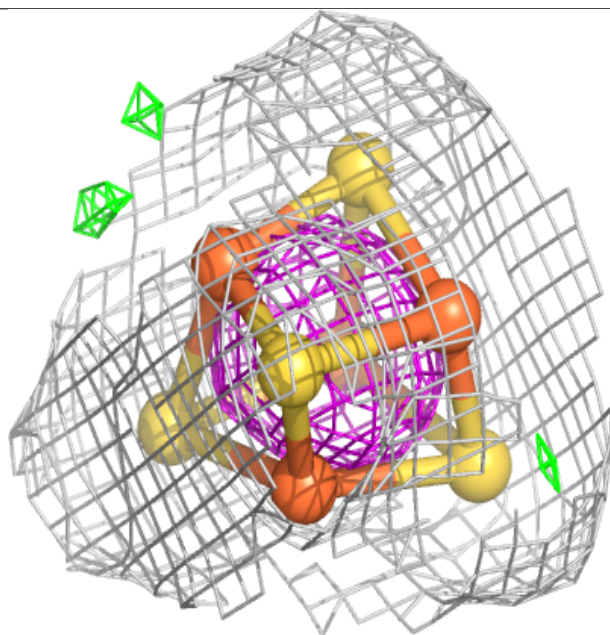
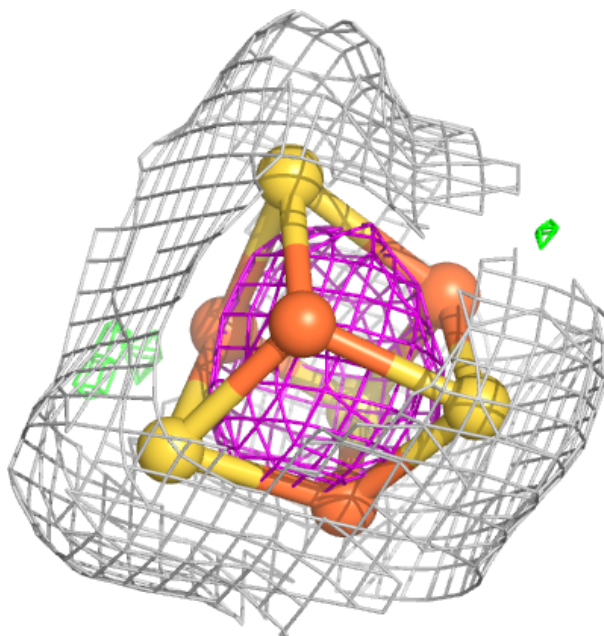
Electron density around SF4 B 1101:

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



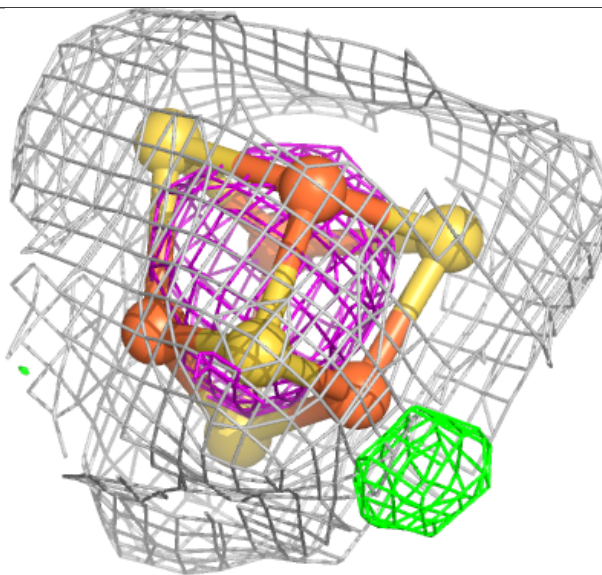
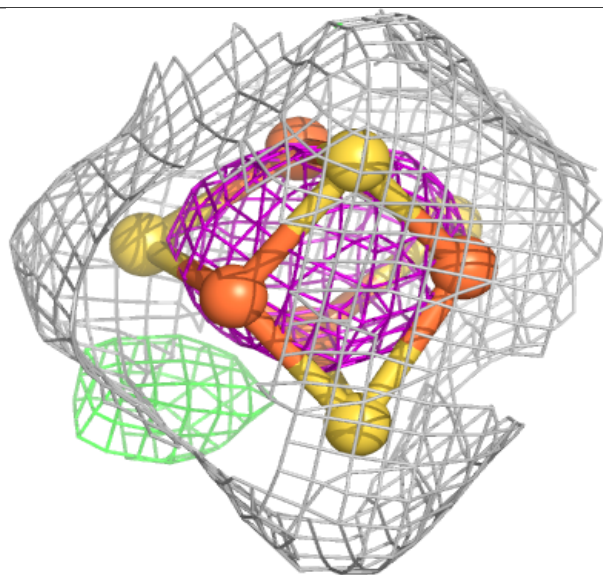
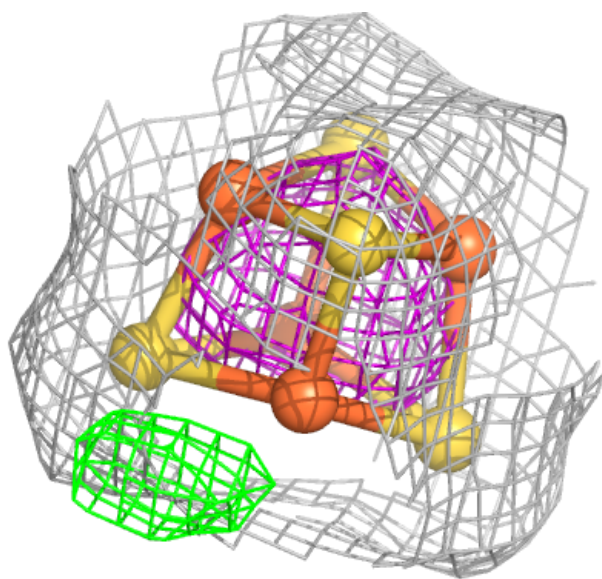
Electron density around SF4 A 1103:

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



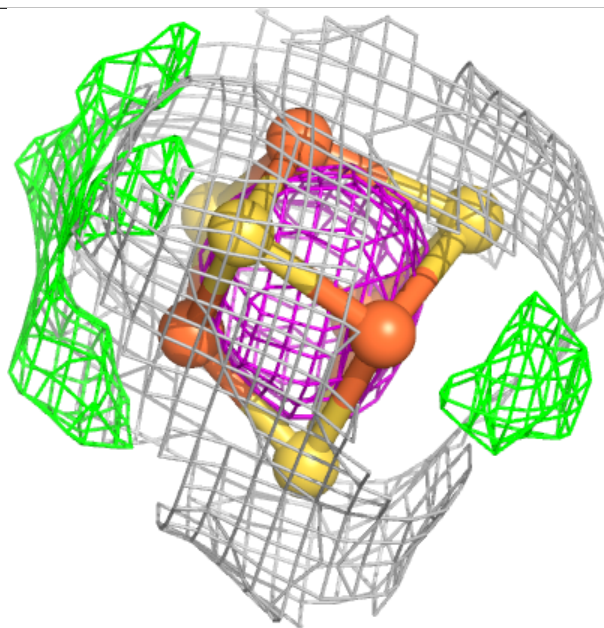
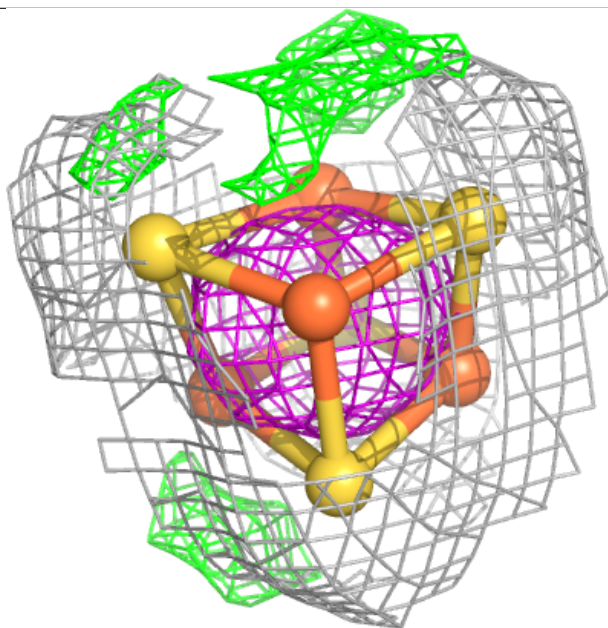
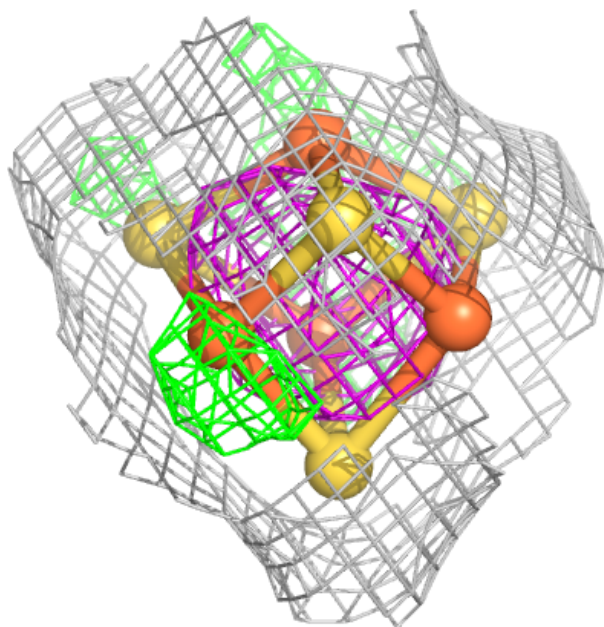
Electron density around SF4 D 1102:

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



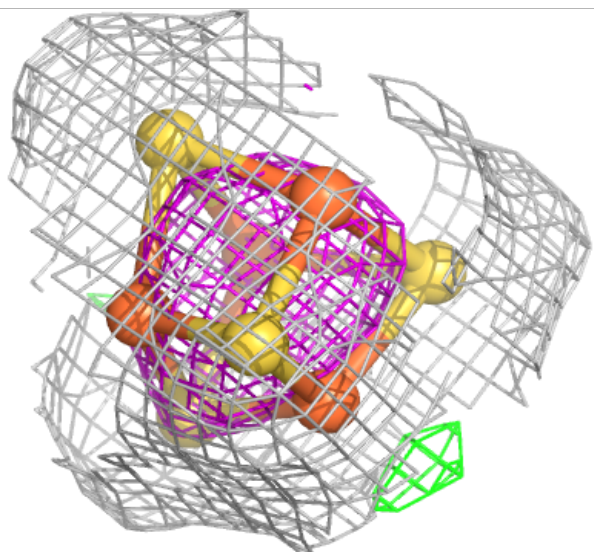
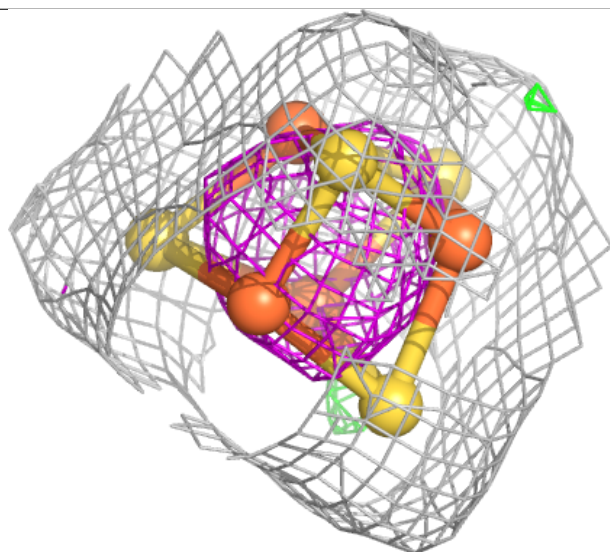
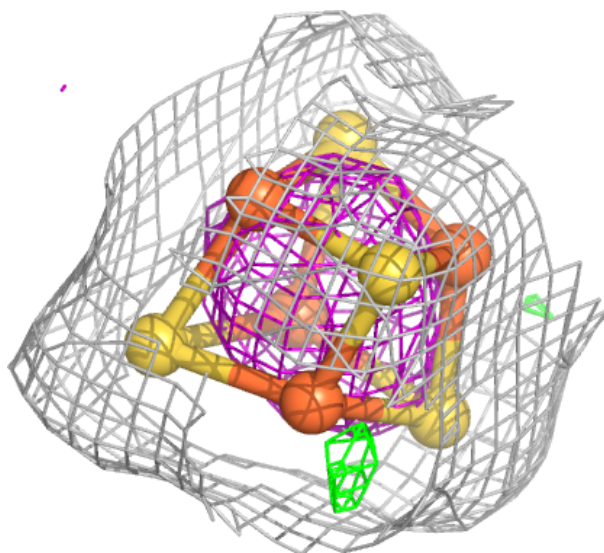
Electron density around SF4 C 1102:

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



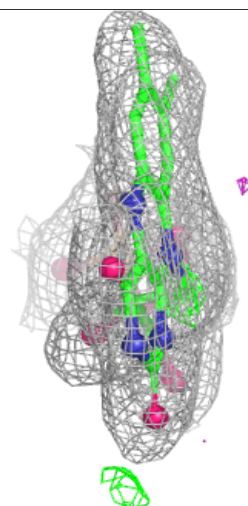
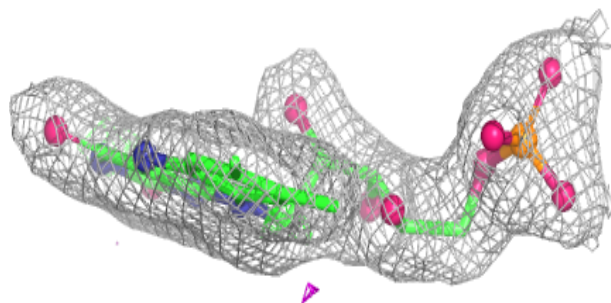
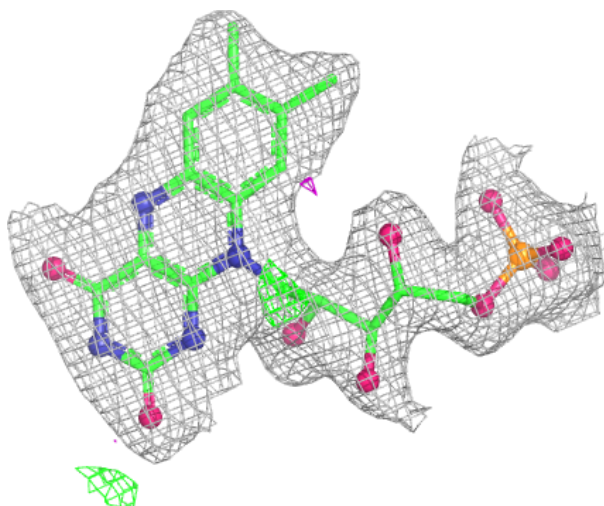
Electron density around SF4 D 1104:

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



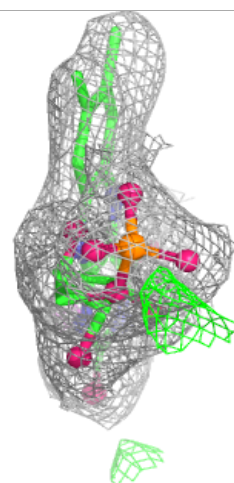
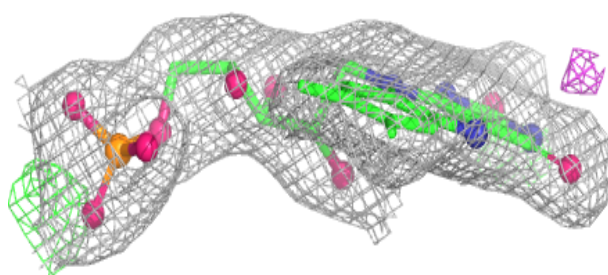
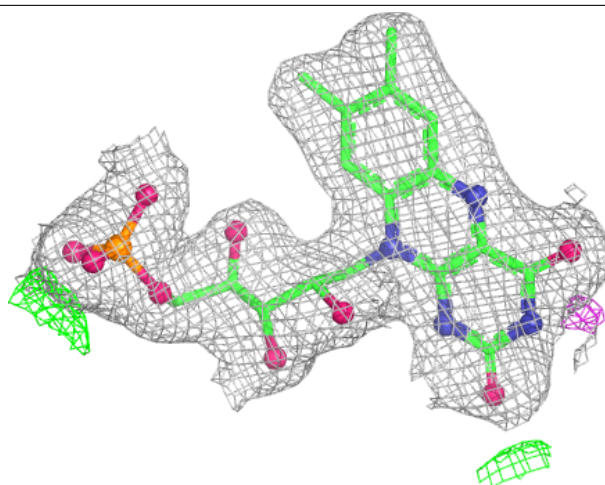
Electron density around FMN C 1105:

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



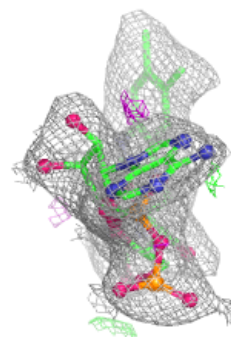
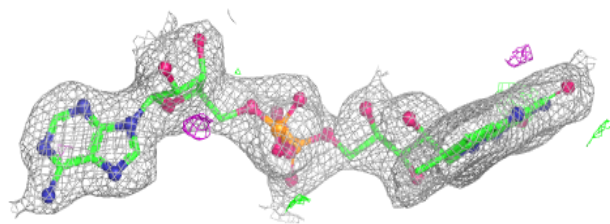
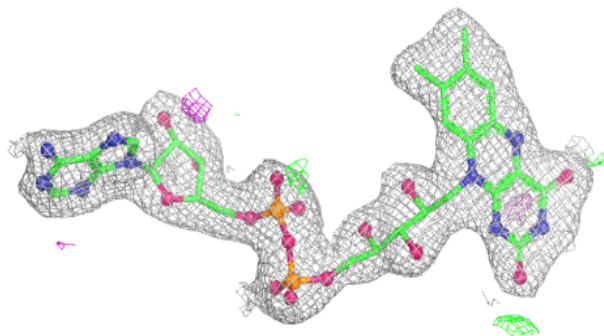
Electron density around FMN D 1105:

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

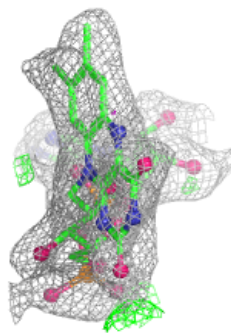
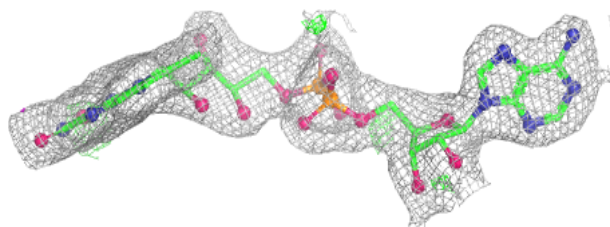
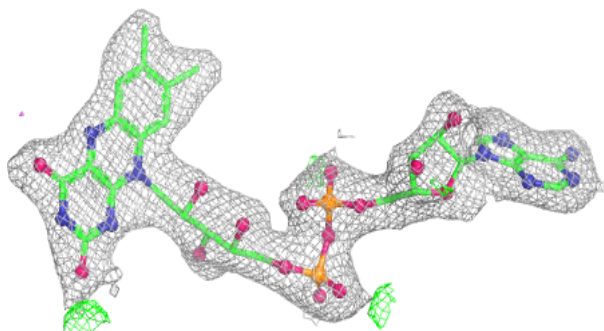


Electron density around FAD A 1106:

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

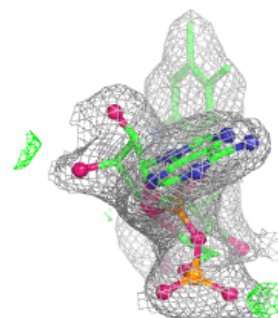
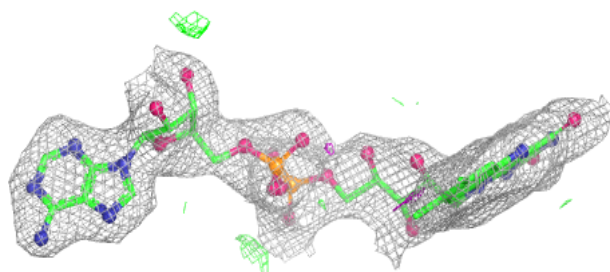
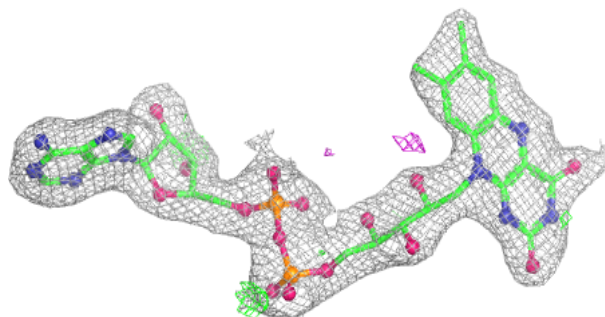
**Electron density around FAD B 1106:**

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

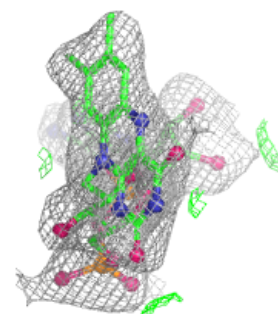
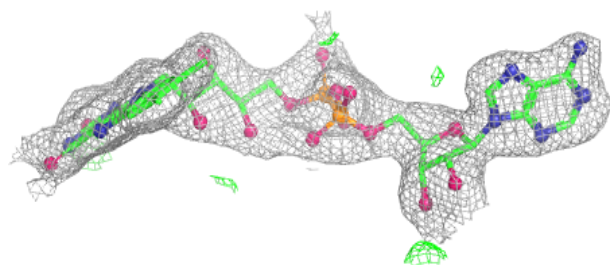
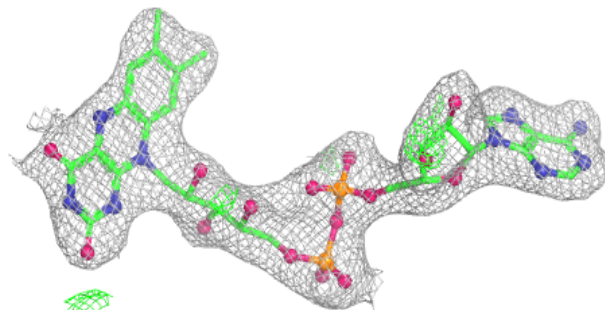


Electron density around FAD C 1106:

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

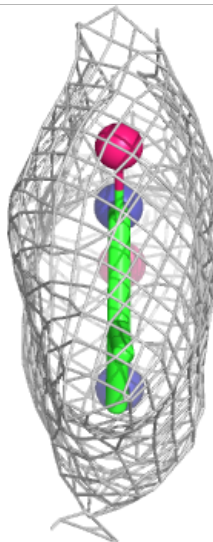
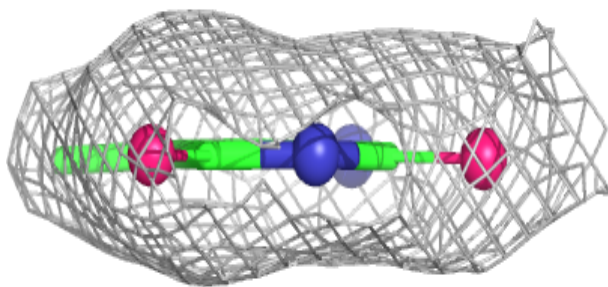
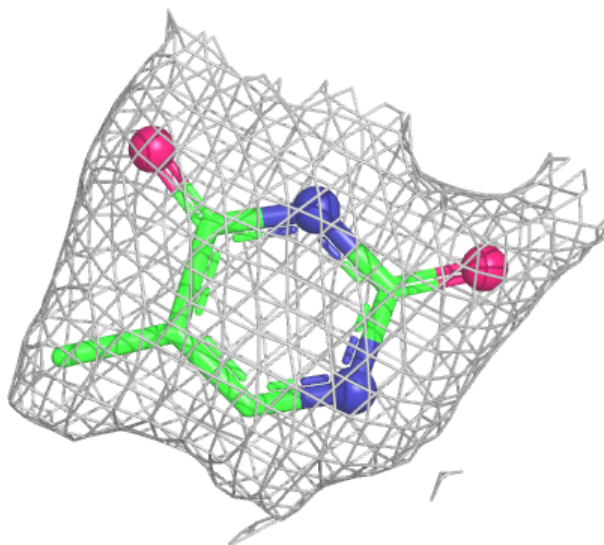
**Electron density around FAD D 1106:**

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



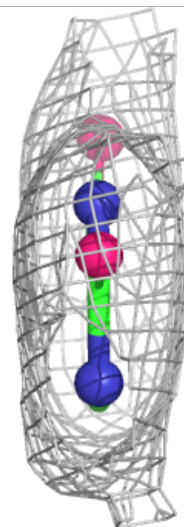
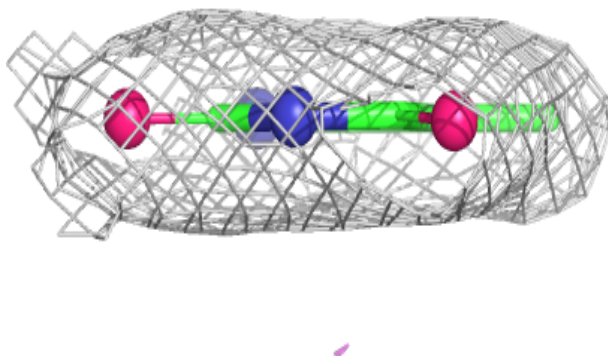
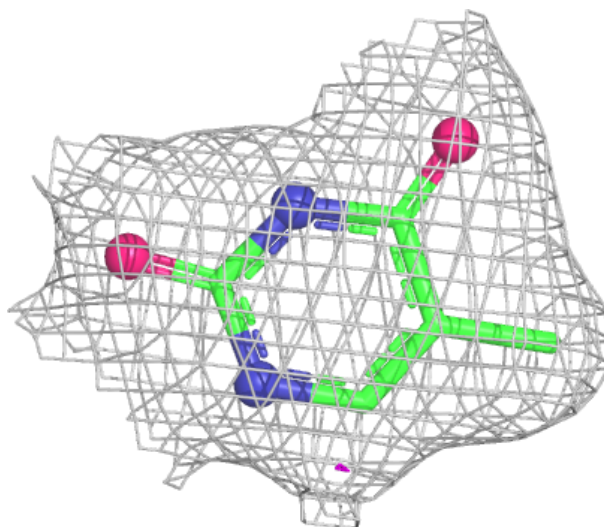
Electron density around TDR A 1107:

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



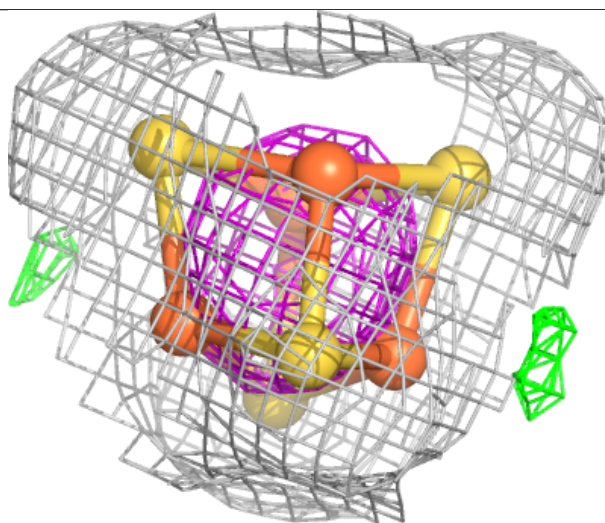
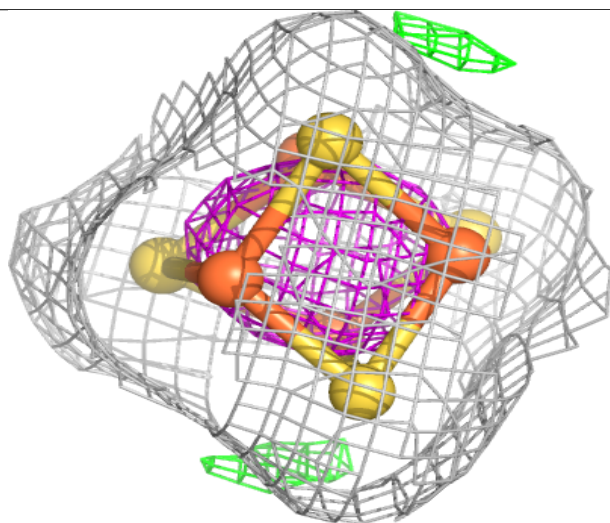
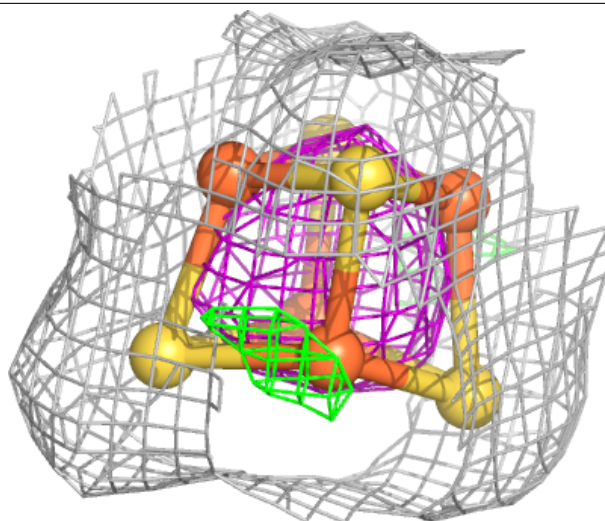
Electron density around TDR B 1107:

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



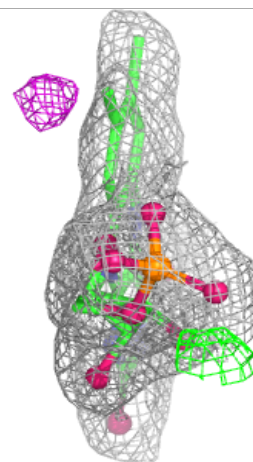
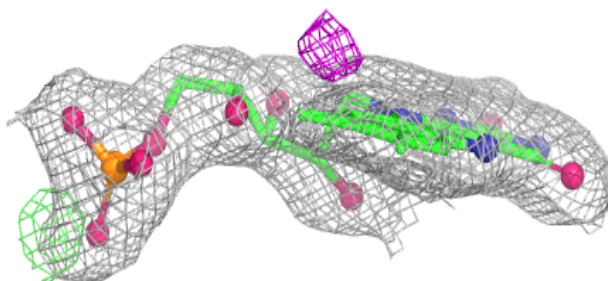
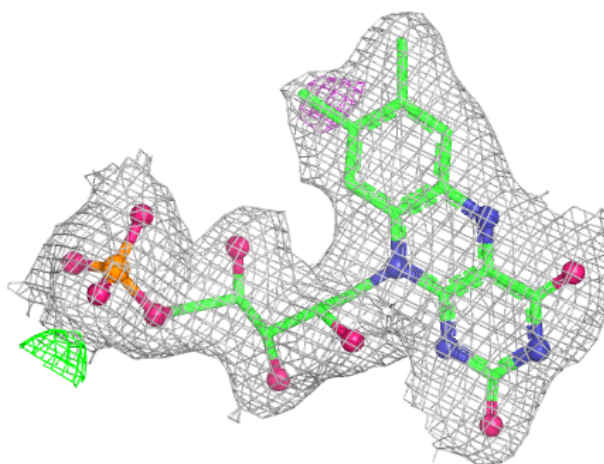
Electron density around SF4 A 1102:

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



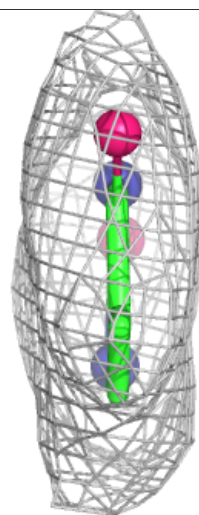
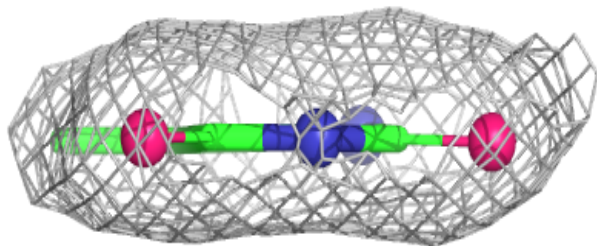
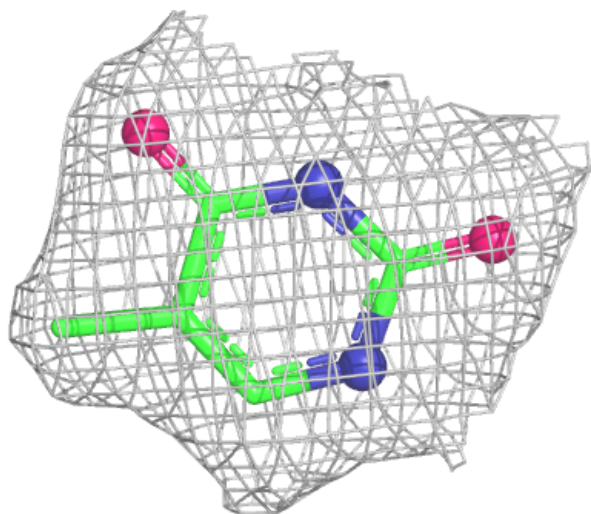
Electron density around FMN B 1105:

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



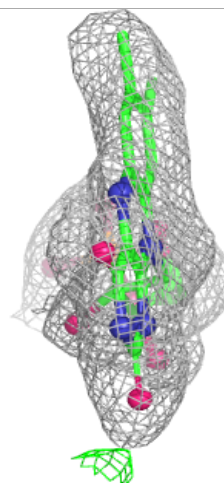
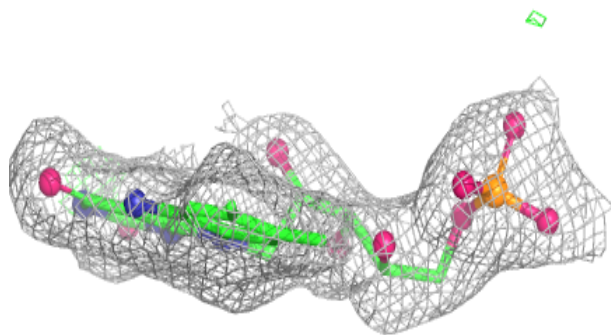
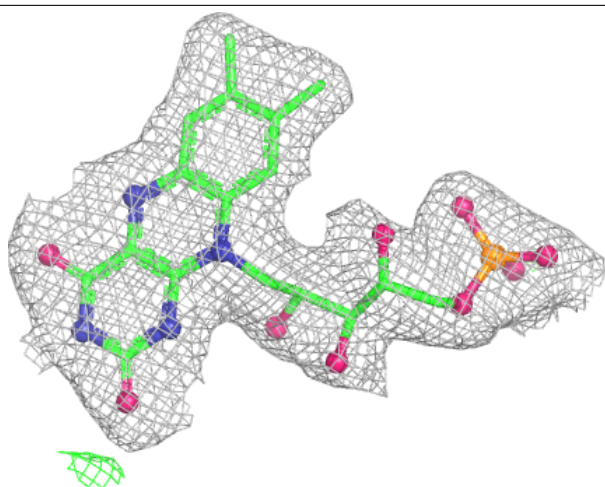
Electron density around TDR C 1107:

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



Electron density around FMN A 1105:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.